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LETTER TO THE EDITOR

Droplet structure in Ising and Potts models

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Abstract. The structure of a recently introduced droplet in the q -state Potts model is analysed. We derive exact relations from which it follows that the incipient infinite droplet at the critical temperature is a self-similar fractal made of links and blobs, just as recently found in random percolation. The number of links N_{links} between two points separated by a distance of the order b is given by $N_{\text{links}} \propto b^{1/\nu_B(q)}$ where $\nu_B(q)$ is the connectedness length exponent when $T = T_c(q)$ and p_B is used as an independent variable. This result and the available calculations of $\nu_B(q)$ indicate that the number of links decreases as q increases.

An analysis of the structure of the usual clusters made of nearest-neighbour sites in a given Potts site configuration is also made. In particular, it shows that for $d = 2$ the incipient infinite cluster is made only of blobs and no links.

A simple theory of phase transitions and metastability is based on droplet models (Fisher 1967, Domb 1976, Binder 1976, Kertesz *et al* 1983). An important problem is the definition of the right droplet whose size diverges at the critical point with the correct exponents. For example, in an Ising model the droplets made up of nearest-neighbour (NN) 'down' spins (the usual Ising clusters) are known to diverge on the coexistence curve below the critical temperature in $d = 3$ dimensions (Müller-Krumbhaar 1974). In two dimensions the mean cluster size diverges at the critical point with an exponent $\gamma^* = 1.91 \pm 0.01$ (Sykes and Gaunt 1976) larger than the susceptibility exponent $\gamma = 1.75$. A recent theory (Bruce and Wallace 1981) and an earlier suggestion (Stauffer 1977) predict $\gamma^* = \gamma + \beta$, where β is the magnetisation exponent.

A more general cluster made of 'down' spins connected by bonds being active with probability p_B has been introduced in the context of polymer gelation (Coniglio *et al* 1979, Coniglio and Peruggi 1982).

Coniglio and Klein (1980) predicted that with the special choice of $p_B = p_B(T) \equiv 1 - \exp(-2J/kT)$, where J is the NN coupling constant, this kind of cluster, which they called Ising droplets, would diverge with Ising thermal exponents. These predictions have been verified by Monte Carlo methods in two and three dimensions (Stauffer 1981, Ottavi 1981, Rousseny *et al* 1982, Heermann and Stauffer 1981, Jan *et al* 1982, Kertesz *et al* 1983).

More specifically from the renormalisation group analysis (Coniglio and Lubensky 1980) it follows that the connectedness length ξ has the scaling form

$$\xi = u^{-\nu_B} f_1(t/u^\phi). \quad (1)$$

Here $t = (T - T_c)/T_c$ and $u = a\varepsilon + bt$ are the scaling variables, $\varepsilon = (p_B(T) - p_B)/p_B(T)$, p_B is the bond probability, a and b are constants such that $u = 0$ if $p_B = p_B(T) \equiv 1 - \exp(-2J/kT)$, ν_B is the connectedness length exponent along the path $t = 0$, $p_B \rightarrow p_B(T)$, $\phi = \nu_B/\nu$ is the crossover exponent and ν is the thermal correlation length exponent, which is 1 for $d = 2$ and $\frac{1}{2}$ for $d \geq 4$. From the Migdal-Kadanoff renormalisation group (MKRG), $\phi = 2.02$ for $d = 2$ and from the ε -expansion $\phi = 4/(2-d)$ near $d = 6$. Therefore ξ diverges with the exponent ν_B along the path $t = 0$, $\varepsilon \rightarrow 0$ and with the thermal correlation length exponent along the path $u = 0$ ($p_B = 1 - \exp(-2J/kT)$).

The mean cluster size has the scaling form

$$S = u^{-\gamma_B} f_2(t/u^\phi) \quad (2)$$

where γ_B is related to the susceptibility exponent γ via $\gamma_B/\gamma = \phi$. $\gamma_B = 3.54$ from MKRG for $d = 2$ and $\gamma_B = 4/(d-2)$ near $d = 6$ from ε -expansion.

A similar analysis was extended by Coniglio and Peruggi (1982) to the q -state Potts model with Hamiltonian $-\mathcal{H} = \sum_{\langle ij \rangle} J(q\delta_{\sigma_i\sigma_j} - 1)$ where $\sigma_i = 1, \dots, q$ are the site variables. It was found that the droplets made of NN sites in a given Potts state connected by bonds with probability

$$p_B = p_B(T) = 1 - \exp(-qJ/kt) \quad (3)$$

diverge at the Potts critical point with the thermal Potts exponents. For $q = 1$ they found $T_c(1) = 0$. Being at $T = 0$ all sites are present, consequently they found that the droplets coincide with the random-bond percolation clusters and $\nu_B(q = 1)$ coincides with the connectedness length exponent in the random-bond percolation problem.

Here we want to study the fractal structure of the incipient infinite droplet as defined above at the critical Potts temperature $T_c(q)$, following closely the analysis made for the incipient infinite cluster in random percolation.

Let us first define the fractal dimensionality (Mandelbrot 1977, Stanley 1977, Stauffer 1979, Kirkpatrick 1979) $d_f(q)$ of the typical droplet of linear dimension ξ as

$$S^*(q) \propto \xi^{d_f(q)} \quad (4)$$

where S^* is the number of sites in the droplet.

With the same analysis as for random percolation one is led to the following expression for the fractal dimensionality of the Potts droplet:

$$d_f(q) = d - \beta(q)/\nu(q) \quad (5)$$

where $\beta(q)$ and $\nu(q)$ are the order parameter and the correlation length exponents of the q -state Potts model. For $q = 1$ equation (5) gives the fractal dimensionality in random percolation.

An immediate application of the fractal concept follows if we view the thermal phase transitions as (nonlinear) processes due to the coalescence of droplets. This is a geometrical mechanism which should be not very sensitive to the details of the Hamiltonian which will mainly affect the shape and size of small droplets. Therefore we expect that the fractal dimensionality, which contains the essential geometric information of the large droplets, should also be roughly independent of the details. This indeed is the case. For example, for the q -state Potts model in $d = 2$, $d_f(q) = 1.896$, 1.875 and 1.866 ($q = 1, 2, 3$) (Nienhuis *et al* 1980, Nienhuis 1982).

This point of view is also a physical interpretation of Suzuki's universality which states that, although the exponents γ , β , ν might be strongly model dependent, the

ratios γ/ν and β/ν , which by means of scaling can be expressed in terms of d_t only, are roughly model independent (Stanley 1977).

We want to study now in more detail the structure of the incipient infinite droplets. We observe that, given two points separated by a distance of the order of the connectedness length ξ , we can always distinguish between dangling bonds or loose ends and backbone bonds. The backbone bonds are made of cutting bonds or links such that if one is cut the droplet breaks in two parts and multiply connected bonds which lump in blobs. This distinction in three categories of bonds was originally introduced by Stanley (1977) for random percolation. We will show now that the number of links is a diverging quantity. To do so we extend exact relations proved for random-bond percolation to Potts correlated-site random-bond percolation (PCSRBP). In particular we will prove the relation

$$p_B(dp_{ij}/dp_B) = \langle \lambda_{ij} \rangle \tag{6}$$

where p_{ij} is the probability that i and j are in the same cluster and $\langle \lambda_{ij} \rangle$ is the average number of cutting bonds between i and j . To be more precise

$$\langle \lambda_{ij} \rangle = \lim_{N \rightarrow \infty} \sum_{\{\sigma_i\}} \exp(-\beta \mathcal{H}) \left(\sum_{C \subseteq E\{\sigma_i\}} \lambda_{ij} p_B^{|C|} (1 - p_B)^{|D|} \right) \left(\sum_{\{\sigma_i\}} \exp(-\beta \mathcal{H}) \right)^{-1} \tag{7}$$

where $E\{\sigma_i\}$ is the set of all bonds in the sublattice made of sites in the site configuration i . C is a subset of $E\{\sigma_i\}$ and $D = E\{\sigma_i\} - C$; $|C|$ and $|D|$ are the number of bonds respectively in the subsets C and D . N is the total number of bonds in the lattice, λ_{ij} is the number of cutting bonds between i and j in the configuration $C\{\sigma_i\}$. Note that $\lambda_{ij} = 0$ if i and j are not connected. Analogously p_{ij} is obtained from (7) substituting λ_{ij} with the connectedness indicator γ_{ij} which is 1 if i and j are in the same droplet and zero otherwise. To prove relation (6) in PCSRBP we use the fact that in random bond percolation relation (6) is valid for any lattice (Coniglio 1982). In particular it is valid for any sublattice $E\{\sigma_i\}$ made up of sites in state 1. If we average over all Potts configurations with the appropriate Boltzmann factor we obtain relation (6) for PCSRBP. From (6), summing over j and dividing by $S = \sum_j p_{ij}$, we obtain

$$p_B S^{-1} dS/dp_B = N_{\text{links}} \tag{8}$$

where $N_{\text{links}} \equiv \sum \langle \lambda_{ij} \rangle S^{-1}$ is the number of links between two points separated by a distance of the order of the connectedness length ξ . From equation (2) generalised to all values of q and (8)

$$N_{\text{links}}(q) \sim u^{-1} f_3(t/u^{\phi(q)}) \tag{9a}$$

or from (1)

$$N_{\text{links}} \propto \xi^{1/\nu_B}. \tag{9b}$$

If $t = 0$ and $\epsilon \rightarrow 0$, $N_{\text{links}} \propto \epsilon^{-1}$ diverge with the super universal exponent 1 for any d , any q and any lattice. If $p_B = p_B(T)$ ($u = 0$) and the critical temperature is approached:

$$N_{\text{links}}(q) \propto t^{-1/\phi(q)}. \tag{10}$$

We will give arguments to show that not only links but also blobs are present.

We consider first the case $d = 2$. If there were only links, two points separated by a distance of the order of ξ would be connected by a self-avoiding chain whose length would be given by $N_{\text{links}} \geq \xi$ since the end-to-end distance is always smaller than any other path. From (9b) it would follow that $\nu_B(q) \leq 1$. On the contrary there is evidence

from MKRG that $\nu_B(q)$ is an increasing function of q (Coniglio and Peruggi 1982) and $\nu_B(q) = \frac{4}{3}$ (den Nijs 1979). Therefore $\nu_B(q) > 1$, and not only links are present but also blobs. If we are right at $t=0$, $\varepsilon=0$ the incipient infinite droplet is then made of links and blobs in such a way that two points separated by a distance of the order b are related to the number of links by $N_{\text{links}} \propto b^{1/\nu_B}$. We should stress that these links are internal links in the sense that if one is broken the two points might still be connected by another chain (see figure 1).

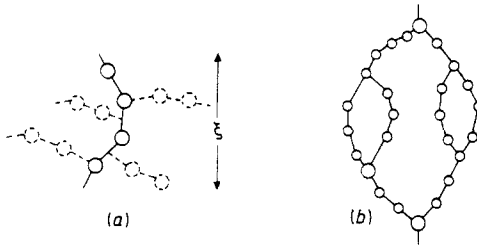


Figure 1. (a) Structure of the incipient infinite 'droplet' in the q -state Potts model as defined in the text. The backbone (full lines) is made of links and blobs. For $q=1$ the 'droplet' coincides with the incipient infinite cluster in the random percolation model. As q increases the number of links decreases for fixed values of ξ . (b) Self-similar structure of the backbone of the incipient infinite 'droplet' at the Potts critical temperature where the droplet size diverges. This is also the structure of the blobs in (a).

Note also that, since $\nu_B(q)$ is an increasing function of q , the number of links for a given distance b decreases. This is rather intuitive due to the fact that the correlation makes the blobs more dominant.

It is interesting to note that Coniglio and Peruggi (1982) using MKRG found a value of $q = q^*$ where $\nu_B^{-1} = 0$. They interpreted this value as the critical value above which the Potts transition becomes of first order. In this context this result implies that for such value of q^* the number of links would vanish, i.e. above q^* the droplets will lose their quasi-one-dimensional character and the coalescence of droplets which gives rise to the transition will lead to a discontinuity in the order parameter.

For $d=3$ there is no calculation of $\nu_B(q > 1)$, but it could be computed by Monte Carlo methods using the same algorithm implemented to study the Ising droplets (Stauffer 1981, Ottavi 1981, Roussenq *et al* 1982, Heermann and Stauffer 1981, Jan *et al* 1982, Kertesz *et al* 1983).

We expect, in analogy with random percolation, that the blobs become less important until they disappear for $d=6$. This is consistent with the result for the Ising model that gives $\nu_B = 2/(d-2)$ near $d=6$ and $\nu_B = \frac{1}{2}$ for $d=6$ which reproduces the Bethe lattice case where no blobs are present.

We want to mention that the behaviour of ν_B indicated above for the Ising model ($q=2$) has been confirmed and extended by a recent result of Benzoni and Cardy (1983). Using ε -expansion techniques these authors proved at all orders in ε the relation

$$\nu_B = 2/(d-2+\eta_1) \quad (11)$$

where η_1 is the algebraic power law decay exponent of the correlation function of the Ising model at T_c . This relation, as they pointed out, seems to break down for low dimensionality. It is interesting to note that the connectedness length exponent of

the Potts droplets diverges with an exponent $\bar{\nu} = 2/(d - 2 + \eta)$ when $T = T_c$ and $p_B = p_B(T_c)$, the density of occupied sites is considered as a variable and η is the algebraic power law decay exponent of the correlation function of the Potts model at T_c . This relation is valid for any d and agrees with the general result of Weinrib and Halperin (1983).

We want now to discuss briefly the structure of the usual clusters (the maximal set of NN 'down' spins) in the Ising model. For $d = 2$ we know that the critical point is characterised by the onset of an infinite cluster of 'down' spins and that the incipient infinite cluster is destroyed only if a bond probability between 'down' spins is below the special value $p_B = 1 - \exp(-2J/kT)$ (Coniglio and Klein 1980). If the incipient infinite cluster of 'down' spins were made only of a quasi-one-dimensional chain of links and blobs, an infinitesimal change of p from $p = 1$ would have destroyed the onset of the infinite cluster. Therefore we argue that the incipient infinite cluster in the Ising model in $d = 2$ is only made of blobs *without* links.

In three dimensions we know that the infinite cluster does not disappear at T_c (Müller-Krumbhaar 1974). Nevertheless we will show that this point is characterised by an anomalous percolation transition which has an effect on the structure of the infinite cluster. We use a theorem which states the following inequality (Coniglio *et al* 1977)

$$\tilde{p}_{ij} \equiv p_{ij} - P_\infty^2 \geq g_{ij}$$

where p_{ij} is the probability that i and j are in the same cluster, P_∞ is the probability that a 'down' spin belongs to the infinite cluster and g_{ij} is the pair correlation function. Summing over j on both sides we obtain

$$\tilde{S} \equiv \sum \tilde{p}_{ij} \geq \sum g_{ij} = \chi.$$

Since $\chi \sim (T - T_c)^{-\gamma}$, $\tilde{S} \sim (T - T_c)^{-\gamma^*}$ with $\gamma^* \geq \gamma$. \tilde{S} is a quantity in random percolation which diverges at the percolation threshold where P_∞ is not zero. In this sense the Ising critical point is characterised by an anomalous percolation transition without the disappearance of the infinite cluster. γ^* is the analogue of the mean cluster size exponent in the two-dimensional Ising model at the critical point. It would be interesting to investigate whether $\gamma^* = \gamma + \beta$ as indicated in the theory of Bruce and Wallace (1983) in low dimensions. In analogy with the two-dimensional case we also expect that the length defined by $\sum r_{ij}^2 \tilde{p}_{ij} / \sum \tilde{p}_{ij}$ will diverge with the correlation thermal exponent ν at the critical point. From what was said it follows that the infinite cluster near the critical point is made of highly correlated regions of linear dimension of the order of ξ connected by strings. The size of the correlated regions diverges with the exponent γ^* .

If we introduce a bond probability we expect in the diagram P_B -magnetisation ($H = 0$) a line where such a transition occurs (see figure 2). This line ends at the value $p_B(T_c) = 1 - \exp(-2J/kT_c)$. In the same diagram is also reproduced another anomalous percolation transition predicted by Delyon *et al* (1981) without the appearance of an infinite cluster.

In conclusion, we have studied the structure of the incipient infinite droplet at the critical point of the q -state Potts model. This is a self-similar fractal made of links and blobs just as in random percolation. The number of links between points separated by a distance b diverges with an exponent $\nu_B(q)$ which coincides with the connectedness length exponent for $q = 1$. For $q > 1$, $\nu_B(q)$ differs from the correlation length exponent $\nu(q)$. This exponent $\nu_B(q)$ has not raised much attention so far. It would be interesting to calculate it for its relation to the structure of the droplets.

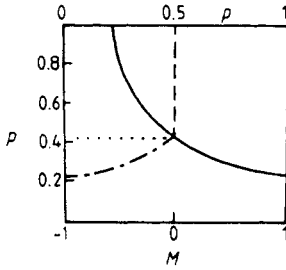


Figure 2. Schematic phase diagram of three-dimensional site Ising correlated random-bond percolation in zero magnetic field (bond probability p_B as function of magnetisation M or site probability $p = \frac{1}{2}(1 + M)$). The broken line corresponds to a percolation transition in the structure of the infinite network, without the vanishing of the infinite cluster. The chain curve corresponds to a percolation transition in the cluster numbers without the appearance of an infinite cluster predicted by Delyon *et al* (1981).

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