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LETTER TO THE EDITOR

Study of droplets for correlated site–bond percolation in two dimensions

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Abstract. We study the droplet size distribution of the correlated site–bond percolation model introduced by Coniglio and Klein, and also the usual clusters of two-dimensional Ising models near the critical point. Equilibrium configurations of the Ising model with nearest-neighbour interaction and also one with nearest- and next-nearest-neighbour interactions are generated through a Monte Carlo simulation, and then a cluster analysis is performed. The exponents β and γ for the Coniglio–Klein droplet distribution are found to agree, for both the nearest-neighbour and the next-nearest-neighbour model, with the corresponding exponents of the Ising model. The usual Ising clusters diverge only at T_c in the Ising model with nearest-neighbour interaction but not for the model with next-nearest-neighbour interaction. The Potts model formulation is used to predict the behaviour of the droplet for general further-neighbour interactions.

Droplet models (Fisher 1967, Kertész *et al* 1982) have been important in understanding critical phenomena and metastability. One fundamental problem is how to define a droplet which will diverge with the correct exponents at the critical temperature.

As an example, consider a ferromagnetic spin-$\frac{1}{2}$ Ising model with nearest-neighbour (NN) interaction J. A naive definition of droplets is a cluster made up of NN 'up' spins which we shall call Ising *clusters*. However, for three dimensions the mean size of the Ising clusters diverge for zero magnetic field $H = 0$ at a temperature below the critical temperature T_c (Muller-Krumbhaar 1974). In two dimensions, on the other hand, they diverge right at T_c. Sykes and Gaunt (1976), using series expansions, found the mean cluster size exponent $\gamma_p = 1.91 \pm 0.01$ to be larger than the corresponding susceptibility exponent $\gamma = 1.75$ in two dimensions. Renormalisation group arguments (Coniglio and Klein 1980) give $\nu_p = \nu = 1$ for the connectedness length exponent ν_p, identical with the Ising correlation length exponent ν. Recently Coniglio and Klein (1980, henceforth abbreviated as CK) suggested that a candidate for a 'droplet' is better defined as a cluster of NN 'up' spins connected by bonds which are activated with probability $p_B = 1 - \exp(-2J/k_B T)$. These we call *CK droplets*. Coniglio and Klein predict, using a Potts Hamiltonian formulation and renormalisation group arguments, that the CK droplets should diverge in size at the Ising critical point with the correct Ising exponents. Their analysis was limited to NN interactions.

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The study of droplets in systems with further-neighbour interactions is important in view of the extension of these concepts to real fluids (Klein 1982) and in the light of studies of metastability in long-range interaction systems (Heermann *et al* 1982) where the usual Ising cluster makes no sense at all.

In particular we evaluate the 'mean cluster size' (more precisely, the second moment of the cluster size distribution) and the density of up-spins in the infinite cluster. Monte Carlo results for the simple cubic lattice have been obtained previously (see Kertész *et al* 1982 for a review); and a study for the square lattice was made by Ottavi (1981).

The computer analysis consisted of two parts: the production of Ising equilibrium configurations; and the subsequent cluster analysis for such a configuration. The generation of the equilibrium configurations of the two-dimensional Ising lattice is made through standard Monte Carlo techniques with efficient multi-spin coding (Zorn *et al* 1981). Then clusters are counted by the Hoshen–Kopelman algorithm (see Stauffer *et al* 1982 for a computer program) applied to both the Ising clusters and the CK droplets.

Ising model with NN *interactions only*

(a) Ising cluster analysis.

The Ising clusters diverge at the Ising critical point; thus we have generated equilibrium configurations for systems of various sizes at the exactly known critical point $T = T_c$ and $H = 0$, and we analysed the data by finite-size scaling (note $\nu = 1$).

We find the magnetisation exponent β (0.135 ± 0.025) to be compatible with the exact result $\frac{1}{8}$. The mean-cluster-size exponent is rather inaccurate (1.83 ± 0.1) but compatible with 1.91 from Sykes and Gaunt (1976). The exponent β_p related to the infinite cluster is about 0.052 ± 0.03. We expected $\beta_p \simeq 0.045$ as obtained from the scaling relation $2\beta_p = 2\nu_p - \gamma_p$ where $\nu_p = 1$ as obtained from renormalisation group analysis (CK). We note that our result is compatible with theoretical expectations and also gives some indications on the reliability of our Monte Carlo data.

(b) CK droplet analysis.

For the CK droplet we find, using the same methods, that the ratio of the density of the infinite droplet to the spontaneous magnetisation is constant (thus $\beta_p \simeq \frac{1}{8}$), in contrast to the case of Ising clusters (figure 1). Our value $\gamma_p \simeq 1.77 \pm 0.03$ agrees within its error bars with the susceptibility exponent $\gamma = \frac{7}{4}$. These results confirm therefore that the CK droplets are a suitable candidate to describe the thermal phase transitions in two dimensions.

Ising model with NN *and* NNN *interactions*

(a) Ising clusters.

The Ising clusters now are made up of NN and NNN up-spins. In this case even in two dimensions the critical point does not correspond anymore to the percolation threshold. In fact, for $T \geq T_c$ in zero field there is always an infinite cluster, and the mean cluster size does not diverge for $T \to T_c$ (note that the concentration of up-spins is 50% and far above the random percolation threshold of 41% (Djordjevic *et al* 1982)) and has a maximum at a temperature above T_c, contrary to the requirements for a good droplet. This feature was found in our simulations for the two cases considered here: $J_2 = J_1$ and $J_2 = \frac{1}{2}J_1$ where J_1 is the NN and J_2 the NNN exchange energy.

(b) CK droplet analysis.

We generalise the CK droplets to the case of NN and NNN interactions, defining a

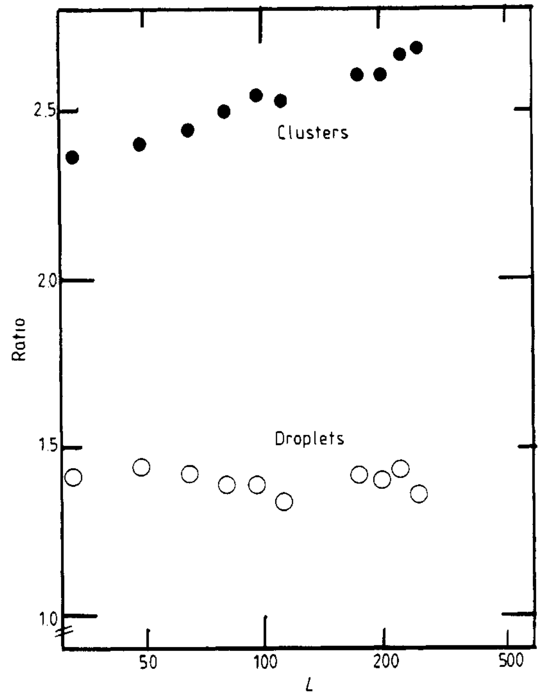

Figure 1. Square lattice Ising model with nearest-neighbour interactions only, at $T=T_c$ for systems of size $L\times L$. We plot against $\log(L)$ the ratio of the density of the infinite cluster to the spontaneous magnetisation. The full circles which indicate a tendency to increase with L refer to the usual Ising clusters, the open circles which scatter about a constant refer to the droplets in the definition of Coniglio and Klein (1980). The statistical errors are less than the size of the symbols used.

droplet as a group of up-spins connected by NN bonds activated with probability $p_{1B}=1-\exp(-2J_1/k_BT)$ or by NNN bonds activated with probability $p_{2B}=1-\exp(-2J_2/k_BT)$. The extension to further-neighbour interactions is obvious and proven below. We expect (see below) these droplets to diverge at the Ising critical point with Ising exponents. This result is confirmed by our analysis of the mean cluster size, which is found to diverge at the Ising critical point with an exponent γ_p (~ 1.65) compatible with γ. We show the data in figure 2 where the mean cluster size is seen to diverge for the CK droplets but not for the Ising clusters.

Potts model formulation

Now we give a formulation for the more general site–bond correlated percolation problem (Coniglio *et al* 1979) for further-neighbour interactions. We will only outline the derivations since they will be a straightforward generalisation of the Potts Hamiltonian formalism employed for the case of NN interactions (see Roussenq *et al* 1982 and Kertész *et al* 1982 for details and further references).

Consider the following asymmetric $(q+1)$-state Potts model:

$$-\mathscr{H}_p/k_BT=\sum_{\langle ij\rangle}J_{ij}^{B}(\delta_{b_ib_j}-1)-2\sum_{\langle ij\rangle}(J_{ij}^{B}-\tfrac{1}{2}K_{ij})\delta_{b_i0}\delta_{b_j0}$$
$$+\Big(\ln q-2H+\sum_{j}(J_{ij}^{B}-\tfrac{1}{2}K_{ij})\Big)\sum_{i}\delta_{b_i0}+\text{constant}$$

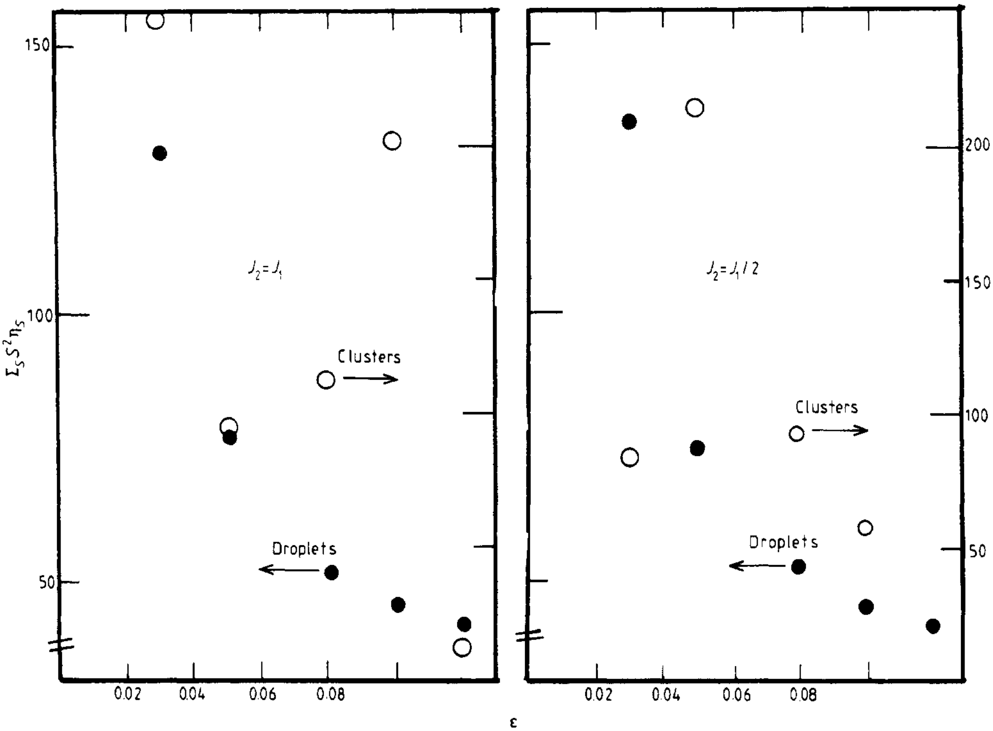

Figure 2. Second moment of the cluster size distribution for 400×400 square lattice slightly above T_c, with interactions to nearest and next-nearest neighbours. In the left part the ratio of interaction strengths is unity, in the right part it is $\frac{1}{2}$. The open circles which seem to scatter about a constant refer to the usual Ising clusters, the full circles which indicate the desired divergence at $\varepsilon \equiv (T-T_c)/T_c = 0$ refer to CK droplets. Note that T_c is different for different interaction ratios J_2/J_1 (Domb and Dalton 1966).

where the double sums run over all pairs (not only NN pairs), δ is Kronecker's symbol, $b_i = 0, 1, \ldots, q$ are the Potts model variables. Following the same procedure as for the NN Ising model it is possible to show that the derivative with respect to q, in the limit $q \to 1$, of this Hamiltonian is related to the generating function of Ising-correlated site–bond percolation in which the clusters are made of up-spins of the Ising model, connected by bonds activated with the probability $p_{ij}^{\mathrm{B}} = 1 - \exp(-J_{ij}^{\mathrm{B}})$ depending on the chosen pair i, j of lattice sites. The spins interact according to the Ising Hamiltonian with coupling constant $J_{ij} = \frac{1}{4}k_{\mathrm{B}}TK_{ij}$ and magnetic field H (more precisely, H = field × magnetic moment/$k_{\mathrm{B}}T$ in our notation).

If we now choose $J_{ij}^{\mathrm{B}} = \frac{1}{2}K_{ij}$, that means $p_{ij}^{\mathrm{B}} = 1 - \exp(-2J_{ij}/k_{\mathrm{B}}T)$; the above Hamiltonian becomes an Ising model with exchange interaction J_{ij} and magnetic field H and therefore shows Ising singularities at the Ising critical point. As a consequence, using the same arguments as for the NN case (Roussenq *et al* 1982, Kertész *et al* 1982) the droplets made of clusters of up-spins connected by bonds randomly with probability $p_{ij}^{\mathrm{B}} = 1 - \exp(-2J_{ij}/k_{\mathrm{B}}T)$ diverge with Ising exponents at the Ising critical point.

The present work continued Ottavi's (1981) efforts and found that for the nearest-neighbour Ising model in two dimensions, the critical exponents of susceptibility and spontaneous magnetisation agree with those of the CK droplets (mean cluster size and largest droplet). This analogy breaks down for the usual Ising clusters where the exponent β_p for the largest cluster was found to be smaller than the β for the spontaneous magnetisation. Ising clusters are even worse for interactions over larger distances where they do not diverge at the critical point. But again the modified definition of CK droplets avoids that discrepancy. In summary, CK droplets seem to be the correct droplet definition, for zero field, even for more complicated cases than just nearest-neighbour interactions.

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