Eur. Phys. J. B **36**, 157–160 (2003)
DOI: 10.1140/epjb/e2003-00329-6

THE EUROPEAN PHYSICAL JOURNAL B

Scaling behavior of jamming fluctuations upon random sequential adsorption

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Received 2 July 2003 / Received in final form 17 October 2003
Published online 8 December 2003 –

Abstract. It is shown that the fluctuations of the jamming coverage upon Random Sequential Adsorption (RSA) (σ_{θ_J}), decay with the lattice size according to the power-law $\sigma_{\theta_J} \propto L^{-1/\nu_J}$, with $\nu_J = \frac{2}{2D-d_f}$, where D is the dimension of the substrate and d_f is the fractal dimension of the set of sites belonging to the substrate where the RSA process actually takes place. This result is in excellent agreement with the figure recently reported by Vandewalle et al. [Eur. Phys. J. B **14**, 407 (2000)], namely $\nu_J = 1.0 \pm 0.1$ for the RSA of needles with $D = 2$ and $d_f = 2$, that gives $\nu_J = 1$. Furthermore, our prediction is in excellent agreement with different previous numerical results. The derived relationships are also confirmed by means of extensive numerical simulations applied to the RSA of dimers on both stochastic and deterministic fractal substrates.

PACS. 05.40.-a Fluctuation phenomena, random processes, noise, and Brownian motion – 02.50.-r Probability theory, stochastic processes, and statistics

Rapid Note

The irreversible deposition of particles on a surface involves two characteristic time scales: the time between depositions, and the diffusion time of the particles on the surface. For very strong interaction between particles and the substrate (chemical adsorption), diffusion becomes irrelevant and the Random Sequential Adsorption (RSA) model provides an excellent description of the underlying processes (for a review on RSA models see [1]). Under these conditions the system evolves rapidly toward far-from equilibrium conditions and the dynamics becomes essentially dominated by geometrical exclusion effects between particles. This kind of effects has been observed in numerous experiments [2].

The RSA of needles (or linear segments) on homogeneous, two-dimensional samples, has very recently attracted considerable interest [3,4]. Particular attention has been drawn to the interplay between the jamming coverage and percolation [3–5]. The percolation problem has also attracted considerable attention in the field of statistical physics due to their relevance for the understanding of processes and phenomena in many other areas such as those occurring in disordered media, porous materials, systems of biological and ecological interest, etc. [6,8,9]. Therefore, a great progress in the field of the statistical physics of far-from equilibrium processes could be achieved by establishing links between RSA and percolation [3–5].

The percolation transition is related to the probability of occurrence of an infinite connectivity between randomly deposited objects, as a function of the fraction p of the substrate occupied by the objects. Close to the percolation threshold p_c, the probability P to find a percolating cluster, on a finite sample of side L, is given by an error function [9]

$$P = \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{p} \exp\left[-\frac{1}{2}\Big(\frac{p' - p_c}{\sigma}\Big)^2\right] dp', \qquad (1)$$

where σ is the width of the transition region. It is well known that σ vanishes in the thermodynamic limit according to [9]

$$\sigma \propto L^{-\frac{1}{\nu}}, \qquad (2)$$

where ν is the exponent that governs the divergence of the correlation length as $\xi \propto |p - p_c|^{-\nu}$.

Very recently it has been suggested that the jamming probability and the fluctuations of the jamming coverage may obey relationships similar to equations (1, 2) [3], respectively. The aim of this note is to provide a qualitative derivation of equation (2) for the case of RSA on both homogeneous and deterministic fractal substrates. The predictions of the obtained equation will be compared with previously published data and further numerical tests

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will be performed. To accomplish these goals, the RSA of dimers on deterministic and stochastic fractals such as a Sierpinski Carpets (SC) [8] and the diffusion front [6,8], has been studied.

Let us first establish a link between the fluctuations of the number of deposited particles (at the jamming state) on a subsystem of side L_0 with those of a system of side L, with $L_0 < L$. Considering a fractal subsystem of side L_0, that has itself Q_0 minimal pattern blocks, and increasing the size of the subsystem n steps λ times until reaching the size L, such as $L(n) = \lambda^n L_0$, then Q_0 will change to $Q(n) = s^n Q_0$. Therefore, eliminating n, it follows that

$$Q = Q_0 \times \left(\frac{L}{L_0}\right)^{d_\mathrm{f}} \tag{3}$$

where $d_\mathrm{f} = \log(s)/\log(\lambda)$ is the fractal dimension.

Let N_0 be the number of adsorbed particles in the starting subsystem of side L_0. For the system of side L the number of adsorbed particles $N(L)$ is given by the sum

$$N(L) = \sum_{\imath=1}^{s^n} N_i, \tag{4}$$

where N_i are the number of adsorbed particles on each subsystem of side L_0 that form the system of side L. Let $\sigma_{N(L_0)}$ be the fluctuations, in the starting L_0-subsystem, of N_0. If the correlation length associated to the random sequential adsorption (ξ_{Rsa}) is short compared with L_0 ($\xi_{Rsa} \ll L_0$), the random variables N_i will be statistically independent an so from equation (4) it follows

$$\sigma^2_{N(L)} = \sum_{\imath=1}^{s^n} {\sigma_i}^2. \tag{5}$$

Furthermore, in the thermodynamic limit, the L_0-subsystems should have identical statistical properties. Thus, their respective fluctuations will be the same. So, from the fact that $s^n = \frac{Q(n)}{Q_0}$ and equations (3, 5) one has

$$\sigma^2_{N(L)} = \frac{\sigma^2_{N_0}}{L_0^{d_\mathrm{f}}} \times L^{d_\mathrm{f}}, \tag{6}$$

then the fluctuation of the density (θ) in the system of size L can be obtained from equation (6) dividing by L^{2D}, so that

$$\sigma_\theta \propto L^{-\frac{1}{\nu_J}}, \tag{7}$$

where

$$\nu_J = \frac{2}{2D - d_\mathrm{f}}. \tag{8}$$

It should be stressed that equations (7, 8) are quite general relationships valid for substrate systems that are both homogeneous and deterministic fractal. Furthermore, the same relationships hold for the case of substrates globally-invariant under translations, such as random fractals, as it has been demonstrated elsewhere [11]. Also, the condition that the correlation length of the RSA process should be smaller than the system size is usually valid for jammed states, where the correlation length is very short. It is also very interesting to notice that, using these relationships it may be possible to evaluate d_f performing both RSA numerical simulations and actual experiments. Furthermore, existing numerical simulations performed in $D = 2$ dimensions with $d_\mathrm{f} = 2$ are in excellent agreement with equations (7) and (8) (notice that for these conditions it follows straightforwardly from equation (8) that $\nu_J = 1$ exactly). In fact, for the jamming upon RSA of needles in two dimensions the value $\nu_J = 1.0 \pm 0.1$ has been reported [3] and this figure is independent of the aspect ratio of the needles. Furthermore, early numerical results of Nakamura for the RSA of square blocks are also consistent with $\nu_J \simeq 1$ [10], while Kondrat et al. [4] have reported $\nu_J = 1.00 \pm 0.05$ for the RSA of segments on the square lattice. Since the obtained values for the exponent are independent (within error bars) of: i) the length of the segments (for all $a = 1, 2, ..., 45$) [4], ii) the aspect ratio of the needles [3] and iii) the size of the square blocks [10], it has been suggested that ν_J is a good candidate for an universal quantity of the jamming process [4]. Within this context, our finding shows that ν_J depends on the dimensionality of the substrate and the set where the RSA processes actually takes place.

On homogeneous samples the jamming coverage (θ) and its fluctuations (σ_θ) can straightforwardly be obtained, since one has to deal with a single stochastic process. However, RSA on nonhomogeneous random substrates requires a careful treatment because two correlated stochastic processes are now involved [11]. One can assume that the fluctuations due to the RSA process are given by an average over M independent samples:

$$\sigma_\theta = \sum_{i=1}^{M} \frac{\sigma^i_\theta}{M}, \tag{9}$$

where σ^i_θ are the fluctuations measured using a **single** substrate sample but taken averages over independent RSA trials. It has been shown [11] that measuring σ_θ with the aid of equation (9) one captures the physical behavior of the RSA process. In contrast, measuring the fluctuations of the average jamming coverage of different samples the physical behavior reflects the properties of the substrate [11].

In order to perform additional tests to the obtained analytical results, the RSA of dimers on both stochastic and deterministic fractals has been studied numerically.

As example of an stochastic fractal, we have used a diffusion front. In order to generate the diffusion front, we considered the diffusion of particles at random, but with hard-core interactions, on a 2D square lattice of size $L \times L$. There is a source of particles at the first row of the lattice $y = 1, 1 \leq x \leq L$ kept at concentration $p(1, t) \equiv 1$. Also, at row $y = L + 1, 1 \leq x \leq L$ there is a well, $p(L + 1, t) \equiv 0$. So, there is a concentration gradient along the source-well direction, while along the perpendicular x-direction periodic boundary conditions are imposed. In the steady state the concentration gradient is constant, so one has

$$\nabla p(y) = L^{-1}. \tag{10}$$

It is well known that the properties of the diffusion front [12,13] are closely related to those of the incipient percolation cluster [6,8,9]. As the concentration $p(y)$ of particles depends on the position, decreasing from the source to the well, one actually has a gradient percolation system. The structure of the diffusion front is identical to the structure of the hull of the incipient percolation cluster [12]. Furthermore, the concentration of particles at the mean front position y_f is the same as the percolation threshold p_c, so that $p(y_f) = p_c$ [12]. The diffusion front is conveniently described by its average width σ_f and the total number N_f of particles that constitute it. Using heuristic arguments it has been suggested that

$$\frac{N_f}{L} \sim |\nabla p(y_f)|^{-\alpha_N} \qquad \text{where} \quad \alpha_N = \frac{1}{\nu+1} \qquad (11)$$

being ν the critical exponent of the correlation length in the percolation problem [6,8]; $\nu = 4/3$ in $2D$, which gives $\alpha_N = 3/7$. So, from equations (10, 11) one has

$$N_f \sim L^{d_{\rm f}^{DF}}, \qquad (12)$$

with $d_{\rm f}^{DF} = \alpha_N + 1 = 10/7 \approx 1.4286$, and the diffusion front is a stochastic self-similar fractal [14].

RSA of dimers on diffusion fronts has been simulated using two rules: according to Rule I only adsorption events of dimers taking place on two nearest-neighbor (NN) sites, such us one of then belongs to the diffusion front and the remaining one is outside it, are considered. On the other hand, using Rule II one only allows the adsorption on NN sites of the diffusion front, disregarding adsorption trials on already occupied sites of the front and sites outside the fractal.

RSA of dimers on deterministic fractals (Sierpinski Carpets [6,8]) is also studied. The SC in $D = 2$ dimensions is generated by dividing a full square into λ^D smaller squares of the same size. Out of these squares, k of them are chosen and removed. In the next iteration, the procedure is repeated by dividing each of the small squares left into λ^D smaller squares removing those k squares that are located at the same positions as in the first iteration. The resultant fractal dimensions are

$$d_{\rm f}(s,\lambda) = \log(s)/\log(\lambda) \qquad (13)$$

where $s = \lambda^D - k$. In principle, this procedure has to be repeated again and again, however for the practical implementation in a computer only a finite number of iterations are actually performed [8,7]. In a square lattice the smaller subdivision is actually a single site and the length is measured in site units. Furthermore there is a minimal pattern of $\lambda^{d_{\rm f}}$ sites. In the present work various generations of SC's of different size L, with periodical boundary conditions, have been employed. In all cases dimers are allow to adsorb only on NN empty sites belonging to the fractal. For SC's with $\lambda = 3$ and $k = 1, 2, 3$, as used in the simulations, the fractal dimensions are $d_{\rm f_I} = \log(8)/\log(3) \approx 1.8928$, $d_{\rm f_{II}} = \log(7)/\log(3) \approx 1.7712$ and $d_{\rm f_{III}} = \log(6)/\log(3) \approx 1.6309$, respectively.

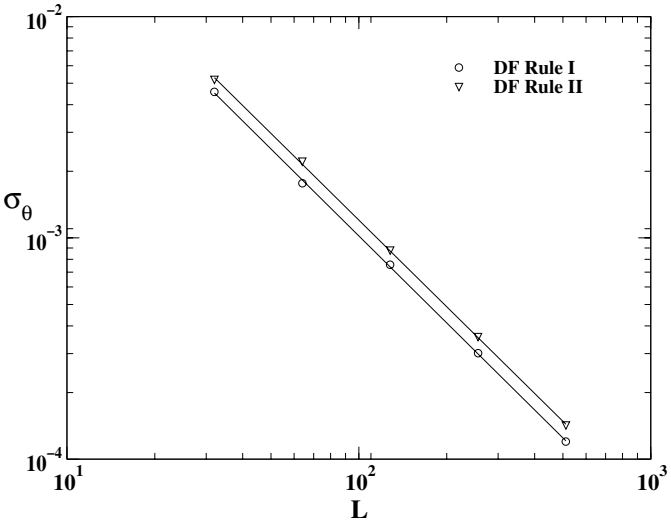

Fig. 1. Log-log plots of σ_θ versus L for the case of RSA of dimers on the random fractal generated by diffusion fronts (DF). Results obtained using two different adsorption rules are shown. For details the adsorption rules see the text.

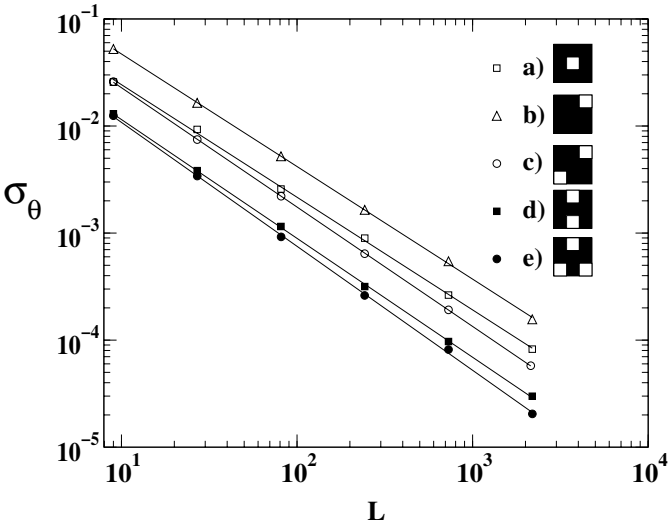

Fig. 2. Log-log plots of σ_θ versus L for the case of RSA on Sierpinski Carpets obtained using different generating patterns as shown in the figure (black squares compose the fractal structure).

Figures 1 and 2 show log-log plots of σ_θ versus L obtained upon RSA of dimers on diffusion fronts and Sierpinski Carpets, respectively. The obtained results, for these kind of fractals, are in excellent agreement with the prediction of equation (8) as follows from the comparison of evaluated and theoretical exponents listed in Table 1. Further support to the theoretical prediction follows from additional results obtained using homogeneous samples, which are also listed in Table 1.

Summing up, it is shown that the exponent ν_J can be obtained as a function of the dimensionality D of the space and the fractal dimension $d_{\rm f}$ of the subset site where the RSA process actually takes place. Our main result

Table 1. Examples of the application of equation (8) to different fractals as listed in the first column: SC ≡ Sierpinski Carpet, DF ≡ Diffusion front, HS2 Homogeneous Substrate in $D = 2$ dimensions. The 2nd column shows the exponents obtained fitting equation (8) to the simulation results while the 3rd one shows the estimations of $d_{\rm f}$ obtained using $\frac{1}{\nu_J} = \frac{2D-d_{\rm f}}{2}$. The 4th column is a list of the exact values of $d_{\rm f}$. Notice that for SC the labels a)-e) allows to identify the generating patterns, as shown in Figure 2.

Substrate	$1/\nu_J$	$d_{\rm f}^*$	$d_{\rm f}$
SC (a)	1.051(4)	1.898(8)	$\ln(8)/\ln(3) \simeq 1.893$
SC (b)	1.052(4)	1.896(8)	$\ln(8)/\ln(3) \simeq 1.893$
SC (c)	1.115(2)	1.770(4)	$\ln(7)/\ln(3) \simeq 1.771$
SC (d)	1.110(7)	1.780(15)	$\ln(7)/\ln(3) \simeq 1.771$
SC (e)	1.16(2)	1.68(4)	$\ln(6)/\ln(3) \simeq 1.631$
DF	1.30(2)	1.40(4)	$10/7 \simeq 1.429$
HS2 (D = 2)	1	-	2

$\nu_J = \frac{2}{2D-d_{\rm f}}$, provides a solid ground to previous numerical data [3,4,10]. Furthermore, in this work, the validity of the proposed relationship is verified by means of extensive numerical simulations, using both homogeneous substrates as well as different fractals.

This work was supported by CONICET, UNLP and ANPCyT (Argentina).

Rapid Note

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14. Notice that scaling N_f as a function of the diffusion width, instead of the lattice size L as in equation (12), one can define a different fractal dimension given by $d_{\rm f}^{*DF} = \nu + 1/\nu = 7/4$