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Clusters and Ising critical droplets: a renormalisation group approach

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Abstract. The Migdal–Kadanoff renormalisation group for two dimensions is employed to obtain the global phase diagram for the site–bond correlated percolation problem. It is found that the Ising critical point ($\vec{K} = \vec{K}_c, H = 0$) is a percolation point for a range of bond probability p_B such that $1 \geq p_B \geq 1 - e^{-2\vec{K}_c}$. In particular, as p_B approaches $1 - e^{-2\vec{K}_c}$, the percolation clusters become less compact and coincide with the Ising critical droplets.

Much attention (Domb 1974, Binder 1976, Stoll *et al* 1972) has been paid to the study of clusters made of nearest-neighbour occupied sites in the lattice gas or Ising model, because of possible connections between the behaviour of such clusters and the thermodynamic properties such as phase transitions, nucleation, etc. For a long time it has been widely believed that these clusters, which we will call Ising clusters, have the same properties as the droplets studied in the droplet model (Fisher 1967)—namely that (i) they diverge at the Ising critical point; (ii) their linear dimension, which we identify with the connectedness length, diverges as the Ising correlation length; and (iii) the mean cluster size S (i.e. the second moment of the cluster size distribution) diverges as the susceptibility.

It has been proven rigorously, in fact, that in two dimensions such clusters diverge at the Ising critical point (Coniglio *et al* 1977) $H = 0, T = T_c$. However, series expansions (Sykes and Gaunt 1976) have shown that the mean cluster size S diverges as $(T - T_c)^{-\gamma_p}$ with $\gamma_p = 1.91 \pm 0.01$, which is definitely larger than the susceptibility exponent in the Ising model, $\gamma = 1.75$. Moreover, in three dimensions Monte Carlo studies and series expansions (Sykes and Gaunt 1976) show that these clusters in the low-density phase diverge at a temperature $T < T_c$. At this stage it is by no means clear what role such clusters play in the study of critical properties of the Ising model. The first question to answer (stated clearly by Binder (1976)) is how to define, in a precise way, a cluster which has the properties (i), (ii) and (iii) of a critical droplet. One would like to define a cluster which carries all the critical information contained in the Ising pair correlation function. The known properties of the Ising clusters suggest that these clusters are too big to describe critical droplets. The reason is that there are two contributions to the Ising clusters: one is due to the correlations, and the other is due to purely geometric effects. The last contribution becomes evident in the limit of infinite temperature and

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zero magnetic field. In this case there are no correlations, although the cluster size is different from zero. This is due to the fact that the density of occupied sites is $\frac{1}{2}$, and these join together to become clusters for purely geometrical reasons. Starting from the Ising clusters, we seek to define a smaller cluster in which the geometrical effect has been eliminated.

For any given configuration of the lattice gas we consider first the Ising clusters made of nearest-neighbour occupied sites. Then we introduce a bond with probability p_B between any nearest-neighbour pair in the Ising cluster (figure 1). These new clusters

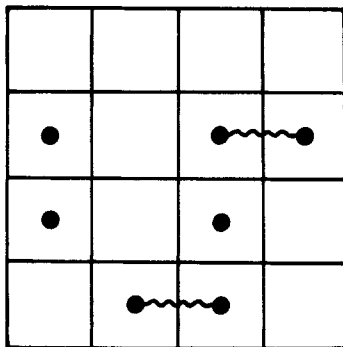


Figure 1. Occupied sites are denoted by dots, and bonds by wavy lines. The configuration in this figure contains two two-site clusters and three one-site clusters.

are made of occupied sites connected by bonds (Coniglio *et al* 1979). The original Ising cluster will either reduce its size or will break into smaller clusters. We will show that there will be a particular value of p_B for which these new clusters behave like critical droplets and obey properties (i), (ii) and (iii). If $p_B = 1$, we obtain the Ising clusters again. This case ($p_B = 1$) is known as the site correlated percolation problem because one looks at the properties of the Ising clusters just as in the random percolation problem (Essam 1973, Stauffer 1979). The main difference is that in random percolation the occupied sites are randomly distributed, while in this case they are correlated according to the lattice gas Hamiltonian. In the infinite-temperature limit one recovers random percolation. The case $p_B \neq 1$ is called site-bond correlated percolation (Coniglio *et al* 1979). Another important reason for studying site-bond correlated percolation is that it has been proposed as a model for the sol-gel transition where the gelation transition occurs near the consolute point. This model has already been solved (Coniglio *et al* 1979) for the Cayley tree, and the phase diagram is in fair agreement with the experimental data of Tanaka *et al* (1979).

A Hamiltonian formalism has been proposed to study site correlated percolation (Murata 1979). We can generalise this formalism to study site-bond correlated percolation. The Hamiltonian that we consider is the S -state dilute Potts model which is given by

$$H = H_{LG} + H_{DP}. \quad (1)$$

Here

$$-\beta H_{LG} = K \sum_{\langle ij \rangle} n_i n_j - \Delta \sum_i n_i \quad (2)$$

is the lattice gas Hamiltonian, where $n = 0, 1$, $\beta = 1/k_B T$, K is the nearest-neighbour coupling constant, related to the Ising coupling \tilde{K} by $\tilde{K} = 4K$, and Δ is the chemical potential, related to the Ising magnetic field H and the coordination number c by $H = \frac{1}{2}(\Delta - \frac{1}{2}cK)$. The sum is over nearest neighbours, and

$$-\beta H_{DP} = J \sum_{\langle ij \rangle} (\delta_{\sigma_i \sigma_j} - 1) n_i n_j + h \sum_i (\delta_{\sigma_i 1} - 1) n_i, \quad (3)$$

where σ_i is the s -state Potts variable. Following the procedure of Murata, we can show that the function G that plays the role of the free energy in the site-bond correlated percolation problem is given by

$$G(K, h, H, J) = dF/ds|_{s=1},$$

where

$$-\beta F = \lim_{N \rightarrow \infty} \frac{1}{N} \ln \left(\text{Tr}_{\sigma_i n_i} e^{-\beta H} \right).$$

The first and second derivatives of G with respect to h are related respectively to the percolation probability P (probability that an occupied site belongs to an infinite cluster) and the mean cluster size S .

The clusters are made of sites distributed with the lattice gas Hamiltonian (2) connected by bonds with probability $p_B = 1 - e^{-J}$.

There is an important property of (1) which allows us to describe the droplet in terms of geometric clusters. Namely, for $J = K/2$ and $H = 0$ equation (1) is equivalent to an $(s+1)$ -state Potts model, i.e.

$$-\beta H = \frac{K}{2} \sum_{\langle ij \rangle} (\delta_{b_i b_j} - 1) + \lg s \sum_i (\delta_{b_i 1} - 1), \quad (4)$$

where b is an $(s+1)$ -state Potts variable. In the limit $s \rightarrow 1$ equation (4) becomes equivalent to the lattice gas (equation (2)); consequently F becomes the lattice gas free energy, and G will have a singularity at the Ising critical point $K = K_c$, $H = 0$. This suggests that the Ising critical point $K = K_c$, $H = 0$ is a percolation point if we choose

$$p_B = 1 - e^{-K/2}. \quad (5)$$

This argument is valid for any dimension. For $d > 2$ and $p_B = 1$ we know (Coniglio *et al* 1977, Müller-Krumbhaar 1974) that for $H = 0$ an infinite cluster of 'down' spins appears at a temperature T below the Ising critical temperature T_c .

The above simple argument shows that, if we instead choose p_B as given by equation (5), these new clusters made of nearest-neighbour 'down' spins connected by bonds will now diverge at T_c . These clusters then are good candidates for Ising droplets near the critical point.

Now we apply the Migdal (Migdal 1976, Kadanoff 1976) renormalisation group to this Hamiltonian on the triangular lattice. After removing bonds and decimating (figure 2), we find the recursion relations

$$x' = \frac{(y^4 z^4 + 1)x^4}{y^4 z^4 (2x^2 - 1) + x^4}, \quad y' = \frac{(y^4 z^4 + 1)(z^4 + 1)}{(y^2 z^4 + 1)^2}, \quad z' = \frac{y^2 z^6 + z^2}{z^4 + 1}, \quad (6)$$

where $x = e^J$, $y = e^K$ and $z = e^{-\Delta/6}$. An important feature of equation (6) is that the expressions for y' and z' reduce to the Ising recursion relations with *no dependence on x* ; that is, the recursion relations are coupled only by the x' dependence on y and z . This

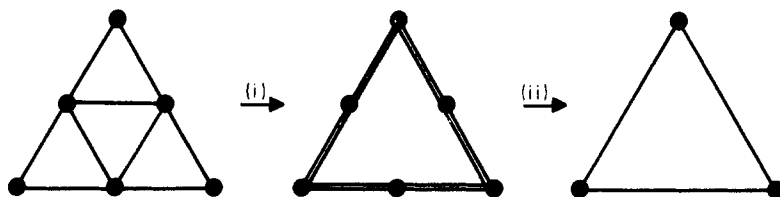


Figure 2. Successive steps of the Migdal renormalisation group on the triangular lattice: (i) bond moving $a \rightarrow b$; (ii) dedecoration $b \rightarrow c$.

decoupling occurs for other renormalisation groups (Coniglio and Lubensky 1980, Coniglio and Klein 1980, to be published), and in fact it seems to be a general property of Hamiltonian (1) in the limit $s \rightarrow 1$. Because of this property, we can predict the exact Ising scaling powers $y_K = 1$, $y_H = 1.875$ and the Ising critical coupling $K = 1.099$, while equation (6) gives the approximate values $y_K = 0.747$, $y_H = 1.879$ and $K = 1.219$. We have also obtained recursion relations for $h \neq 0$, the details of which will be published elsewhere (Coniglio and Klein 1980, to be published).

The fixed points and flow lines are shown in figure 3(a), and the eigenvalue exponents are in table 1. Analysis of these fixed points shows that there exists a line of

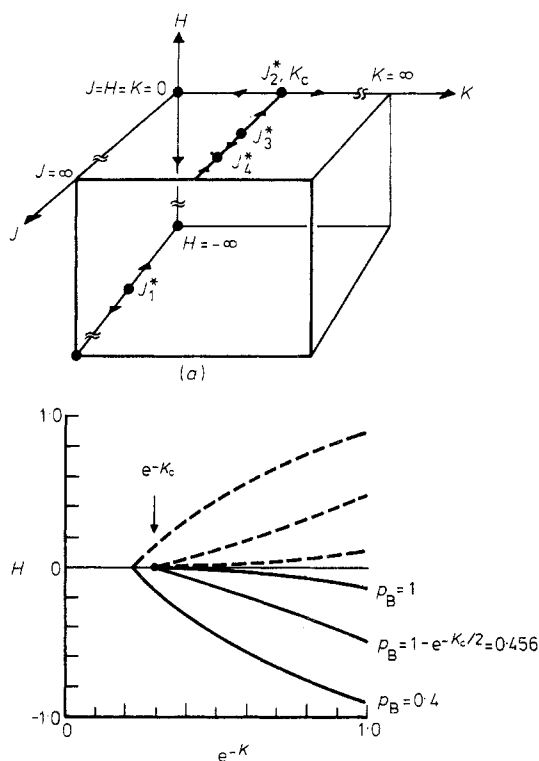


Figure 3. (a) Schematic representation of the flow lines generated by the recursion relations of equations (6). (b) Phase diagram for different values of the bond probability p_B . The full curves are percolation critical lines for 'down' spins (occupied sites). The broken curves, which are a mirror image of the full curves, represent the critical lines of the 'up' spins (empty sites).

Table 1. The fixed point values and scaling powers associated with the phase transitions in our model. The fixed point J_1^* is reached from all values of J, K, H at which there is a percolation transition, except $K = K_c, H = 0$, whereas the fixed points J_3^* and J_4^* are obtained only for $K = K_c, H = 0$.

Fixed points		J^*	y_J	y_h
J_1^*	Pure random percolation	0.481 (0.427) ^a	0.6115 (0.7375 ± 0.08) ^b	1.904 (1.898 ± 0.003) ^b
J_3^*	Ising droplets	0.609 = $K^*/2$	0.535	$y_h = y_H$
J_4^*	Ising clusters	2.324	<0	1.964 (1.955 ± 0.005) ^c
$1 - e^{-K/2} < p_B \leq 1$				
Ising	$K^* = K_c$	y_K	y_H	
K^*	1.219 (1.099) ^d	0.747 (1) ^d	1.879 (1.875) ^d	

^a Exact results (Sykes and Essam 1964).

^b Large cell renormalisation group (Reynolds *et al* 1978).

^c Series expansion (Sykes and Gaunt 1976). This value y_h is obtained from the series expansion calculation $\gamma_p = 1.91 \pm 0.01$ using the scaling relation $\gamma_p = (2y_h - 2)/y_K$ and the exact value $y_K = 1$.

^d Exact results.

percolation points where the Ising clusters diverge. Such lines end at the Ising critical point (figure 3(b)), in agreement with rigorous results (Coniglio *et al* 1977). The critical exponents along this line are the same as those of random percolation, in agreement with other results (Klein *et al* 1978, Stoll and Domb 1978), but at the Ising critical point there is a change in the behaviour and we find that the connectedness length $\xi_p \sim (K - K_c)^{-\nu_{\text{Ising}}}$, where $\nu_{\text{Ising}} = 1$ and the mean cluster size $S \sim (K - K_c)^{-\gamma_p}$, with $\gamma_p = 1.89$. The crossover exponent is given by the Ising gap exponent, $\frac{15}{8}$.

This result gives a complete picture of two-dimensional *Ising clusters* at the Ising critical point. Although the linear dimension ξ_p diverges as the Ising correlation length (Klein *et al* 1978), the mean cluster size S diverges faster than the susceptibility χ , in very good agreement with the series result (Sykes and Gaunt 1976) $\gamma_p = 1.91 \pm 0.01$. The conclusion is that the Ising clusters satisfy the properties (i) and (ii) but do not satisfy (iii). The Ising clusters due to the geometrical effects are too compact to describe Ising critical droplets.

If we instead choose $p_B = p_B^* = 1 - e^{-K/2}$, we find another percolation line below the line $p_B = 1$ (cf figure 3(b)). This line ends at the Ising critical point, which is a higher-order critical point for percolation. Along this line (except for the Ising critical point) we again find random percolation exponents. At the Ising critical point we find $\xi_p \sim (K - K_c)^{-\nu_{\text{Ising}}}$ and $S \sim (K - K_c)^{-\gamma_{\text{Ising}}}$, where $\gamma_{\text{Ising}} = 1.75$. The 'bond dilution' has not shown any effect on the critical behaviour of the linear dimension of the clusters, but the size is now changed. The clusters are less compact now and behave like *critical droplets*; namely, they satisfy all the properties required, (i), (ii) and (iii). To complete our description, if we choose $p_B < p_B^*$, we find percolation lines (cf figure 3(b)) between the line $p_B = 1$ and p_B^* with the same critical behaviour as for the case $p_B = 1$. For

$p_B > p_B^*$ the percolation line ends at a temperature below the Ising critical temperature. The exponents along the line are the same as random percolation exponents (Reynolds *et al* 1978).

It is appropriate at this point to make a brief comment on the Migdal renormalisation group we employ. We find in our calculations that some lattice-dependent properties agree with the known values for the triangular lattice (percolation threshold for the pure bond problem, Ising critical temperature), while others are more appropriate to the square lattice (percolation threshold for the pure site problem). This is due to the fact that the Migdal renormalisation group generally does not distinguish different lattice types (Nicoll 1979).

In conclusion, we have considered a Hamiltonian formalism for studying the site-bond correlated percolation problem. A general result, valid in all dimensions, has led us to the identification of the Ising critical point with the onset of an infinite cluster. Such a cluster is made of nearest-neighbour occupied sites, linked by random bonds with a probability p_B given by equation (5). We have employed the Migdal renormalisation group in two dimensions to show that these clusters in fact describe critical droplets near the Ising critical point. The fixed point which describes such droplets is related to a higher-order phase transition in the percolation problem which has not been studied previously. The study of this new point in higher dimensions is under way.

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