LE JOURNAL DE PHYSIQUE-LETTRES

J. Physique — *LETTRES* 43 (1982) L-703 - L-709

15 OCTOBRE 1982, PAGE L-703

Classification

Physics Abstracts

05.50

Study of droplets for correlated site-bond percolation in three dimensions

J. Roussenq

Département de Physique des Systèmes Désordonnés,
Université de Provence, Centre de St-Jérôme, 13397 Marseille Cedex 13, France

A. Coniglio (*) and D. Stauffer (**)

Center of Polymer Studies (***), Boston University, Boston MA 02215, U.S.A.

(Reçu le 8 juillet 1982, accepté le 6 septembre 1982)

Résumé. — Au moyen d'un programme de simulation numérique type Monte-Carlo, on étudie la distribution statistique des tailles de gouttes dans le modèle de percolation corrélée site-lien de Coniglio et Klein. L'exposant γ de cette distribution est trouvé en bon accord avec l'exposant correspondant du modèle d'Ising. On discute la relation entre la susceptibilité et le second moment en utilisant le formalisme du modèle de Potts dilué pour ce problème de percolation.

Abstract. — Using a Monte-Carlo simulation, we study the droplet size distribution in the correlated site-bond percolation model of Coniglio and Klein for three dimensions. The exponent γ for that distribution is found to agree well with the corresponding exponent of the Ising model. We discuss the relation between susceptibility and second moment by using the dilute Potts formulation of such a percolation problem.

During the last years in percolation theory particular attention was paid to find new, more sophisticated models which could be applied better to problems for which the elementary model could not give satisfactory results. In particular correlations between a site or bond and its neighbours were introduced. These models are then called correlated percolation.

More recently, Coniglio and Klein [1, 2] (we abbreviate Ref. [1] as CK) proposed a theory with Ising-model correlation where site and bond aspects were intermixed. Let us look at a three-dimensional Ising model in zero field at temperature T . The « up » spins which are nearest neighbours form Ising clusters; one finds that the infinite cluster is formed at a temperature below the critical temperature T_c . To make the percolation threshold coincide with the critical

(*) Permanent address : Istituto di Fisica Teorica, Università di Napoli, Mostra d'Oltremare, Pad. 19, 80125 Napoli, Italy.

(**) Permanent address : Institut für Theoretische Physik, Cologne University, 5000 Köln 41, West-Germany.

(***) Supported in part by grants from ARO, NSF and ONR.

temperature, CK suggest to consider as clusters only those up spins which are connected by a randomly active bond. The probability p_B for such a bond to be active is given by $p_B = 1 - \exp(-2J/kT)$ where J is the Ising interaction energy and kT the thermal energy ($2J$ is the energy necessary to transform two parallel isolated spins into two antiparallel ones).

We see that this model combines elements of percolation and Ising models. For $p_B = 1$ it reduces to the usual Ising problem; but if p_B becomes smaller these usual Ising clusters are cut into smaller clusters which we call *droplets*. For temperatures far below T_c , p_B is close to unity; but the model is expected to be good up to T_c . Previous work [3] showed that droplet percolation occurs at $T = T_c$ apart from effects due to the finite size of the systems studied. The phase diagrams for this model were discussed by Ottavi [4] in two and by Heermann and Stauffer [5] in three dimensions.

The average number (per site) of droplets, in the sense of CK, containing s up spins each is called $n_s = n_s(T)$. Roussenoq [6] studied previously the droplet size distribution with respect to nucleation phenomena, to which this model seems relevant. The present work is complementing these results by studying the second moment of the size distribution, using more precise data on the basis of more computer runs. And we clarify in an appendix that the magnetic susceptibility is proportional to but not identical with this second moment or « mean cluster size ».

1. Simulation technique. — Our simulation consisted of two parts. First we simulated a simple cubic $16 \times 16 \times 16$ Ising model in zero field and looked for its thermal equilibrium, using multi-spin coding [7]. At the beginning all spins are down, and each spin is examined N times. N is called the number of Monte-Carlo Steps (MCS) per spin. In equilibrium after N such steps some spins have flipped and are oriented upwards; these up spins form the Ising clusters.

Now we use a bond percolation program [6] to analyse the droplets in this sample. For this purpose we examine the bonds between up spins as realized in the first part. For each bond, a random number between 0 and 1 is selected; if this number is smaller than p_B the bond is defined as active, otherwise it is regarded as cut. The value for p_B can be chosen as independent variable [2]; as special case we may give it the value $p_B = 1 - \exp(-2J/kT)$ of CK.

With the help of this procedure we arrive at the statistical distribution of the droplet sizes. We made two types of simulations :

In the first, for one single temperature $T = 0.8 T_c$, we produced an equilibrium configuration of Ising spins after 500 MCS per spin. Then p_B was varied between 0 and 1, with 100 realizations of bond configurations for each p_B .

In the second, for each equilibrium configuration at different temperatures T we look at only two values of p_B , i.e. $p_B = 1 - e^{-2J/kT}$ (CK droplets) and $p_B = 1$ (Ising clusters). We used 100 configurations for the first value of p_B and only one, of course, for the second which corresponds to Ising-correlated site percolation.

2. Results. — The first series of computer experiments confirms our previous results [6] that for p_B close to its CK value the variation of n_s with s is described well by the law predicted by Delyon *et al.* [8], as illustrated in figure 1.

In the second series we verified that at the critical temperature n_s decays with some power law as function of s . Theoretically we expect [9] n_s to vary as $s^{-\tau}$ with $\tau \simeq 2.2$. The data in figure 2 correspond to $\tau \simeq 2.25$.

The second moment $S(T) = \sum_s s^2 n_s$ of the droplet size distribution takes into account all finite droplets of up spins, with p_B taken as the CK value $1 - e^{-2J/kT}$ for each temperature. Figure 3 gives its variation with $t = |T - T_c|/T_c$ for temperatures below (Fig. 3a) and above (Fig. 3b) T_c in a log-log plot.

Our effective critical temperature T_c assumed in that analysis is taken as 2% above the true critical temperature, as determined earlier [3] for samples of the same size as used here. The experimental points fit well a straight line with a slope γ close to 1.2 both above and below T_c .

Fig. 1. — Variation of n_s with $s^{2/3}$ at $T/T_c = 0.8$ and $p_B = 1 - \exp(-2 J/kT)$.

Fig. 2. — Log-log plot of n_s versus s at $T/T_c = 1.02$. (The slope of the straight line is 2.25.)

Fig. 3. — Variation of second moment S as function of $|T - T_c|/T_c$ for $p_B = 1 - \exp(-2J/kT)$ below (Fig. 3a) and above (Fig. 3b) T_c (logarithmic scales). Below T_c , the phase with most spins down was investigated.

3. **Discussion.** — The results of the computer simulations are in good agreement with theoretical expectations and confirm more accurately our previous results [6] on the variation of n_s with s . For the second moment S , the analogies between magnetism and percolation suggest a variation proportional to the magnetic susceptibility with a critical exponent γ , according to CK. This susceptibility diverges [10] with an exponent 1.24 above and below T_c , in good agreement with our results and drastically different from the exponent 1.8 of random percolation. This result is another confirmation of the good agreement between the statistical description of droplets by CK and the magnetic properties of the Ising model.

We have also evaluated the ratio A_+/A_- of the critical amplitudes of the second moment S . Our appendix shows that one should expect $S = A_{\pm} t^{-\gamma}$ for the second moment but

$$\chi = (2A_{\pm} + B_{\pm}) t^{-\gamma}$$

for the susceptibility, where the subscript + (or -) corresponds to temperature above (or below) T_c . We find a value A_+/A_- of about 27 for the second moment, whereas the corresponding ratio of the susceptibility amplitudes is about 5 [11]. This strong difference shows that while second moment and susceptibility are described by the same critical exponent they have different amplitudes, as explained in the appendix.

(Our system is rather small : but work for 40^3 and 60^3 sites seems to confirm our results : J. Kertesz, private communication [16].)

In summary the suggestion of CK seems to give a good description of the zero field susceptibility in the Ising model with the help of droplets.

Acknowledgments. — We thank J. Kertesz for advance information about his work. D. Stauffer thanks the University of Provence for its hospitality during the initiation of this research. We also wish to thank B. Souillard for helpful comments.

Appendix. — This appendix explains the differences in the critical amplitudes of the magnetic susceptibility and the second moment of the droplet size distribution.

It is well known [12] that the q -state Potts model describes, in the limit $q \rightarrow 1$ random bond percolation. Analogously it has been shown [1, 13] that Ising-correlated site-bond percolation is obtained from the following dilute q -state Potts model, in the limit $q \rightarrow 1$, for any lattice of N sites in d dimensions :

$$- \beta \mathcal{H}_{\text{DP}} = J_{\text{B}} \sum_{\langle ij \rangle} (\delta_{\sigma_i \sigma_j} - 1) n_i n_j + h \sum_i (\delta_{\sigma_i 1} - 1) n_i + K \sum_{\langle ij \rangle} n_i n_j - \Delta \sum_i n_i \quad (1)$$

where the double sum runs over all pairs of nearest neighbours, δ is Kronecker's symbol, $\sigma_i = 1 \dots q$ are the Potts variables, $n_i = 1/2 (1 + S_i)$ are the lattice gas occupation numbers and $S_i = \pm 1$ are the Ising spins, $K = 4 \beta J$ is the (dimensionless) coupling constant of the lattice gas ($\beta = 1/kT$), Δ the dimensionless chemical potential related to the Ising magnetic « up » field H (more precisely, $H = \beta \times \text{field} \times \text{magnetic moment}$) and coordination number c by

$$- H = 1/2(\Delta - 1/2 cK), \quad p_{\text{B}} = 1 - \exp(-J_{\text{B}})$$

is the bond probability and h the Ising field coupled to the $\sigma_i = 1$ state. The Ising droplet of CK are obtained for the special case $J_{\text{B}} = 2 \beta J = 1/2 K$.

If

$$Z_{\text{DP}}(q) = \sum \exp(-\beta \mathcal{H}_{\text{DP}}) \quad (2)$$

is the partition function of the model Hamiltonian (1), with the sum running over all possible values for the σ_i and n_i , then the free energy $F_{\text{DP}}(q) = \lim_{N \rightarrow \infty} N^{-1} \ln Z_{\text{DP}}(q)$ is related to the generating function G for the Ising-correlated site-bond percolation problem *via* [1],

$$G = dF_{\text{DP}}/dq |_{q=1} \quad (3)$$

from which the second moment of the cluster size distribution, S is obtained :

$$\partial^2 G / \partial h^2 = S = \sum_s s^2 n_s. \quad (4)$$

Here the n_s are numbers (per lattice site) of clusters containing s spins each, averaged over both thermal fluctuations of the lattice gas and bond configurations of the percolation problem. It has also been shown [1, 13] that the Hamiltonian of equation (1) is equivalent to the following asymmetric $(q+1)$ -state Potts model :

$$\begin{aligned} - \beta \mathcal{H}_{\text{P}}(q+1) = & J_{\text{B}} \sum_{\langle ij \rangle} (\delta_{b_i b_j} - 1) - 2(J_{\text{B}} - K/2) \sum_{\langle ij \rangle} \delta_{b_i 0} \delta_{b_j 0} + \\ & + \{ h - 2H + c(J_{\text{B}} - K/2) + \ln q \} \sum_i \delta_{b_i 0} + h \sum_i \delta_{b_i 1} + \text{const.} \end{aligned} \quad (5)$$

where $b_i = 0 \dots q$ are the variables of this new Potts model. More precisely,

$$Z_{\text{DP}}(q) \equiv \sum \exp(-\beta \mathcal{H}_{\text{DP}}) = \sum \exp(-\beta \mathcal{H}_{\text{P}}) \equiv Z_{\text{P}}(q+1) \quad (6)$$

where the first sum runs over all values for the σ_i and n_i , the second over all values for the b_i . Consequently the free energies agree :

$$F_{\text{DP}}(q) = F_{\text{P}}(q+1) \quad (7)$$

where $F_p(q+1) = \lim_{N \rightarrow \infty} N^{-1} \ln Z_p(q+1)$. From equations (4), (7) the second moment S of the cluster size distribution is given by

$$S = \frac{\partial^2}{\partial h^2} dF_p(q+1)/dq|_{q=1}. \quad (8)$$

On the other hand, for the special value $J_B = 2\beta J$ corresponding to the Ising droplets of CK, Hamiltonian (5) for $q=1$ becomes an Ising model with coupling constant J and dimensionless magnetic field H , with a free energy $F_{\text{Ising}} = F_p$ and a magnetic susceptibility

$$\chi = \partial M / \partial H = \partial^2 F_p / \partial H^2 \quad (9)$$

with F_p evaluated at $q+1=2$.

In order to relate the second moment S to the susceptibility χ , we write $Z_p(q+1)$ using standard techniques [13, 14] in the following way :

$$Z_p(q+1) = \sum p_B^A (1-p_B)^{N'-A} \prod_c \{ (q-1) e^{(2H-h-\ln q)s_c} + e^{(2H-\ln q)s_c} + 1 \} \quad (10)$$

with $p_B = 1 - e^{-J_B}$; the sum runs over all possible distributions of bonds in the lattice, where A is the total number of active bonds and $N' (= 1/2 cN)$ the total number of possible bonds. The number of sites in a cluster c is denoted by s_c , and the product runs over all clusters in the given configuration of active bonds. (Here clusters are groups of arbitrary sites connected by active bonds, i.e. neither Ising clusters nor droplets in the CK sense.)

From equations (8), (9) we now find for second moment and susceptibility :

$$S = \langle \sum_c s_c^2 e^{-hs_c} (1 + e^{-2Hs_c})^{-1} \rangle \quad (11)$$

$$1/4 \chi = \langle \{ \sum_c s_c (1 + e^{-2Hs_c})^{-1} \}^2 \rangle - \{ \langle \sum_c s_c (1 + e^{-2Hs_c})^{-1} \rangle \}^2 + \langle \sum_c s_c^2 e^{-2Hs_c} (1 + e^{-2Hs_c})^{-2} \rangle \quad (12)$$

where the brackets stand for averages with the statistical weight ($q=1$ in (10))

$$p_B^A (1-p_B)^{N'-A} \prod_c (1 + e^{2Hs_c}). \quad (13)$$

For $H = h = 0$, we get

$$S = 1/2 \sum_c \langle s_c^2 \rangle \quad (14a)$$

$$\chi = 2S + \Delta R^2 \quad (14b)$$

$$\Delta R^2 = \langle (\sum_c s_c)^2 \rangle - \langle \sum_c s_c \rangle^2. \quad (14c)$$

We see that the second moment S of the droplets in the Ising model is given by half of the second moment of the cluster size distribution in a particular bond percolation problem where a configuration of bonds is weighted according to (13), while the susceptibility χ also includes the quantity ΔR^2 related to the fluctuation of the order parameter in that percolation problem. We expect ΔR^2 to diverge near the phase transition [15] as S . Since χ diverges at T_c with an exponent γ and ΔR^2 and S are both positive quantities, we have with $t = |T - T_c|/T_c \rightarrow 0$:

$$S = A_{\pm} t^{-\gamma} \quad (15a)$$

$$\chi = (2A_{\pm} + B_{\pm}) t^{-\gamma} \quad (15b)$$

$$\Delta R^2 = B_{\pm} t^{-\gamma} \quad (15c)$$

where the subscripts $+$ and $-$ refer to quantities above and below T_c , respectively. Thus, the susceptibility amplitude $2 A_{\pm} + B_{\pm}$ is larger than twice the amplitude $A_{\pm}$ of the second moment S , as we said in the main text confirmed numerically ($A = 0.02$, $2 A_{\pm} + B_{\pm} = 0.2$). (For T below T_c , this discussion as well as our numerical data refer to the low density phase where no infinite droplet exists. In the high density phase much larger S were observed.)

References

- [1] CONIGLIO, A., KLEIN, W., *J. Phys. A* **13** (1980) 2775.
 - [2] CONIGLIO, A., STANLEY, H. E., KLEIN, W., *Phys. Rev. Lett.* **42** (1979) 518 and *Phys. Rev. B* **25** (1982) in press.
 - [3] STAUFFER, D., *J. Physique-Lett.* **42** (1981) L-99.
 - [4] OTTAVI, H., *Z. Phys. B. Condensed Matter* **44** (1981) 203.
 - [5] HEERMANN, D. W., STAUFFER, D., *Z. Phys. B. Condensed Matter* **44** (1981) 339.
 - [6] ROUSSENQ, J., *J. Aerosol Sci.* **12** (1981) 437.
 - [7] ZORN, R., HEERMANN, H. J., REBBI, C., *Comput. Phys. Commun.* **23** (1981) 337.
 - [8] DELYON, F., SOUILLARD, B., STAUFFER, D., *J. Phys. A* **14** (1981) L243.
 - [9] STAUFFER, D., *Phys. Rep.* **54** (1979) 1.
ESSAM, J. W., *Rep. Progr. Phys.* **43** (1980) 843.
 - [10] STANLEY, H., *Introduction to phase transitions and critical phenomena* (Oxford University Press, Oxford) 1971.
 - [11] FISHER, M. E., *Rep. Progr. Phys.* **30** (1967) 615, in particular page 671.
 - [12] FORTUIN, C., KASTELEYN, P. W., *J. Phys. Soc. Japan* **26**, Suppl. 11 (1969).
 - [13] CONIGLIO, A., DI LIBERTO, F., MONROY, G., *J. Phys. A* **14** (1981) 3017.
 - [14] WU, F. Y., *J. Stat. Phys.* **18** (1978) 115.
 - [15] CONIGLIO, A., STAUFFER, D., *Lett. Nuovo Cimento* **28** (1980) 33.
 - [16] KERTESZ, J., STAUFFER, D., CONIGLIO, A., Preprint (1982), to be submitted to *Israel Phys. Soc.*
-