Determination of percolation probability from the use of a concentration gradient

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Using the idea that the percolation hull is the limit of a diffusion front, we are able to propose a very precise value for the percolation critical probability p_c. For a two-dimensional square lattice, we obtain $p_c = 0.592\,802 \pm 10^{-5}$.

Percolation is widely studied as a simple representation to critical phenomena in disordered systems.[1,2] Usually the percolation problem is defined in a lattice with a constant concentration probability. We have, however, introduced in a previous paper[3] the idea that interesting new features appear in systems where the concentration probability is made to vary over the lattice. In the case of the concentration gradient obtained by diffusion, we have defined a diffusion front which was shown to be very similar to the percolation hull defined by Voss.[4] In particular, it has the same fractal dimension.[3,5] The length and the width of this front follow power laws,[3] the exponents of which are directly related to the critical exponent ν of the correlation length in the percolation problem. The mean position of this front was found to be in a concentration region very close to the percolation probability p_c. In the present Brief Report we show that this last property may be used to obtain a simple and accurate determination of p_c in a 2D lattice.

As far as the determination of p_c is concerned, our preceding approach was found to present the difficulty that the concentration of diffused particles varies nonlinearly with position; we use here a constant gradient of concentration. Besides, because we were interested in the frontier of the diffused region, the diffusion front was situated on occupied sites; we use in this paper a different definition presented in the following paragraph, in which empty and occupied sites play a more equivalent role.

In the usual site percolation problem for a square lattice,[1] a cluster is defined as an ensemble of occupied sites linked via nearest-neighbor connections (four possible connections); we call this cluster an A cluster. The percolation probability is the minimum concentration probability for the onset of an infinite A cluster. Considering now the remaining empty sites, we define in a similar manner a B cluster as being composed of empty sites connected via first- and second-nearest-neighbor connections (eight possible connections). A and B clusters are defined on two lattices with different coordination numbers (four or eight possible connections for each site).[6] In opposition to the usual percolation problem, in the case of a monotonous concentration gradient ranging from zero to one, we remark that there exist both infinite A and B clusters. The infinite A cluster is located in the high-concentration region, whereas the infinite B cluster is in the low-concentration region. They are in contact with each other (Fig. 1). The sites of the infinite A cluster which are connected with sites in the infinite B cluster (via first- or second-nearest-neighbor connections) constitute the frontier as defined in Ref. 3. We call this frontier f_A; its definition is similar to that given by Voss for the hull[4] and we have shown[3] that the frontier should be found in a region where the concentration is very close to p_c. Similarly, we define the frontier f_B as composed with the sites of the infinite B cluster which are connected with the sites of the infinite A cluster via first-nearest-neighbor connections (see Fig. 1). Following Ref. 3, we consider for each frontier f_A or f_B the following parameters: the mean positions x_{fA} and x_{fB}, the widths σ_{fA} and σ_{fB}, and the numbers of sites N_{fA} and N_{fB}. We introduce now the new entity f_{AB}, defined as the union of frontiers f_A and f_B; its position x_{fAB} is simply the mean position of all the lattice points belonging to the frontiers f_A and f_B, and one can easily find

$$x_{fAB} = \frac{N_{fA}x_{fA} + N_{fB}x_{fB}}{N_{fA} + N_{fB}} \quad . \tag{1}$$

We determine the parameters characterizing the frontiers by using a simulation procedure similar to that described in Ref. 3. For each site of abscissa x in a sample of size L by L' (L columns by L' rows), we choose a number n_p at random between 0 and 1; the site is occupied if $n_p < p(x)$ and

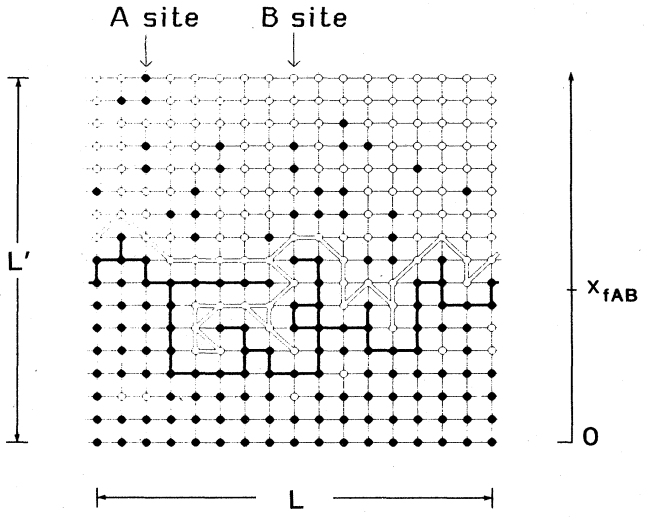

FIG. 1. Schematic picture of frontiers f_A and f_B in a lattice with a gradient of concentration; the concentration of A sites decreases with increasing x. A and B sites are shown as black and white circles, respectively. The frontier f_A is the set of black circles connected by the thick black line. f_B is the set of white circles connected by the thick white line.

empty if $n_p > p(x)$, where the concentration $p(x)$ of A sites is simply given by the following expression:

$$p(x) = 1 - x|\nabla p| \ , \tag{2}$$

where ∇p is the imposed constant concentration gradient. We determine the frontiers f_A and f_B assuming periodical boundary conditions in the direction perpendicular to the gradient. The parameters characterizing the frontiers are averaged over a large number of samples in order to reduce statistical uncertainty.

In accordance with our previous observations[3] we find that

$$\sigma_{fA} \simeq \sigma_{fB} \propto |\nabla p|^{-0.57} \ , \tag{3}$$

which corresponds to relation (7) of Ref. 3. This was explained on the basis of simple arguments relating the width of the diffusion front to the correlation length of percolation.[3] This dependence permits a considerable reduction of the computation time because it is sufficient to consider only a number of rows L' such that the frontier remains within the limits of our sample. As the gradient ∇p decreases, we only need to investigate a concentration region limited by concentrations p_1 and p_2, where $(p_1 - p_2)$ varies as $|\nabla p|^{-0.57}$. Besides, for a given gradient ∇p, the largest finite A or B clusters have a spread of the order of σ_{fA}.[3] Therefore the lateral extent of our samples must be larger than σ_{fA} to prevent any possible confusion between such large clusters and the frontier itself. In the present calculation, L has systematically been taken larger than $10\ \sigma_{fA}$.

Relying upon the rapid convergence to p_c observed in Ref. 3, we consider the variation of the position x_{fAB} when the concentration gradient decreases to zero. We define the quantity $p_c^*(\nabla p) = p(x_{fAB})$. For each concentration gradient ∇p, we average the calculation of $p_c^*(\nabla p)$ on 10 000 samples of lateral size $L = 2048$. The statistical uncertainites are then reduced to about 2×10^{-5} for each point. We observe in Fig. 2 that $p_c^*(\nabla p)$ varies linearly as a function of ∇p. Assuming that this can be extrapolated to zero gradient, we propose to determine p_c as the limit $p_c^*(0)$. We then obtain

$$p_c = 0.592\ 802 \pm 10^{-5} \ . \tag{4}$$

This result is obtained from a linear regression through the points of Fig. 2, with a very good correlation coefficient of 0.9997. This result is compatible with the most recent values for p_c.[7,8] However, we have gained a factor of 5 in the statistical precision compared with the best available result,[8] and it should be stressed that this calculation only required 20 h of calculation on an IBM 3033 class computer. This has two main reasons. First, we may investigate relatively small samples as mentioned above. Second, the identification of the frontier is quite short compared to the cluster recognition in usual percolation problems. Another superiority of our method arises from the fact that the frontier is well defined as soon as L is large enough compared to the width σ_{fA}; the errors due to cutting both lateral ends may be expected to be negligible for periodic boundary conditions. The results obtained from our simulation indeed show a complete independence (within statistical uncertainty) of lateral size L as soon as L is larger than a few σ_{fA}.

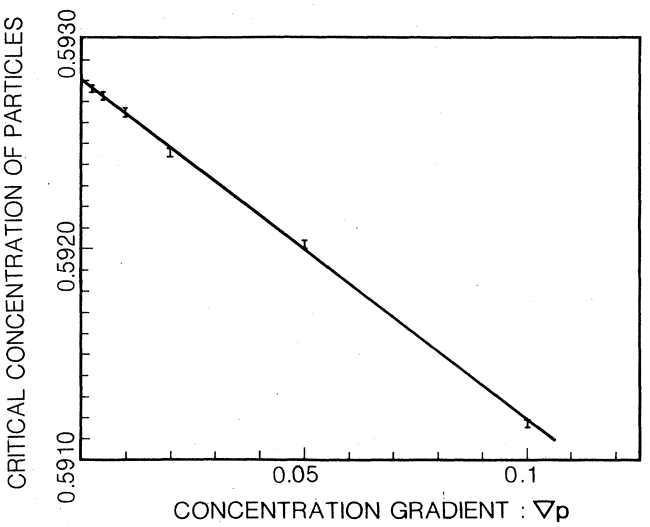

FIG. 2. Variation of the probability $p_c^*(\nabla p)$ as a function of the concentration gradient ∇p. The error bars represent the standard deviations obtained on 10 000 samples. The probability $p_c^*(\nabla p)$ is found to vary almost linearly as a function of ∇p. The straight line is the best fit for these points, obtained by linear regression. We take for p_c the value on this line obtained for $\nabla p = 0$.

In conclusion, this paper confirms beyond doubt the stabilization of the double frontier at p_c. This fact can be justified from scaling arguments.[9] We have shown that the concentration at the mean barycenter of the double frontier converges very rapidly to p_c, allowing for a very precise determination of this quantity. Although there is no theoretical proof for this result at the present time, it can be shown from symmetry considerations that in the triangular lattice $p_c^*(\nabla p)$ is exactly equal to p_c for any gradient.[9] We expect that the calculations presented in this paper could very efficiently be generalized to other lattices, especially in higher dimensions, where rapid convergence should be of great help.

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