



Percolation of dimers on square lattices

W. Lebrecht^a, J.F. Valdés^a, E.E. Vogel^a, F. Nieto^b, A.J. Ramirez-Pastor^{b,*}

^a Departamento de Física, Universidad de La Frontera, Casilla 54-D, Temuco, Chile

^b Dpto. de Física, Instituto de Física Aplicada, Universidad Nacional de San Luis - CONICET, Ejército de los Andes 950, 5700 San Luis, Argentina

ARTICLE INFO

Article history:

Received 29 June 2012

Received in revised form 14 August 2012

Available online 25 August 2012

Keywords:

Percolation

Multisite occupancy

Critical exponents

Scaling phenomena

ABSTRACT

A theoretical approach, based on exact calculations of configurations on finite rectangular cells, is applied to study the percolation of homonuclear dimers on square lattices. An efficient algorithm allows us to calculate the detailed structure of the configuration space for $M = L_x \times L_y$ cells, with M varying from 16 to 36. The percolation process has been monitored by following the percolation function, defined as the ratio between the number of percolating configurations and the total number of available configurations for a given cell size and concentration of occupied sites. The percolation threshold has been calculated by means of two complementary methods: one based on well-known renormalization techniques and the other based on determining the inflection point of the percolation function curves. A comparison of the results obtained by these two methods has been performed. The study includes the use of finite-size scaling theory to extrapolate numerical results towards the thermodynamic limit. The effect of jamming due to dimers is also established. Finally, the critical exponents ν , β and γ have been obtained and values compared with numerical results and expected theoretical estimations. The present results show agreement and even improvement (in the case of γ) with respect to some numeric values available in the literature.

© 2012 Elsevier B.V. All rights reserved.

1. Introduction

The percolation problem is a topic being increasingly considered in statistical physics. One reason for this current interest is that it is clear that generalizations of the pure percolation problem are likely to have extensive applications in science and technology [1–5]. Although it is a purely geometric phenomenon, the phase transition involved in the process can be described in terms of a usual continuous phase transition. This mapping to critical phenomena has made percolation a full part of the theoretical framework of collective phenomena and statistical physics.

In this context, percolation of monomers (particles occupying one lattice site each) has been one of the most studied models in the literature, and the corresponding percolation threshold p_c has been measured to high precision for decades [6–10]. The problem becomes considerably difficult when some sort of correlation exists, such as particles that occupy several k contiguous lattice sites (k -mers). Consequently, there have been fewer studies devoted to the problem of percolation of structured objects. Among them, Leroyer and Pommiers [11] studied the percolation behavior of a random sequential adsorption (RSA) of linear segments with different sizes, and Gao and Yang [12] and Cherkasova et al. [13] analyzed the percolation of dimers. In all cases, the dependence of the percolation threshold on the parameters of the problem and the universality of the phase transition have been discussed. However, Ref. [11] is limited due to finite-size effects, while Refs. [12,13] are just restricted to the case $k = 2$ (dimers). In fact, Leroyer and Pommiers found that, as the

* Corresponding author.

E-mail address: antorami@unsl.edu.ar (A.J. Ramirez-Pastor).

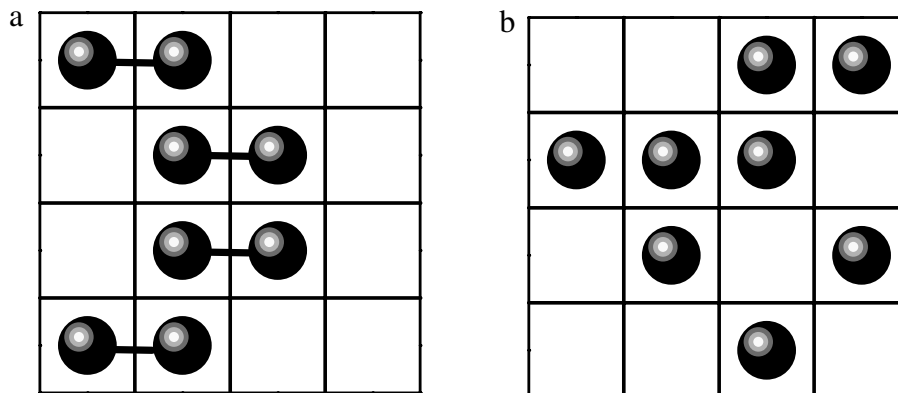


Fig. 1. (a) Snapshot corresponding to one of the possible configurations for a system of four dimers on a 4×4 cell. Full circles and empty squares represent dimer units and empty sites, respectively. (b) As part (a) for a system of eight monomers on a 4×4 cell. Full circles and empty squares represent monomers and empty sites, respectively.

segment length grows, the percolation threshold decreases, goes through a minimum, and then increases slowly for large segments. Further studies by Cornette et al. [14] showed a monotonic dependence of the percolation threshold on the size of the deposited element, in contrast with the results of Ref. [11]. This discrepancy was explained because of the finite-size effect not being considered in Ref. [11].

As discussed in the previous paragraph, it took until 2003 to elucidate the dependence of p_c on k for tortuous and rigid k -mers deposited according to an RSA process. In addition, the phase transition predicted by Monte Carlo (MC) techniques in Refs. [11–14] has not been corroborated yet by analytical methods. In this framework, the main objective of the present work is, using an analytical technique, to determine the full set of characteristic parameters of percolation (percolation threshold and critical exponents) for a system of dimers, randomly and irreversibly deposited on a square lattice.¹ We make use of the opportunity of considering the effect of jamming on the coverage of square lattices upon using dimers. The study is based on (i) exact calculation of configurations on finite $M = L_x \times L_y$ cells, with M varying from 16 to 36 and (ii) the use of finite-size scaling techniques [15–17].

The rest of the paper is organized as follows. In Section 2, the theoretical formalism is presented. The analysis of the results and discussion are given in Section 3. Finally, the conclusions are drawn in Section 4.

2. Theory

In the filling process, rigid dimers are deposited sequentially and irreversibly on an initially empty square cell of $M = L_x \times L_y$ sites with the following restrictions: (1) the depositing objects contain two identical units; (2) the distance between dimer sites is assumed in registry with the lattice constant a ; hence exactly two sites are occupied by a dimer when deposited; (3) the incoming particles must not overlap with previously added objects; and (4) the elements remain frozen in the lattice. In any case, the procedure is iterated until N dimers are placed on the cell and the desired concentration (given by $p = 2N/M$) is reached. A configuration is a distribution of empty and occupied sites on the cell. Fig. 1(a) shows one of the possible configurations corresponding to a system of four dimers on a 4×4 cell. In part (b), one possible configuration of monomers at the same concentration as that in part (a) is plotted. Note that the configuration in part (b) is not available for dimers. Thus, not all the available configurations of empty and occupied sites can be reached by dimer deposition.

A central idea of percolation theory is based on 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 of the system to the opposite one. This particular value of the concentration rate is named the critical concentration or percolation threshold p_c , and it determines a phase transition in the system. In the monomeric random percolation model, any single site (or a bond connecting two sites) is occupied with probability p . For the precise value of p_c , the percolation threshold of sites (bonds), at least one spanning cluster connects the opposite borders of the system (indeed, there exists a finite probability of finding $n (> 1)$ spanning clusters [18–21]). In that case, a continuous phase transition appears at p_c which is characterized by well-defined critical exponents.

Let us define $p(t)$ as the fraction of lattice sites covered at time t by the deposited objects. Due to the blocking of the lattice by the already randomly adsorbed elements, the limiting or jamming coverage, $p^j = p(t \rightarrow \infty)$, is less than that corresponding to close packing ($p^j < 1$). Consequently, p ranges from 0 to p^j for objects occupying more than one site. An extensive overview of this field can be found in the excellent work by Evans [22] and the references therein. In the case of

¹ The dimer is the simplest case of a polyatomic adsorbate, and it contains all the properties of multisite-occupancy adsorption.

Download English Version:

<https://daneshyari.com/en/article/10480635>

Download Persian Version:

<https://daneshyari.com/article/10480635>

[Daneshyari.com](https://daneshyari.com)