Multicritical behaviour in the q-state Potts lattice-gas

LETTER TO EDITOR

Multicritical behaviour in the q-state Potts lattice-gas

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Abstract. The phase diagram of the q-state Potts lattice-gas is determined exactly on a Cayley tree for $q < 2$. We use this result to make some conjectures concerning the lower-dimensional cases. It is argued that there should be a tetracritical point, different from the transition point where Ising droplets diverge, in the case of three-dimensional correlated site–bond percolation ($q = 1$). In two dimensions, the critical exponent γ_p of the mean cluster size at the Ising critical point is derived from the extended den Nijs conjectures: $\gamma_p = \frac{91}{48} = 1.896$.

The diluted version of the q-state Potts model (Wu 1982) has been used to describe the changeover in the nature of the transition occurring in the pure system at q_c depending only on the lattice dimension d (Nienhuis *et al* 1979). The Hamiltonian of the diluted system can be defined as

$$\mathcal{H} = -J \sum_{(ij)} [(\delta_{s_i, s_j} - 1) t_i t_j + \alpha t_i t_j] + \sum_i [\mu - h(\delta_{s_i, 1} - 1)] t_i \tag{1}$$

where $t_i = 0$ ($t_i = 1$) if the lattice site i is vacant (occupied) and s_i assumes one of the values $1, 2, \ldots, q$ if $t_i = 1$. The Potts interaction is given by the Kronecker delta, while the parameter α characterises the lattice-gas coupling. The density of 'magnetic' atoms is governed by the chemical potential μ and the last term in (1) breaks the symmetry of the Potts spins preferring the state 1 for a positive magnetic field. Only nearest-neighbour ferromagnetic interactions ($J, \alpha \geq 0$) are considered.

Depending on the values of q, d and α the q-state Potts lattice-gas defined by Hamiltonian (1) exhibits very different phase diagrams with first-order, critical and even multicritical points. Nienhuis *et al* (1979) found a tricritical point separating the critical and first-order transition surfaces for $q \leq q_c(2)$ and $\alpha = 1$. In two dimensions renormalisation-group investigations for $q = 1$ (Coniglio and Klein 1980), $q = 2$ (Berker and Wortis 1976, Kaufman *et al* 1981) and $q = 3$ (Berker *et al* 1978) showed that a line of tricritical points existed for the whole range $0^+ \leq \alpha < 2$ and ended at the pure $(q+1)$-state Potts transition point for $\alpha = 2$. The third thermal eigenvalue of the tricritical fixed point, however, was found to become relevant for $q < q_m(d)$ in some larger dimensions with $1 \leq q_m(d) \leq 2$ (Nienhuis *et al* 1981). Thus a tetracritical point appeared in the system and Nienhuis *et al* (1981) argued that tricritical behaviour was governed by a classical (Gaussian) fixed point for $q < q_m(d)$.

At least in one case we can exactly check whether this tetracritical point exists or not. We can determine the whole phase diagram of Hamiltonian (1) (for $h = 0$) on

the Cayley tree which can be considered as an infinite-dimensional lattice. The tetracritical point will be located and the topology of the phase diagram analysed for $q < 2 = q_c(d = \infty)$ in order to make some conjectures concerning the three-dimensional $q = 1$ and $q = 2$ cases.

It is well known that thermodynamic properties are influenced essentially by boundary effects on a Cayley tree because of the finite surface to volume ratio in this case. The zero-temperature limit of the phase boundary, for example, depends on how the single-site variables in Hamiltonian (1) are divided between the incident bonds. It will be shown in a more detailed paper that ground state properties on regular lattices change abruptly at $H \equiv \frac{1}{2}caJ - \mu = 0$ where c is the coordination number (Temesvári and Herényi 1983). To ensure that this zero-temperature transition be correctly reproduced, Hamiltonian (1) must be regrouped in the following manner:

$$\mathcal{H} = -J \sum_{(ij)} [(\delta_{s_i,s_j} - 1)t_i t_j + \alpha t_i t_j - \tfrac{1}{2}\alpha(t_i + t_j)] - \sum_i [H + h(\delta_{s_i,1} - 1)]t_i.$$

Another difficulty arises from the definition of the order parameters. For regular lattices, the following definitions seem to be convenient:

$$m_1 \equiv \frac{q}{q-1} N^{-1} \sum_i (\langle t_i \delta_{s_i,1}\rangle - q^{-1}\langle t_i\rangle) = \frac{q}{q-1} (\langle t_0 \delta_{s_0,1}\rangle - q^{-1}\langle t_0\rangle), \qquad (2a)$$

$$m_2 \equiv \frac{q+1}{q} N^{-1} \sum_i [\langle 1 - t_i\rangle - (q+1)^{-1}] = \frac{q+1}{q}[\langle 1 - t_0\rangle - (q+1)^{-1}], \qquad (2b)$$

where $\langle \ldots \rangle$ means thermal averages and the lattice consists of N sites. Here $m_1(m_2)$ is the q-state Potts (the lattice-gas) order parameter and the homogeneity of the lattices has been utilised in deriving the second equation (the index '0' refers to the site at the origin). This homogeneity, however, is absent for the Cayley tree. The spontaneous magnetisation was found to be zero for all temperatures in the case of the pure Ising and Potts models (Eggarter 1974, Wang and Wu 1976), while the averages at the orgin showed the usual behaviour of an order parameter vanishing at the transition point with mean-field exponents. Therefore we adopt as the definition of the order parameters the second parts of equations $(2a)$ and $(2b)$.

The method to calculate thermodynamic functions on Cayley trees is well known (see e.g. Eggarter 1974, Wang and Wu 1976) and is displayed in figure 1: the summation over surface variables can be performed successively, renormalising the single-site parameters at the boundary in each step. Using the notations

$$X \equiv e^{-H/kT}, \qquad Y \equiv e^{-\alpha J/2kT}, \qquad Z \equiv e^{-J/kT}, \qquad (3)$$

the recursion relations can be obtained as follows:

$$X_{n+1} = X\left(\frac{X_n + Y[1 + (q-1)\exp(-h_n/kT)]}{X_n Y + 1 + (q-1)Z\exp(-h_n/kT)}\right)^{c-1},$$

$$\exp(-h_{n+1}/kT) = \exp(-h_n/kT)\left(\frac{X_n Y + Z + [1 + (q-2)Z]\exp(-h_n/kT)}{X_n Y + 1 + (q-1)Z\exp(-h_n/kT)}\right)^{c-1}. \qquad (4)$$

Eliminating all the degrees of freedom but those at the origin and its surrounding sites, the field variables go to a fixed point X^*, h^* in the thermodynamic limit. As a last step, equation (4) is used with c, instead of $c - 1$, and $X_n = X^*$, $h_n = h^*$ to obtain a single site with $X_{\text{eff}} = \exp(-H_{\text{eff}}/kT)$ and h_{eff}. The order parameters can be expressed
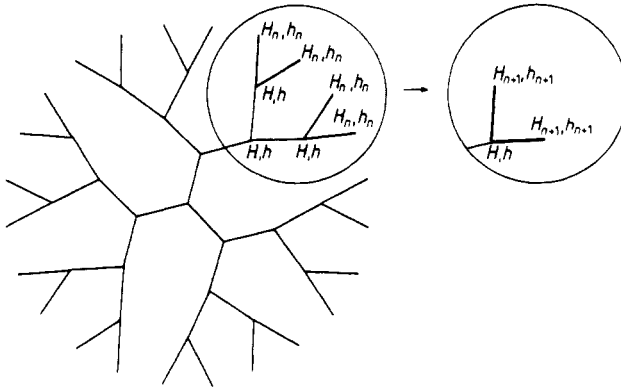
Figure 1. Cayley tree (or Bethe lattice) with branching ratio two ($c = 3$) and the method for obtaining recursion relations of (4): after summing over the variables in the nth generation (surface sites), the single-site parameters (H and h) of the ($n+1$)th generation will be renormalised.

by these effective fields:

$$m_1 = \exp(H_{eff}/kT) \frac{1 - \exp(-h_{eff}/kT)}{1 + \exp(H_{eff}/kT)[1 + (q-1)\exp(-h_{eff}/kT)]},$$

$$m_2 = \frac{1 - q^{-1}\exp(H_{eff}/kT)[1 + (q-1)\exp(-h_{eff}/kT)]}{1 + \exp(H_{eff}/kT)[1 + (q-1)\exp(-h_{eff}/kT)]}. \tag{5}$$

We will consider only the $c = 3$ case. The lattice-gas and q-state Potts transitions can be located by analysing equation (4). There is always a zero-field fixed point X_0^*, $h^* = 0$ when $h = 0$:

$$X_0^* = X[(X_0^* + qY)/(X_0^* Y + 1 + (q-1)Z)]^2. \tag{6}$$

From (6) we can deduce that a first-order lattice-gas transition takes place in two cases: (i) when the initial value X gets from the region of attraction of one fixed point to that of another and (ii) when an attractive fixed point becomes marginal and finally disappears. A q-state Potts transition is obtained when the zero-field fixed point becomes unstable against a small perturbation of the magnetic field: the ordered phase is characterised by a finite-field fixed point. Omitting the calculational details (see Temesvári and Herényi 1983) we only cite the result. Near the transition ($c_1 \approx 0$)

$$h^*/kT \approx -[4q/(q-2)]c_1 \tag{7}$$

where $c_1 > 0$ ($c_1 < 0$) in the ordered (disordered) phase and is given by

$$c_1 = 2(1-Z)/[X_0^* Y + 1 + (q-1)Z] - 1. \tag{8}$$

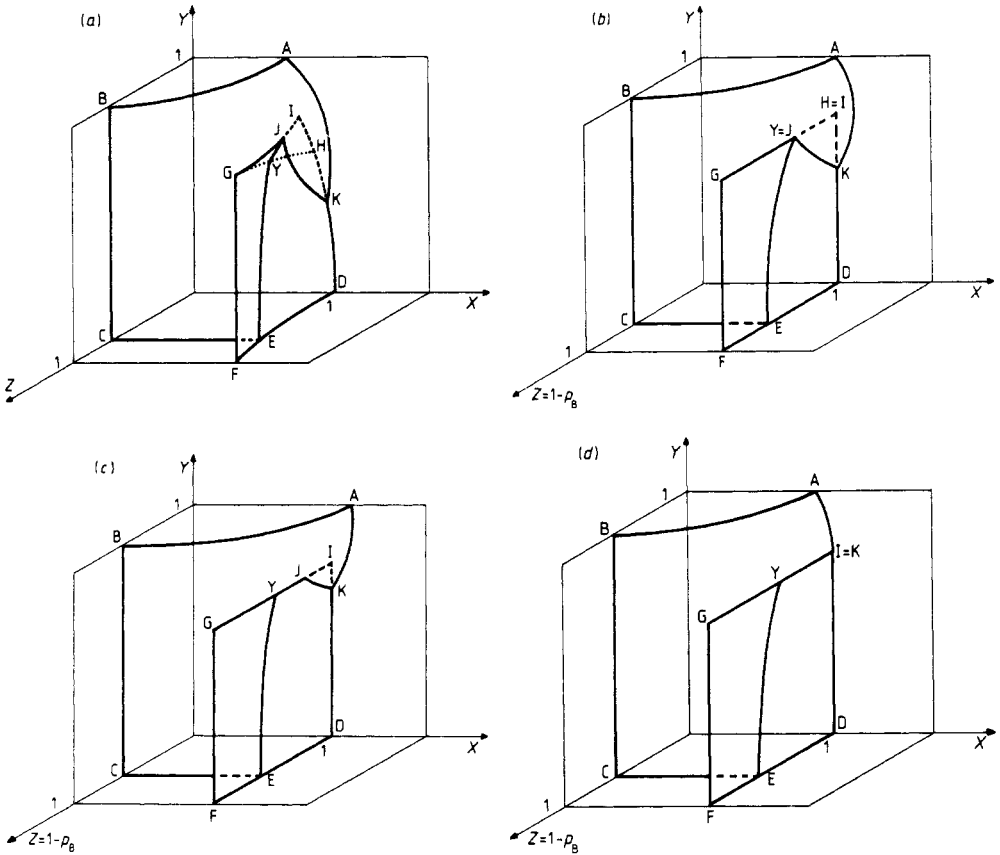Thus for $q < 2$ we can write using (4), (5), (7) and the definition of the critical exponent β:

$$m_1 \sim h_{eff} \sim h^* \sim c_1 \sim |T - T_c|^\beta.$$

Since Y and Z are analytical at T_c, it follows from (8) that X_0^* approaches its critical value (for fixed J, μ and α) with the same exponent β. Therefore we can determine β by investigating the cubic equation (6).

The results for the phase diagram in the case $q < 2$ are summarised in table 1 and its topology is shown in figures 2(a) and (b). Here the tricritical line, as contrasted with the $q = 2$ case (Temesvári and Herényi 1983), coincides with the intersection of the q-state Potts and lattice-gas transition surfaces. Three different values were

Table 1. Transition surfaces, lines and points for the q-state Potts lattice-gas on a Cayley tree with branching ratio two ($1 \le q < 2$). The notation $u \equiv q^{-1}[1 + (q-1)Z]$ is used. There is a first-order q-state Potts transition also on a part of the lattice-gas surface bounded by the lines EY, YJ, JK, KD and DE.

Name and/or notation	Boundary lines or points	Defining equation
Lattice-gas transition surface (with fixed point changing)	GI, FD, DH and HG	$X = q\dfrac{u - Y}{1 - Y} \equiv X_{LG}$
Lattice-gas transition surface (with a marginal fixed point)	GH, HI and IG	$X = \dfrac{qu(u + 3Y^2 + v)^2}{8Y(u - 3Y^2 + v)} \equiv X'_{LG}$ with $v \equiv (u^2 - 10uY^2 + 9Y^4)^{1/2}$
q-state Potts transition surface	BC, CE, EY, YJ, JK, KA and AB	$X = \dfrac{4qY(1 - u)^2[2 - (q+1)u]}{(q-1)[2 - (q+1)u + (q-1)Y^2]^2}$ $\equiv X_{Potts}$
Lattice gas critical line	I and G	$u = 9Y^2$ and $X = 27qY^3$
Tricritical line	Y and J	$Y^2 = \dfrac{Z[2 - (q+1)u]}{3 - (q+2)u}$ and $X = X_{Potts}$
Line separating the two types of lattice-gas surfaces	H and G	$u = \dfrac{Y(2 - 3Y)}{1 - 2Y}$
Line of type-I critical endpoints	J and K	$X = X_{Potts} = X'_{LG}$ and $X = X_{Potts} = X_{LG}$
Line of type-II critical endpoints	E and Y	$X = X_{Potts} = X_{LG}$
Pure $(q+1)$-state Potts transition point Y		$X = 1 (\alpha = 2)$
Tetracritical point J		$Y^2 = [3(2q+1)]^{-1}\left(\alpha = 1 + \dfrac{\ln 3}{\ln(2q+1)}\right)$
E		$Y = 0$
K		$Z = 0$
I		$Z = 0$
G		$Z = 1$

Figure 2. The topology of the phase diagram (see table 1 for notation). (*a*) Exact result for the Cayley tree (*c* = 3) in the case $1 < q < 2$. The dotted line (GH) separates the two types of lattice-gas transition. (*b*) Exact result for the Cayley tree (*c* = 3) in the case of percolation ($q = 1$). The tetracritical point (J) and the transition point where Ising droplets diverge (Y) coincide. The lattice-gas transition surface with the marginal fixed point disappears at $q = 1$ (H = I). (*c*) Conjectured phase diagram for three-dimensional percolation. The tricritical line YJ is expected to have classical exponents. (*d*) Two-dimensional phase diagram for percolation. The Ising critical point I is now also the place where the system begins to percolate (I = K). YI is the one-state Potts tricritical line.

obtained for the critical index β: (i) $\beta = 1$ on the q-state Potts surface and along type-I and type-II critical endpoints; (ii) $\beta = \frac{1}{2}$ along the tricritical line; (iii) $\beta = \frac{1}{3}$ in the tetracritical point. Type-I critical endpoints were investigated, in the Ising case, by Ziman *et al* (1982) and they are characterised by phase diagrams with a lattice-gas critical point in the ordered phase. This line of type-I critical endpoints becomes a tricritical line through the tetracritical point at

$$\alpha = 1 + \ln 3 / \ln(2q + 1), \qquad q < 2.$$

The q-state Potts lattice-gas model becomes the Ising-correlated site–bond percolation problem in the limit $q = 1^{+}$ (Coniglio and Klein 1980, Wu 1981). On the Cayley tree this problem has been investigated in many papers (Coniglio 1975, 1976, Coniglio *et al* 1979, 1982, di Liberto *et al* 1983). We are interested here in how the phase diagram

changes when q reaches 1. As can be seen from figure 2(b), the lattice-gas transition surface with the marginal fixed point disappears for $q = 1$. This is related to the fact that $1 = q_c(\infty) - 1$ and thus the $(q + 1)$-state Potts transition becomes continuous just in the case of percolation (for details see Temesvári and Herényi 1983). Furthermore, the tetracritical point and the $(q + 1)$-state Potts transition point merge and form a new multicritical point where Ising droplets diverge (Coniglio and Klein 1980, Kertész *et al* 1982). The order parameter of Ising droplets has the critical exponent $\beta = \frac{1}{2}$, instead of $\beta = \frac{1}{3}$, and the two types of critical endpoints join together in this new multicritical point.

We expect, however, another type of phase diagram when $q < q_m(d)$ and $q < q_c(d) - 1$ in lower dimensions (see figure 2(c) with $d = 3$ and $q = 1$): since the tetra-critical point must disappear continuously at $q_m(d)$ (this is not the case on the Cayley tree because of the abrupt change in the phase diagram at $q = 2$ (Temesvári and Herényi 1983)), it moves away from Y when q increases toward $q_m(d)$. They are connected with a line of classical tricritical points (Nienhuis *et al* 1981). Taking into account that the upper tricritical dimensionalities of the Ising and Potts models are three and four, respectively, we can draw $q_m(d)$ schematically as in figure 3 (see also Nienhuis *et al* 1981).
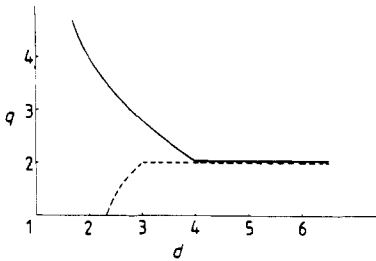
Figure 3. $q_c(d)$ and $q_m(d)$ are drawn schematically with full and broken lines, respectively. For $q \leqslant q_m(d)$ a tetracritical point can be found in the system and tricritical behaviour should be classical. At $q_c(d)$ the nature of the Potts transition changes from second to first order (it is taken from Wu (1982)).

The most important consequences of the tetracritical point on the phase diagram are obtained in the percolational case ($q = 1$). In two dimensions (figure 2(d)), where $1 > q_m(2)$, for a bond probability p_B which is unity ($p_B = 1 - Z$, see Kasteleyn and Fortuin 1969, Coniglio and Klein 1980, Wu 1981), i.e. for Ising-correlated site percolation, the Ising critical point (I) lies on the percolational transition surface (Coniglio *et al* 1977, Coniglio and Klein 1980) and it is actually a tricritical point in the context of the $q \to 1$ limit of the diluted Potts model. In three dimensions (figure 2(c)), however, the system percolates on the coexistence curve below the Ising critical temperature (Müller-Krumbhaar 1974, Sykes and Gaunt 1976) at the point K which is now a type-I critical endpoint. As has been stated, we expect that the tetracritical point, where the line of type-I critical endpoints merges with the Ising (or lattice-gas) critical line, should be at a bond probability p_B^J which is larger than that of Ising droplets p_B^Y. We think that figure 4 in Heermann and Stauffer (1981) supports this idea: p_B for the two types of critical endpoints are shown as functions of the temperature and the two curves do not meet at the Ising critical temperature. However, in discussions of Monte Carlo results a phase diagram similar to that on the Cayley tree ($p_B^J = p_B^Y$)

was always suggested (Stauffer 1981, Heermann and Stauffer 1981, Kertész *et al* 1982). Further Monte Carlo work would be useful to investigate this point.

Finally the exponent γ_p of the mean cluster size when approaching the Ising critical point along the temperature axis will be derived. In two-dimensional correlated site percolation ($p_B = 1$) γ_p was found to differ from both the Ising and random percolational values (Sykes and Gaunt 1976, Coniglio and Klein 1980). From the usual scaling law $\gamma_p = (2 - \eta)\nu$ we can calculate γ_p using the probably exact values for the thermal and magnetic eigenvalues of the tricritical fixed point (den Nijs 1979, Nienhuis *et al* 1979, 1980, Pearson 1980, Nienhuis 1982):

$$\nu = y_{T2}^{-1} = 1 \qquad \text{and} \qquad 2 - \eta = 2y_h - d = \tfrac{91}{48}.$$

Thus

$$\gamma_p = \tfrac{91}{48} = 1.896 \qquad (d = 2, p_B^Y < p_B \leqslant 1)$$

which can be compared with the series result $\gamma_p = 1.91 \pm 0.01$ (Sykes and Gaunt 1976) and renormalisation-group value $\gamma_p = 1.89$ (Coniglio and Klein 1980). Although the scaling law used here has been stated by Coniglio and Klein (1980), they did not identify the Ising critical point with the $q = 1$ Potts tricritical point.

The classical value of γ_p can also be calculated. When $p_B^J > p_B > p_B^Y$ in three dimensions, the tricritical fixed point should be classical:

$$y_{T2} = 1 \qquad \text{and} \qquad \eta = 0,$$

thus

$$\gamma_p = 2 \qquad (d = 3, p_B^Y < p_B < p_B^J).$$

This value for γ_p in three dimensions should also be checked, together with the determination of γ_p in the tetracritical point ($p_B = p_B^J$), by further numerical work.

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