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Surface effects for percolation

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Résumé. — On se place dans le cas où la surface de dimension $d - 1$, d'un milieu semi-infini de dimension d , est dopée avec une probabilité p_s différente du dopage volumique p_B . On peut imaginer que la percolation est possible même lorsque p_s et p_B sont simultanément inférieures l'une au seuil de percolation pour la dimension $d - 1$, l'autre au seuil de la dimension d . Nous donnons des arguments simples, confirmés en partie par une expérience Monte-Carlo, qui montrent que cet effet existe pour $d = 3$ et non pour $d = 2$. Nous discutons également le cas d'une ligne de défauts unidimensionnelle dans un réseau tridimensionnel.

Abstract. — If a $(d - 1)$ -dimensional surface of a d -dimensional semi-infinite medium has a concentration p_s different from the bulk concentration p_B one may imagine that percolation is possible even if both p_B and p_s are below the d - and $(d - 1)$ -dimensional threshold, respectively. We give simple arguments, partly confirmed by Monte Carlo experiment, why this effect occurs for $d = 3$ but not for $d = 2$. We also discuss the case of a defect line immersed in a three-dimensional medium.

1. Introduction. — This paper deals with the role of a surface limiting a half-infinite medium for bond percolation. As examples we have in mind a square or simple cubic lattice in the semi-infinite medium, with a bulk concentration p_B of active bonds in the interior of the lattice and a surface concentration p_s of active bonds on the surface. This « surface » is a one-dimensional line for the two-dimensional lattice, and a two-dimensional plane in the three-dimensional case. The first case is denoted here as (1D, 2D), the second as (2D, 3D). We also look at the case (1D, 3D) where a one-dimensional line is in the interior of the three-dimensional lattice, with a concentration p_s on this line only, differing from the bulk concentration p_B . We are interested mainly in the case of p_s very close to the threshold p_{sc} where the surface alone starts to percolate. This limit received little attention in previous studies of percolation surface effects [1-4], in contrast to the other region of interest where p_s is nearly equal to p_B . Thus we take p_B smaller than the value p_{Bc} of the bulk percolation threshold, and p_s smaller than p_{sc} , with

$$\varepsilon \equiv p_{sc} - p_s \quad (1)$$

Fig. 1. — *a*) Schematic phase diagram; p_s is the concentration of active bonds on the surface and p_B that in the bulk phase. The solid line separates the conducting region for large concentrations from the insulating region for small concentrations; the insulating region is shadowed. *b*) A link missing in the one-dimensional chain is bridged by three bonds of the two-dimensional bulk phase.

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positive and very small. Often also p_B will be taken as very small. For our above examples we have $p_{Sc} = 1/2$, $p_{Bc} = 0.25$ for the case (2D, 3D), $p_{Sc} = 1$, $p_{Bc} = 1/2$ for (1D, 2D), and $p_{Sc} = 1$, $p_{Bc} = 0.25$ for (1D, 3D). Figure 1a shows these quantities schematically.

2. The case (1D, 2D). — A $n \times n$ square lattice in bond percolation is called conducting if it contains a cluster extending from the first line to the last (n th) line. The first column which is now our « surface » has a probability p_s for its bonds to be active, which is different from the probability p_B for all the other bonds to be active in the rest of the lattice (including the bonds linking column 1 with column 2). How does the phase diagram look like in the p_s - p_B plane? Let us calculate the probability $R_{12} = R_{12}(p_B, p_s, n)$ that our system conducts. Since $\varepsilon \equiv 1 - p_s$ is very small only a few isolated bonds are missing in the surface line. We make the hypothesis that each of these missing links can be bridged independently with probability $p_3 = p_3(p_B)$. Such a bridge consists of (at least) three bulk bonds as shown in figure 1b; therefore $p_3 \rightarrow p_B^3$ for small p_B where larger bulk clusters are extremely improbable. In the average $M = \varepsilon n$ links are missing in our surface, and we neglect the fluctuations in M . If all M missing links are bridged the system conducts :

$$R_{12} = p_3^M = p_3^{\varepsilon n}. \quad (2)$$

For large p_B close to p_{Bc} complicated crossover effects occur [1-4] since due to large bulk clusters also large bridges may exist with a length exceeding the distance between two missing links, invalidating eq. (2). But in the limit $\varepsilon \rightarrow 0$ at fixed p_B these complications should vanish.

In the limit of large n one gets the correct percolation threshold by setting the probability R_{12} of conduction equal to 1/2 or some other constant [5]. Then equation (2) gives $p_3^{\varepsilon n} = \text{const.}$, or

$$\varepsilon \propto 1/n \quad (\text{fixed } p_B < p_{Bc}) \quad (3)$$

as the condition for the percolation threshold. Thus for large n the surface percolation threshold approaches unity with an $1/n$ law; in other words the presence of the two-dimensional bulk phase does not assist the one-dimensional surface to lower its percolation threshold below unity.

We tested this simple theory by a Monte Carlo computer simulation, including a value of p_B close to the percolation threshold of the bulk phase. (Whereas the theory is made for bond percolation in order to make the bridge concept transparent the simulation was made for site percolation; therefore we used here the symbols p' and p instead of p_s and p_B . The bulk percolation threshold p_c is now near 0.59. The reader can easily transform the above arguments to the case of site percolation too.)

Apart from test runs we used about half an hour time on a CII Iris 80 computer. For each sample we

kept the occupational status of the $n - 1$ right columns fixed and varied only the occupation probability p' for the left most column, until we found by dichotomy [6] with sufficient accuracy the conduction threshold p'_c for that sample. We averaged these thresholds over 9 samples for each pair p and n of parameters to get the average threshold $\langle p'_c \rangle$. (First we checked if the bulk part conducts already without the help of the special surface, by setting $p' = 0$. If the system then conducts we set $p'_c = 0$ for this sample.) We used $n = 10, 20, 30, 40, 50, 100, 150, 200, 250, 300$ and 350 at $p = 0.55$ slightly below the bulk threshold, and $n = 100$ for $p = 0.1; 0.2; \dots 0.8$.

Figure 2 shows the resulting phase diagram. The continuous curve separates the p' - p plane into two regions : Below the curve or on its left side the system is insulating; on the top and right of the curve it conducts. One sees that for a bulk concentration p below the bulk threshold the surface threshold is very close to unity, as predicted above, except for p very close to the bulk threshold.

In order to check if these deviations of the surface threshold from unity are real or arise from our finite

Fig. 2. — Monte Carlo phase diagram. The average surface percolation threshold is plotted for 100×100 samples against the bulk concentration.

Fig. 3. — Log-log plot of the finite-size effect at a bulk concentration of 0.55. The solid line has slope -1 .

system size, we plot in figure 3 the difference ε of the threshold from unity as a function of system size n at fixed $p = 0.55$ slightly below the bulk threshold. We see now clearly that for an infinite sample the surface threshold approaches unity, with an accuracy better than one percent. And the straight line in our log-log plot, which has a slope of minus unity, shows that $\varepsilon \simeq 2.5/n$ in agreement with equation (3).

3. Case (1D, 3D). — The above argument may be extended immediately to a one-dimensional « defect » line of length n surrounded by a $n \times n \times n$ lattice. Let us call p_3 the probability that a missing isolated link on the defect line is bridged by bonds of the three-dimensional medium. Each bridge again consists of at least three bonds. But now up to 4 bridges are possible for a single link in the cubic lattice; thus $p_3 = 4 p_B^3$ for $p_B \rightarrow 0$. For $\varepsilon \equiv 1 - p_s \rightarrow 0$ the probability that the system conducts, i.e. that all $M = \varepsilon n$ missing links are bridged, is

$$R_{13} = p_3^M = p_3^{\varepsilon n} \quad (4)$$

for p_B below p_{Bc} . This means that equation (2) is again valid for the surface percolation threshold: For p_B below the bulk threshold the single special line does not help the system to become conducting except when, in the thermodynamic limit, the line itself is conducting at $p_s = 1$.

4. Case (2D, 3D). — In this case the simple concept of missing links becomes useless since a single missing bond no longer prevents the surface from conduction: the $n \times n$ surface is now two-dimensional. Series results of de'Bell and Essam [4] have, in agreement with predictions of Bray and Moore [1] (see Carton [2] for the special case of percolation), shown that for (2D, 3D) one has a phase transition line $p_s = p_s(p_B)$ with $p_s < p_{sc}$ extending from $p_s = p_{sc}$ at $p_B = 0$ to $p_s = p_{Bc}$ at $p_B = p_{Bc}$. Thus in contrast to the two previous cases surface and bulk now cooperate to produce conduction under conditions where neither the bulk alone nor the surface alone conduct.

(If one would treat the n columns of the surface as statistically independent one would get a lower bound for the probability R_{23} of conduction, i.e.

$$R_{23} = 1 - (1 - p_3^{\varepsilon})^n \quad (5)$$

which approaches np_3^{ε} for large n . The resulting lower bound for ε , $\varepsilon > \log(n)/n$ for large n , is of little interest since actually [4] ε remains finite.)

Instead a somewhat different argument can be used for $p_B \rightarrow 0$, $\varepsilon \rightarrow 0$, $n \rightarrow \infty$: compared with a typical configuration just at the threshold $p_s = p_{sc}$ for an isolated plane, the surface at concentration $p_s = p_{sc} - \varepsilon$ has $2 \varepsilon n^2$ of its $2 n^2$ bonds missing. The absence of a single of these links has, in contrast to one dimension, no catastrophic effects since other conducting paths may exist in the plane. Again for the surface bounding

the three-dimensional half-space each missing surface link can be bridged with probability $p_3 = p_B^3$ by a suitable cluster of three bulk bonds; larger clusters are now extremely improbable. These bridges are rather isolated and distributed randomly over the surface. A fraction $p_s \simeq p_{sc} = 1/2$ of them are wasted since they cover already active surface bonds. Thus, in the average, if the number of not wasted bridges, $(1 - p_{sc}) 2 p_3 n^2$, equals the number of missing links, $2 \varepsilon n^2$, conduction is restored (we neglect here fluctuation effects in the thermodynamic limit). Thus the phase transition line in the corner near $p_s = p_{sc}$, $p_B = 0$, is reached if $\varepsilon = (1 - p_{sc}) p_3$ or

$$p_s = p_{sc} - \frac{1}{2} p_B^3 + \dots \quad (p_B \rightarrow 0). \quad (6)$$

This result was generalized by T. W. Burkhardt (private communication, March 1981) in an exact calculation for the Q -state Potts model. We are working in this laboratory on an experimental conduction study using random mixtures of conducting and insulating powders where we take into account the surface effect. No series or Monte Carlo results are known to us to test this exact limiting relation.

5. Conclusion. — Using the concept of bridges to cross missing links in the lattice (not in our arguments) we explained in a simple way why surface effects for the two-dimensional half-space are so different from those in the three-dimensional case. And we generalized this argument to the case of a « wire » immersed in a three-dimensional lattice. In one of these cases Monte Carlo data confirmed our theory and its finite-size result. We thus reconfirmed [3, 4] that a one-dimensional surface does not cooperate with the two-dimensional bulk to produce percolative conduction.

These results are in full accord with a more sophisticated theory of Bray and Moore [1] who predicted such surface-bulk cooperation only for the case where the bulk correlation exponent ν is smaller than unity. For two-dimensional percolation we have $\nu = 4/3$ presumably exactly [7], meaning no cooperation, whereas in three dimension $\nu < 1$, resulting in a surface phase transition curve. Finally a presumably exact result is given for this transition curve in the limit of very small bulk concentrations, equation (6). It is straightforward to generalize our arguments to different lattices or different dimensions. For a d' -dimensional « surface » bounding a d -dimensional bulk phase or immersed into it we expect for $d \geq 2$ that surface and bulk cooperate to lower the percolation threshold only for $d' \geq 2$ and not for $d' = 1$.

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