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COMMENT

A–B droplets for a two-dimensional antiferromagnetic Ising model in external field H

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Abstract. The A–B site–bond percolation in the antiferromagnetic Ising model in an external field H is studied with the infinitesimal Migdal–Kadanoff renormalisation group. It is shown that for $H=0$ the clusters of holes and particles diverge at the Ising critical point $K=K_c$ with the bond concentration p_B in the range $1-\exp(-|K_c|/2)\leq P_B\leq 1$ as in the Coniglio–Klein model.

For $H\neq 0$ the thermal antiferromagnetic critical line coincides with the percolation lines for a wider range of p_B, i.e. $p_{B_{min}}(K)\leq p_B(K)\leq 1$ where $p_{B_{min}}(K)<1-\exp(-|K|/2)$.

The correlated percolation problem has been widely used in the area of critical phenomena (see e.g. Stoll and Domb 1979, Stauffer 1979, Essam 1980, Kertesz *et al* 1983).

The site–bond correlated percolation is a generalisation of the correlated percolation. It provides a geometrical interpretation of the Ising critical droplets (Fisher 1967, Bruce and Wallace 1981, 1982). It has been studied both in the case of equal particles (A–A percolation) (Coniglio and Klein 1980, Coniglio *et al* 1982b) and for particles of different type (A–B percolation) (Coniglio *et al* 1982a).

In the A–A site–bond correlated percolation the clusters in an attractive lattice gas or ferromagnetic Ising model are defined as the maximal sets of nearest-neighbour particles connected by active bonds; the probability of a bond being active is p_B and non-active $1-p_B$.

It has been shown that this type of cluster diverges at the Ising critical point in any dimension d with Ising exponents, provided that $p_B=1-e^{-K/2}$ where K is the nearest-neighbour coupling constant (Coniglio and Klein 1980, Heermann and Stauffer 1981, Ottavi 1981, Roussenq 1981, Coniglio *et al* 1981, di Liberto *et al* 1983).

These special clusters ('droplets'), however, diverge also along a line which is in the region where the external field, H, is $H>0$; in this region no singularities are expected in the thermal free energy.

For a repulsive lattice gas ($K<0$) or antiferromagnetic Ising model it has been suggested (Coniglio *et al* 1982a, Monroy *et al* 1982) that for $H=0$ the clusters which diverge at the critical point with the right exponents are the A–B 'droplets', i.e. A–B clusters with $p_B=1-e^{-|K|/2}$.

An A–B cluster is a cluster made of nearest-neighbour particles (A) and holes (B) with antiferromagnetic order, connected by bonds active with probability p_B. At $H=0$

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the A–B percolation problem for a two-sublattice antiferromagnet can be mapped on to the A–A problem in the ferromagnetic region, by reversing the spins on one sublattice. For this last problem the answers are already known (Coniglio *et al* 1981): therefore the A–B 'droplets' must have the stated property.

More intriguing is the case $H \neq 0$. It is known that in an antiferromagnet there is indeed a line of thermal critical points for $H \neq 0$. Do the A–B droplets diverge along the thermal critical line? Monroy *et al* (1982) have already shown that this is not the case in the Bethe approximation.

Here we investigate this problem for $d = 2$ with a new version of the infinitesimal Migdal–Kadanoff renormalisation group.

The A–B site-bond correlated percolation problem can be obtained as the $Q = 1$ limit from a suitable dilute Q-state Potts model. This has been shown elsewhere (Coniglio *et al* 1982a, Monroy *et al* 1982); we give here for convenience a brief outline of the procedure, to show that the previous definition of 'droplet' (i.e. $p_B = 1 - e^{-|K|/2}$) is not expected to work at $H \neq 0$.

Let us consider a square lattice of N sites made of sublattices A and B and let a site be active if it belongs to sublattice A and is occupied or if it is vacant and belongs to sublattice B.

The interaction between particles is repulsive and due to the Hamiltonian

$$-\beta\mathcal{H}_{LG} = K \sum_{\substack{\langle i,j\rangle \\ i\in A}} n_i n_j + \Delta \sum_{i\in A\cup B} n_i$$

where $n_i = 1$ if site i is occupied, $n_i = 0$ otherwise, $\beta = 1/K_B T$, $K < 0$ is the nearest-neighbour coupling constant related to the Ising constant K_I by $K_I = K/4$, Δ is the chemical potential related to the Ising magnetic field H and the coordination number c by $-H = \frac{1}{2}(\Delta - cK/2)$. The sum $\Sigma_{\langle i,j\rangle}$ is over nearest-neighbour pairs.

An A–B cluster is made of active sites connected by active bonds, a bond being active with probability p_B and not active with probability $1 - p_B$ (figure 1).

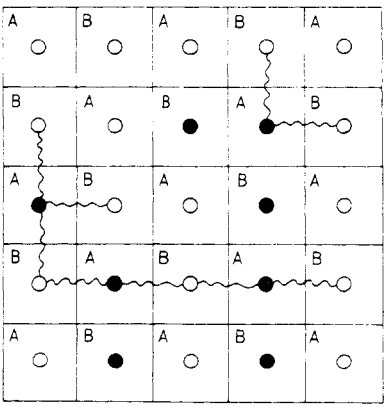

Figure 1. Full circles denote particles and open circles holes. The labels A and B single out one of the two antiferromagnetic ground states. Bonds are denoted by wavy lines. The case $p_B = 1$ is reported. The configuration in this figure contains one eight-site cluster (three particles and five holes) and one three-site cluster (one particle and two holes). Observe that the probability of a bond being active between the other particles and the neighbouring holes is zero since these particles are located on the sublattice B.

Therefore in the A–B site-bond percolation the average of quantities of interest can be written as follows:

$$\langle \ldots \rangle = \lim_{N\to\infty} \sum_{\{n_i\}} \ldots \exp(-\beta\mathcal{H}_{\mathrm{LG}}) \sum_{C\subseteq E\{n_i\}} p_{\mathrm{B}}^{|C|}(1-p_{\mathrm{B}})^{|D|}\Big(\sum_{\{n_i\}} \exp(-\beta\mathcal{H}_{\mathrm{LG}})\Big)^{-1} \tag{1}$$

where $E\{n_i\}$ is the set of the bonds in the sublattice made of active sites in the configuration $\{n_i\}$, C is a subset of $E\{n_i\}$, $D = E\{n_i\} - C$, $|C|$ and $|D|$ are the number of bonds in C and D. Of course for every configuration we have $\Sigma_{C\subseteq E\{n_i\}} p_{\mathrm{B}}^{|C|} \times (1-p_{\mathrm{B}})^{|D|} = 1$.

The probability distribution (1) can be obtained in the $Q = 1$ and $h = 0$ limit from the following asymmetric $(Q+1)$-state Potts Hamiltonian:

$$-\beta\mathcal{H}(b_i) = J \sum_{\substack{\langle i,j\rangle \\ i\in A}} (\delta_{b_i b_j} - 1) - (2J + K) \sum_{\substack{\langle i,j\rangle \\ i\in A}} \delta_{b_i 0}\delta_{b_j 0}$$

$$+ (cJ - \Delta + \ln Q) \sum_{\substack{i \\ i\in A}} \delta_{b_i 0} + (cJ - \Delta + \ln Q) \sum_{\substack{j \\ j\in B}} (1 - \delta_{b_j 0}) \tag{2}$$

where $b_i = 0, 1, \ldots, Q$ (Coniglio *et al* 1982a).

The Hamiltonian (2) in the $Q = 1$ limit is equivalent to a two-state Potts model. If $J = -K/2$ ($K < 0$), i.e. $p_{\mathrm{B}} = 1 - \mathrm{e}^{-|K|/2}$, then Hamiltonian (2) becomes a symmetric two-state Potts model with ferromagnetic coupling constant $|K|/2$ and staggered field $2H = -(\Delta - \frac{1}{2}cK)$ which is equivalent to the Ising model with coupling constant $|K|/4$ and staggered field H.

This, on the other hand, is equivalent to an antiferromagnetic Ising model with coupling constant $-|K|/4$ and homogeneous field H which exhibits a line of critical points in the H–K plane with Ising exponents.

Therefore for $H = 0$ also the clusters of holes and particles connected by active bonds with probability $p_{\mathrm{B}} = 1 - \mathrm{e}^{-|K|/2}$ should diverge at the antiferromagnetic critical point $K = K_{\mathrm{c}}$, with Ising exponents.

For $H \neq 0$ this is not necessarily true. In fact the linear term in H breaks the symmetry and again generates (in the renormalisation group language) a term proportional to $\delta_{b_i 0}\delta_{b_j 0}$. This consideration could invalidate the suggestion that even for $H \neq 0$ the choice $p_{\mathrm{B}} = 1 - \mathrm{e}^{-|K|/2}$ would have reproduced the features of the 'droplets' (Coniglio *et al* 1982a).

The Migdal–Kadanoff renormalisation group (MKRG) approach for Potts models has been widely used in the percolation problem (Coniglio and Klein 1980, Coniglio and Peruggi 1982, Coniglio *et al* 1981). As is already known (Nicoll 1979), the Migdal–Kadanoff procedure for a Hamiltonian

$$-\beta\mathcal{H} = \sum_{\langle i,j\rangle} \mathcal{H}(\mu_i, \mu_j),$$

where μ_i is a site variable and $\Sigma_{\langle i,j\rangle}$ runs over the nearest-neighbour sites, gives rise to relations

$$T' = T^b(T^b(\mu_i, \mu_j)) \tag{3}$$

where $T(\mu_i, \mu_j) = \exp \mathcal{H}(\mu_i, \mu_j)$ and T' is a matrix whose elements are expressed in terms of the renormalised Hamiltonian $\mathcal{H}'(\mu_i', \mu_j')$, i.e. $T'(\mu_i', \mu_j') = \exp \mathcal{H}'(\mu_i', \mu_j')$.

The right-hand side of relations (3) is the product of b matrices T, the elements of which are $T^b(\mu_i, \mu_j)$ with b as scaling factor. In the infinitesimal MKRG, b is infinitesimally near to 1.

In our case Hamiltonian (2) depends on A and B sublattices; therefore we have to modify the general procedure and define the two asymmetric matrices

$$(T^b_A)_{ij} = T^b(\mu_i, \mu_j), \qquad (T^b_B)_{ij} = T^b(\mu_j, \mu_i).$$

These enable us to write the renormalisation relations

$$T' = T^b_A (T^b_B T^b_A)^{b'}, \qquad b' = \tfrac{1}{2}(b-1).$$

In the $Q = 1$ limit and for an $h = 0$ ghost field the diagonalisation of these matrices gives the following recursion relations:

$$w' = [w^b(\nu+\delta)+\tau]/(\tau+\delta-\nu), \tag{4a}$$

$$y' = w^b y^b [(\nu+\delta)+y^{-b}w^{-b}\tau]^2/[w^b(\nu+\delta)+\tau][\tau+\delta-\nu], \tag{4b}$$

$$x' = 1-(1-x^b)2(\alpha^2+4)^{1/2}/\beta[(\mu+\delta)+y^{-b}w^{-b}\tau], \tag{4c}$$

where $w = e^{-H}$, $y = e^{-K} = e^{|K|}$, $x = e^{-J}$, $w' = e^{-H'}$, $y' = e^{|K'|}$, $x' = e^{-J'}$ and

$$\alpha = \frac{w^b-1}{w^{b/2}y^{b/2}}, \qquad \varepsilon = \frac{2y^b w^b + 1 + w^{2b}}{y^{b/2}w^{b/2}(w^b+1)}, \qquad G' = \left(\frac{\varepsilon+(\alpha^2+4)^{1/2}}{\varepsilon-(\alpha^2+4)^{1/2}}\right)^{b'},$$

$$\nu = \alpha(G'-1), \qquad \delta = (\alpha^2+4)^{1/2}(G'+1), \qquad \tau = 2w^{b/2}y^{b/2}(G'-1),$$

$$\beta = (1+w^b)[\varepsilon-(\alpha^2+4)^{1/2}]/2w^{b/2}y^{b/2}(1-x^b)^2.$$

We point out that as in the ferromagnetic case also here the renormalisation equations for y and w are decoupled from the x equation.

Equations (4a) and (4b) which describe the thermal behaviour give the following relevant fixed points in the H–K plane:

(1) $\qquad H = \tfrac{1}{2}(\Delta - \tfrac{1}{2}cK) = 0, \qquad K_c = -4|K_{ONS}|,$

where $|K_{ONS}| = \frac{1}{2}\ln(\sqrt{2}+1) = 0.4407$ with the following scaling powers:

$$y_{H=0} = 0.12, \qquad y_{K_c} = 0.75,$$

which describe the critical behaviour at $H = 0$, $K = K_c$;

(2) the spurious fixed points

$$H^* = \pm 0.7844, \qquad K^* = -2.1015,$$

with scaling powers

$$y_{H^*} = 0.06, \qquad y_{K^*} = 0.66,$$

which describe the critical behaviour on the phase boundary for $H \neq 0$.

However, it is believed that there is only one critical behaviour all along the phase boundary, including $H = 0$. The presence of the spurious fixed point, which is also found by Coniglio *et al* (1981) and Mujeeb and Stinchcombe (1982), is presumably due to the Migdal–Kadanoff approximation.

At $H = 0$, $K = K_c$ there are three fixed points: $J_2 = \frac{1}{2}K_c = 2K_{ONS} = 0.8814$, $J_1 = 0$, $J_3 = 3.3068$. The fixed points J_1 and J_3 are stable in the J direction. The scaling power at J_2 is $y_{J_2} = 0.50$.

The fixed point J_2 describes the critical behaviour of the Ising A–B droplets which diverge with Ising exponents. The fixed point J_3 describes percolation at the Ising critical point for

$$1-e^{-|K|/2}<p_B\leqslant 1. \tag{5}$$

Therefore we find that for $H=0$ the A–B clusters diverge at the antiferromagnetic critical point for all the values of p_B in the range $1-e^{-|K|/2}\leqslant p_B\leqslant 1$. For all these values the connectedness length exponent and the correlation length exponent coincide because of the decoupling of equations (4). The A–B droplets are defined only for $p_B=1-e^{-|K|/2}$ because only for this particular choice of p_B do the cluster size exponent and the thermal susceptibility exponent coincide (Coniglio and Klein 1980).

All these results are expected because of the mapping of the A–B percolation problem onto the A–A percolation problem in the ferromagnetic region, as pointed out before. However, they are a useful test for the Hamiltonian (2) and the related equations (4). In addition to that, we find at $H=0$ and $K=-\infty$ a fixed point $J_4=0.693$ which corresponds to the pure random bond percolation (i.e. $p_B=0.5$). The percolative critical line for this value of p_B is at $T=0$ (i.e. $1/|K|=0$) on the H/K axis, inside the phase boundary (figure 2). The scaling power at this fixed point is $y_{J_4}=0.61$ which implies a connectedness exponent $\nu_p=y_{J_4}^{-1}=1.63$. This point describes all the percolative transitions which occur inside the phase boundary.

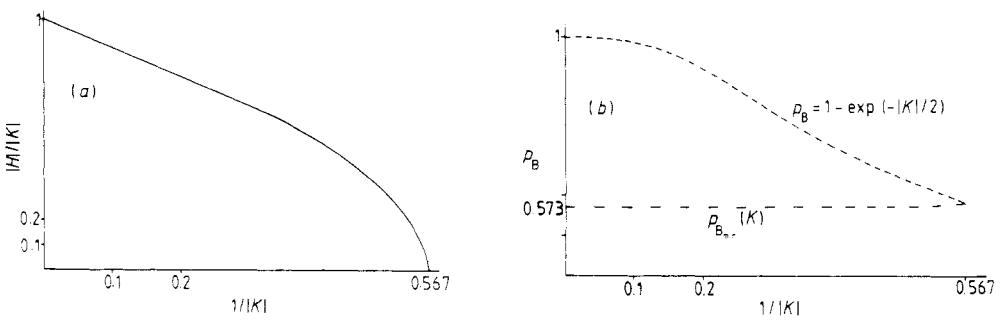

Figure 2. (*a*) The A–B percolation critical lines for $p_B(K)$ in the range $p_{B_{min}}(K)\leqslant p_B(K)\leqslant 1$ coincide with the antiferromagnetic phase boundary. The antiferromagnetic phase boundary can be regarded as a function of T (i.e. $1/K$) which goes from $H=0$ at $T=T_c$ to $H=\pm H_c$ at $T=0$. (*b*) $p_{B_{min}}(K)$ together with $p_B=1-e^{-|K|/2}$ is reported as a function of $1/K$. For each K the percolation critical point coincides with the phase boundary point $H(T)$ for p_B in the range $p_{B_{min}}(K)\leqslant p_B\leqslant 1$.

For $H\neq 0$ we find that the thermal antiferromagnetic critical line coincides with the percolation line for a range of p_B wider than that given by relation (5). In fact, at the spurious fixed point $H=H^*$ and $K=K^*$ we find the fixed points

$$J_5=0, \qquad J_6=0.8613, \qquad J_7=3.4439.$$

J_6 is unstable; it is the analogue of J_2 at $H\neq 0$ but it is smaller than $|K^*|/2$.

In figure 2 we give the $p_{B_{min}}(K)$ such that the percolation line for $p_B(K)$ in the range $p_{B_{min}}(K)\leqslant p_B(K)\leqslant 1$ coincides with the phase boundary. In this figure we report for comparison $p_B=1-e^{-|K|/2}$ too. Except for $K=K_c$ we have $p_{B_{min}}<1-e^{-|K|/2}$.

Finally, because of the decoupling of equations (4), we have that the connectedness length exponent is given by $y_{K^*}^{-1}$ for $p_{B_{min}}(K)\leqslant p_B\leqslant 1$. No analysis has been made for

the mean cluster size exponent, but we expect that the percolation exponent γ_p is the thermal Ising exponent γ_I only for $p_B(K) = p_{B_{min}}(K)$.

The results obtained here lead us to the following conclusions. The A–B droplets made of nearest-neighbour particles (A) and holes (B) connected by bonds active with probability $p_B = 1 - e^{-|K|/2}$ diverge with the right exponents if $H = 0$ as in the Coniglio–Klein droplet model.

For $H \neq 0$ the thermal antiferromagnetic critical line coincides with the percolation lines for p_B in the range $p_{B_{min}}(K) \leqslant p_B(K) \leqslant 1$ where $p_{B_{min}}(K) < 1 - e^{-|K|/2}$. Therefore the extension of the Coniglio–Klein droplet model at $H \neq 0$ is obtained for the choice $p_B(K) = p_{B_{min}}(K)$.

For three dimensions we expect that at $H = 0$ the A–B droplets are obtained for $p_B = 1 - e^{-|K|/2}$, but at $H \neq 0$ the $p_B(K)$ would not be such a simple function. Therefore the resulting percolative phase diagram for three dimensions would be similar to that found for the Bethe lattice (Monroy *et al* 1982).

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