Remark on percolative phase transitions without infinite network

LETTER TO THE EDITOR

Remark on percolative phase transitions without infinite network

W Klein†§ and D Stauffer‡

† IFF, KFA Jülich, 5170 Jülich 1, West Germany.
‡ Institut für Theoretische Physik, Universität, 5000 Köln, West Germany

Abstract. For Ising-correlated site–bond percolation, Delyon, Souillard and Stauffer predicted a phase transition in the number of finite droplets, without the appearance of an infinite network. We interpret their result as due to percolation of active bonds within very large but finite Ising clusters.

Correlated site–bond percolation has often been studied in recent years (Coniglio *et al* 1979, Coniglio and Klein 1980, Delyon *et al* 1981, Stauffer 1981, Roussenq 1981, Ottavi 1981, Chakrabarti *et al* 1981, Stanley 1981), in particular for the case of Ising correlation. Then lattice sites are occupied or empty as in the pure lattice gas (Ising model) in thermal equilibrium. Between two occupied sites which are nearest neighbours, bonds are defined as being active with probability p_B and passive with probability $1 - p_B$, where p_B can be regarded as a variable independent of temperature and "magnetisation" (or field). A *cluster* is a group of occupied neighbour sites; for $p_B < 1$ each such cluster can split up into several smaller 'droplets' which are defined as groups of occupied neighbour sites connected by *active* bonds, whereas clusters can also be held together by passive bonds.

For this model, Delyon *et al* (1981) suggested a phase transition in the droplet numbers n_s without appearance of an infinite network of active bonds. Let n_s be the average number of droplets (per lattice site) containing s occupied sites each; and let ζ be defined by:

$$\log n_s \propto -s^{\zeta} \qquad (s \to \infty). \tag{1}$$

For temperatures below the critical temperature T_c of phase separation, Delyon *et al* (1981) predict, on the coexistence curve, that ζ changes from 1 for $p < p_{Bc}$ to $1 - 1/d$ for $p > p_{Bc}$, where the phase transition point p_{Bc} depends on magnetisation M, and d is the dimensionality. This result holds for liquid droplets in both the liquid phase (positive M, point A in our figure) and the vapour phase (negative M, point B in our figure). Presumably one has $p_{Bc}(-M) = p_{Bc}(+M)$, as suggested by Delyon *et al* (1981). But whereas at point A, i.e. for large liquid droplets in the liquid phase, an infinitely large droplet starts to appear, no such percolation of droplets is possible at point B where all droplets remain finite. The present note suggests a simple explanation for this effect.

§ Present and permanent address: Center for Polymer Studies and Physics Dept., Boston University, Boston MA 02215, USA.
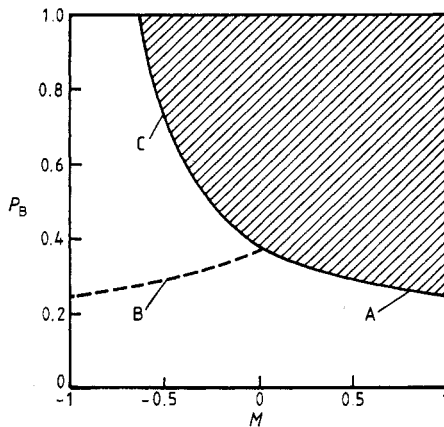
Figure 1. Schematic phase diagram for simple cubic lattice: bond activation probability p_B versus magnetisation M for Ising-correlated site–bond percolation; after Delyon *et al* (1981). In the shadowed region, an infinite droplet percolates throughout the system; above the broken phase transition curve of Delyon *et al*, droplets percolate throughout the very large but finite Ising clusters. Points A, B and C are located on these transition lines.

(Stanley (1981) compared the phase transition of Delyon *et al* 1981 with that predicted by Griffiths (1969) for quenched dilute ferromagnets. Our explanation does not necessarily contradict that analogy.) (See also Aizenman *et al* 1980.)

Very large but finite clusters (radius $\gg$ correlation length) have been studied numerically in detail for random percolation (Stauffer 1979 and 1981). Above the percolation threshold, their internal structure is the same as that of the infinite network. Much earlier (Binder and Stauffer 1972), large but finite clusters were studied on the coexistence curve for the Ising model; for temperatures T far below T_c, the internal structure of these 'raindrops in the vapour phase' is the same as that of the bulk liquid phase with which they may coexist. For correlated site–bond percolation below T_c in the vapour phase, the active and passive bonds are distributed randomly within the Ising clusters; these cluster sites thus have the same density and correlation as the numerous occupied sites on the bulk liquid side, provided the cluster to which they belong is much larger than the Ising correlation length.

On the liquid side, point A in our figure, the active bonds within the bulk liquid phase just start to percolate throughout the sample. On the vapour side, point B in our figure, the active bonds just start to percolate throughout the very large (and very rare) clusters of occupied sites. They cannot percolate through the whole sample since no infinite cluster exists; but for droplet sizes s much smaller than the cluster size l, these droplets will not feel this limitation and will behave at point B as if they were in the symmetric liquid phase at point B. Therefore the number n_s of finite large droplets in an extremely large Ising cluster will be the same at point A as in a bulk liquid sample of the same size at point B. In this way we propose an explanation for the suggested phase transition of Delyon *et al* (1981). The numbers of finite clusters near point B feel the singularity of point A.

More quantitatively, let n_s^{drop} be the number of droplets (per lattice site) of size s within the infinite cluster (point A) or within the interior of an extremely large cluster (point B); if the number of sites in that cluster, l, is much larger than the number of sites in the droplet, s, we expect n_s^{drop} to be independent of l. By definition, $l \geq s$; and the

radius of the s-droplet is also much larger than the correlation length. On the liquid side, at point A, the majority of occupied sites belong to the infinite Ising cluster, and thus

$$n_s \simeq n_s^{\text{drop}}. \qquad (2a)$$

If we go closer to the endpoint of the phase transition line at $p_B = 1$, i.e. if we are near point C, only a small fraction P_∞ of occupied sites belongs to the infinite cluster, and equation $(2a)$ is generalised to

$$n_s = P_\infty n_s^{\text{drop}}. \qquad (2b)$$

(We neglect in (2) the contribution from finite clusters and also trivial factors like the concentration $(1+M)/2$ of up-spins.).

On the vapour side, point A, within one extremely large cluster of size l, we have $l\,n_s^{\text{drop}}$ smaller (but still very large) droplets. If we have $N_l = N_l(M)$ such clusters (per lattice site) on the coexistence curve, they contain altogether

$$n_s = \sum_l l N_l n_s^{\text{drop}} \qquad (3)$$

droplets, where the sum runs from s to infinity. What is happening close to the phase transition $p_B = p_{Bc}$?

In three dimensions, for p_B slightly above p_{Bc} we expect

$$n_s^{\text{drop}} \sim \exp[-c_1(p_B - p_{Bc})^{\beta\delta 2/3} s^{2/3}] \qquad (4a)$$

whereas for p_B slightly below p_{Bc}

$$n_s^{\text{drop}} \sim \exp[-c_2(p_{Bc} - p_B)^{\beta\delta} s] \qquad (4b)$$

apart from pre-exponential factors which are less important for large s. (The c_i depend on M; β and δ are the critical exponents of random percolation, and we used the scaling law for random percolation (Stauffer 1979).) At point B, where no infinite Ising cluster is present, presumably (Müller-Krumbhaar 1979) the numbers N_l of Ising clusters decay as

$$N_l \sim \exp(-c_3 l^{2/3}). \qquad (4c)$$

(For magnetisations larger than about -0.6, but still negative, another exponential decay might hold.)

Combining equations (3) and (4) we get, apart from pre-exponential factors, for large s at A:

$$n_s \sim \exp(-c_3 s^{2/3}) n_s^{\text{drop}} \qquad (5)$$

or

$$-\log[n_s(p_B > p_{Bc})] \simeq [c_3 + c_1(p_B - p_{Bc})^{\beta\delta 2/3}] s^{2/3} \qquad (6a)$$

$$-\log[n_s(p_B < p_{Bc})] \simeq c_3 s^{2/3} + c_2(p_{Bc} - p_B)^{\beta\delta} s. \qquad (6b)$$

(Note $|p_B - p_{Bc}|^{\beta\delta} s \gg 1$ in both cases.) It will be difficult to test these predictions by direct Monte Carlo simulation of n_s, since due to the factor $\exp(-c_3 s^{2/3})$ the numbers n_s are always extremely small. Moreover this factor ensures, as observed by Roussenq (1981), that the second moment of the droplet size distribution always remains finite; a change is seen only in the asymptotic decay of the droplet numbers ('essential singularity').

In conclusion, we have explained the transition of Delyon *et al* (1981) by the percolation of active bonds within the extremely large but finite Ising clusters in the

vapour phase. Since these clusters are very rare, they hardly affect easily measurable quantities. Monte Carlo simulations in restricted ensembles, like the study of large Ising clusters at fixed size l (Binder and Stauffer 1972, Binder and Kalos 1980), might test the present assertions at least qualitatively, whereas a quantitative test of our predictions for droplets numbers, equations (6a, b) will be much more difficult.

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