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# Dependence of the percolation threshold on the size of the percolating species

V. Cornette, A.J. Ramirez-Pastor, F. Nieto\*

*Surface Chemical Physics Group, Dpto. de Física, Universidad Nacional de San Luis—CONICET, Chacabuco 917, 5700 San Luis, Argentina*

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## Abstract

Site and bond percolation of  $k$ -mers of different structures and forms deposited on 2-D regular lattices is studied. In addition, the percolation threshold for percolating  $k$ -mers on a Bethe lattice is analytically obtained. By using finite-size scaling theory, the analysis of the results is performed in order to determine the behavior of the percolation threshold which exhibits an exponential decrease with the  $k$ -mer size. Characteristic parameters of that function are dependent not only on the form and structure of  $k$ -mers but also on the properties of the lattice where they are deposited. An expression for the percolation threshold as a function of the parameters of the problem is proposed and discussed.

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## 1. Introduction

Percolation theory has been known for several decades [1–6] and applied to a wide number of problems in a large variety of fields, even outside physics, proving to be a very general, powerful and useful tool. Although it is a purely geometric phenomenon, the phase transition involved in the process can be described in terms of the usual second-order phase transition. This mapping to critical phenomena made percolation a full part of the theoretical framework of collective phenomena and statistical physics.

Upon site or bond dilution, a sharp change is found to occur in the connectivity of the system at some threshold  $p_c$  in the density of occupied sites or bonds. Despite

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\* Corresponding author. Tel.: +54-2652-436151; fax: +54-2652-430224.

*E-mail address:* [fnieto@unsl.edu.ar](mailto:fnieto@unsl.edu.ar) (F. Nieto).

the simplicity of its definition, its mathematical ground and its success, percolation theory (and the evaluation of the corresponding percolation threshold) has resisted exact calculations. Most known data are numerical estimates from both Monte Carlo simulations and series expansions. In particular, analytical calculations of percolation threshold have proven to be a rather difficult task only overcome for a given number of simple geometries. From simulations percolation thresholds have been found to be dependent on both the dimension of the system  $d$  and the connectivity of the lattice  $c$ . Only in the known Cayley trees have been solved exactly to yield  $p_c = 1/(c - 1)$ . This expression which holds for both bonds and sites, yields good results at high dimensions. Several contributions in the literature have tried to generalize the above expression in order to include the known values of the percolation threshold of several geometries and dimensions. Galam and Maugier [7,8] have used the following expression as a natural generalization of the Cayley tree's percolation threshold:

$$p_c = p_0[(d - 1)(c - 1)]^{-a}, \quad (1)$$

where  $p_0$  and  $a$  are fitting parameters.

The behavior of the percolation threshold as a function of the size of the percolating species has been studied in several contributions in the literature. However, the problem has not been fully exhausted. In the present work, the percolation of  $k$ -mers on several regular lattices is studied in the framework of a Monte Carlo (MC) analysis. The aim of the paper is to generalize Eq. (1) in order to include the size of the percolating species.

The paper is organized as follows. In Section 2, an exact analytical result for percolation threshold of  $k$ -mers deposited on a Bethe lattice is obtained. In Section 3, the basis of the model of deposition of  $k$ -mers on either sites or bonds of a regular lattice are given. Monte Carlo results for  $p_c(k, c)$  are also presented and discussed. Conclusions are drawn in Section 4.

## 2. Percolation of polyatomic species on the Bethe lattice

Let us assume  $N$   $k$ -mers distributed at random on a Bethe lattice of size  $M$  and connectivity  $c$  (see Fig. 1(a)). Then, the coverage (fraction of occupied lattice sites) is given by  $p = kN/M$ . One can now think of mapping the original lattice  $\mathbf{L}$  to an *effective lattice*  $\mathbf{L}'$  where each empty site of  $\mathbf{L}$  transforms into an empty one of  $\mathbf{L}'$ , while each set of  $k$  sites occupied by a  $k$ -mer in  $\mathbf{L}$  is represented by an occupied site in  $\mathbf{L}'$  (see Fig. 1(b)). Thus, the total number of sites in  $\mathbf{L}'$  is  $M' = M - (k - 1)N$ , and the coverage of  $\mathbf{L}'$

$$p' = N/M' = (p/k) / \left[ 1 - \frac{(k - 1)}{k} p \right]. \quad (2)$$

The effective lattice can be characterized by two connectivities,  $c'_o$  and  $c'_e$ , associated to occupied and empty sites, respectively. From simple arguments, (a)  $c'_o = 2(c - 1) + (k - 2)(c - 2)$  and (b)  $c'_e = c$ . These relationships make complete the mapping from the original problem of  $k$ -mers percolation on  $\mathbf{L}$  to an effective monomer percolation on  $\mathbf{L}'$ .

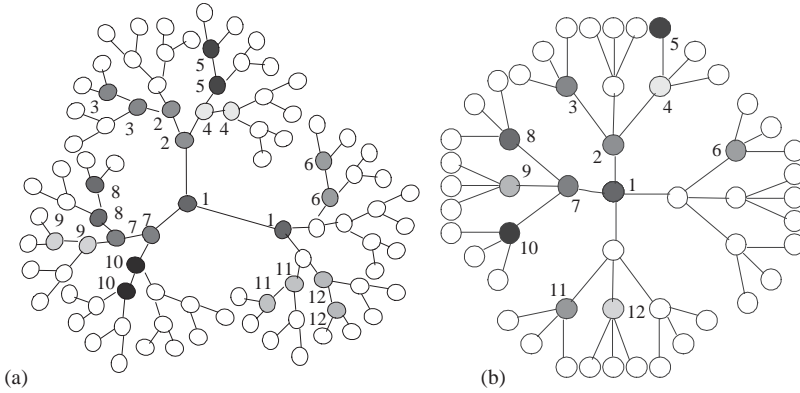


Fig. 1. (a) Dimers (labeled according their respective numbers, as indicated) deposited on a Bethe lattice with coordination  $c$ . (b) Effective lattice of the Bethe lattice (a) according to the rules given in the text.

Let us now find the percolation threshold in the effective lattice. We start at the origin and check if there is a chance of finding an infinite path of occupied neighbors, starting from that site. If we go on such a path in the outward direction, we find  $(c'_o - 1)$  new bonds emanating from every new site, apart from the direction from which we came. Each of these  $(c'_o - 1)$  bonds leads to one new neighbor, which is occupied with probability  $p'$ . Thus on average we have  $(c'_o - 1)p'$  new occupied neighbors to which we can continue our path. If this number  $(c'_o - 1)p'$  is smaller than unity, the average number of different paths leading to infinite decreases at each generation by this factor  $< 1$  and the probability of finding a contiguous path of occupied neighbors goes to zero exponentially with path length, if  $p' < 1/(c'_o - 1)$ . Therefore, the percolation threshold,  $p'_c$  in the effective lattice  $\mathbf{L}'$  has been derived as  $p'_c = 1/(c'_o - 1)$ .

By using the relationships between  $\mathbf{L}$  and  $\mathbf{L}'$  and replacing in  $p'_c$ , the percolation threshold  $p_c$  in  $\mathbf{L}$  can be obtained. Thus,

$$\frac{p_c}{k - (k - 1)p_c} = \frac{1}{2(c - 1) + (k - 2)(c - 2) - 1} \tag{3}$$

Finally, the percolation threshold is obtained:  $p_c = 1/(c - 1)$ .

This equation shows that the size of the percolating species does not modify the percolation threshold for this very peculiar lattice which can be considered of infinite dimensionality [2]. In addition, this result does not guide us for a generalization of Eq. (1) which include the influence of  $k$  on  $p_c$  for regular lattices of finite dimensionality. Then, MC simulations emerge as an important tool in order to determine the influence of  $k$  on  $p_c$  for regular lattices in 2-D.

### 3. Numerical results

We consider a periodic lattice of linear size  $L$  on which we deposit at random  $k$ -mers, each one occupying  $k$  sites of the lattice. The procedure to realize this non-reversible

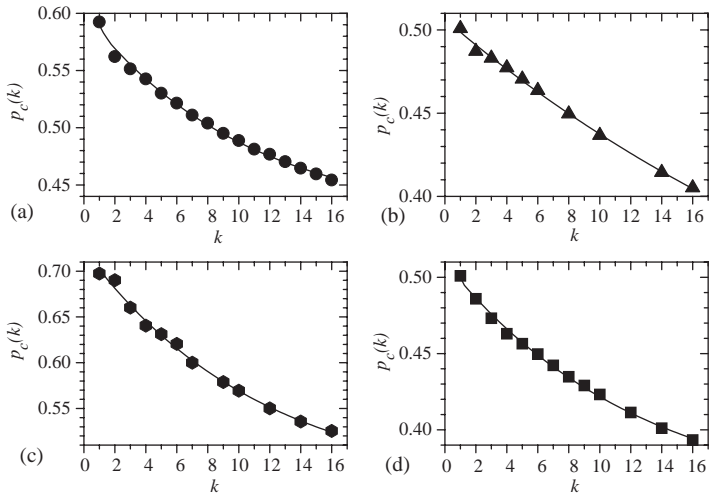


Fig. 2. Percolation threshold as a function of  $k$  for site percolation in a (a) square lattice, (b) triangular lattice, (c) honeycomb lattice and (d) for bond percolation in a square lattice. Symbols represent results from MC data obtained after a detailed finite size scaling analysis while solid lines are fitting by using Eqs. (1) and (4).

adsorption is the following. We select at random a site of the lattice; if it is vacant, one of its  $c$  neighbors is randomly chosen. If this new site is empty, we repeat the process until either  $k$  free sites are found and the  $k$ -mer is then deposited on those sites or an occupied site is selected and the attempt is rejected. In any case, we iterate the procedure until  $N$  of those  $k$ -mers are adsorbed and we reach a desired concentration given by  $p = (kN)/L^2$ . In the same manner, it has also been considered the process when only the bonds are occupied by  $k$ -mers.

The central idea of the percolation theory is based in finding the minimum concentration  $p$  for which a cluster (a group of occupied sites in such a way that each site has at least one occupied nearest-neighbor site) extends from one side to the opposite side of the system. The important point is that, as long as the structure of the background lattice is the same, the value  $p_c$  is always the same in spite of the random configuration of the percolating cluster which varies from sample to sample. As is was already mentioned, the main goal of this paper is (a) to determine how the numerical value of the percolation threshold is modified whether the size of the  $k$ -mer increases and (b) generalize Eq. (1) in order to include the case of polyatomic species.

In Fig. 2(a), we have plotted the percolation threshold for  $k$ -mers as a function of its size  $k$ .  $k$ -mers are adsorbed only on sites of the lattices. At the beginning, for small values of  $k$ , the curve rapidly decreases. However, it flattens out for larger values of  $k$  and finally asymptotically converges toward a definite value as  $k \rightarrow \infty$ . In previous studies of the same problem [9,10], an abrupt increment of  $p_c(k)$  is observed for values of  $k > 10$ . This discrepancy with our results is explained because of finite size effect not considered in Refs. [9,10]. In Figs. 2(b) and (c) are presented the behaviors

of the percolation threshold as a function of  $k$  for triangular and honeycomb lattices, respectively. Fig. 2(d) shows the corresponding curve for a square lattice where the  $k$ -mers only can be deposited on its bonds.

From the above results, the Galam and Maugier equation, Eq. (1) can be generalized for including the case when  $k$ -mers are deposited. All solid curves in Fig. 2 correspond to fitting with the expression given by Eq. (1) with

$$a(k) = A_a \exp\left(-\frac{k}{B_a}\right), \quad p_0(k) = A_{p_0} \exp\left(-\frac{k}{B_{p_0}}\right) \quad (4)$$

being  $A_a=0.366\pm 0.021$ ,  $B_a=30.703\pm 0.003$ ,  $A_{p_0}=0.911\pm 0.005$  and  $B_{p_0}=30.147\pm 0.001$  fitting parameters.

#### 4. Conclusions

In the present paper, the behavior of the percolation threshold of site and bond percolation when  $k$ -mers of different size and structure are deposited on regular lattices is presented. For the different situations considered, a monotonic decreasing function is observed when  $p_c$  is plotted as a function of  $k$ . In order to include the cases treated here, which correspond to regular 2-D lattices, a generalization of Eq. (1) is presented where the influence of the parameter  $k$  is explicitly considered. This shows the importance of the effect of this particular degree of local correlation, determined by the  $k$ -mers, on the percolation threshold.

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