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LETTER TO THE EDITOR

Irreversible deposition on disordered substrates

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Abstract. We report results of a Monte Carlo study of the kinetics of random sequential deposition of line segments (mostly dimers) on the 1D lattice substrate, already occupied with point-like quenched impurities at low concentration. The area covered by the placed objects grows with time and finally reaches a jamming limit when no more deposition is possible. The jamming coverage values, obtained by numerical simulations, depend on the segment length and on the previous occupation of the substrate by impurities. The rate of late-stage deposition is not disturbed by presence of forbidden sites when the process of deposition starts ($t=0$). Numerical results, shown in semi-log scale, confirm that area coverage $\theta(t)$ approaches the jamming limit $\theta(\infty)$ exponentially, with the same exponent factor -1 multiplying scaled time, as in the case of random sequential deposition of line segments on the clean 1D lattice (initially non-occupied).

Irreversible deposition, or random sequential adsorption (RSA) is a process in which objects of finite size are randomly deposited on a substrate. The overlapping of deposited objects is not permitted. The relaxation time of placed objects is much longer than the time needed for the system to reach saturation. Therefore objects stay permanently fixed, once deposited. The dominant effect in RSA is the blocking of the available substrate area by the already deposited particles. In earlier studies this problem was defined as 'the car parking problem [1]. The quantity of interest is the relative coverage $\theta(t)$, which is the fraction of the substrate area covered by the adsorbed particles. The kinetics of the process of RSA is characterized by the time evolution of the coverage. Due to the blocking effect, the jamming coverage $\theta(\infty)$ (in $t\to\infty$ limit) is smaller than 1, which is close to the packing value. The only exception is deposition of point-like objects, when jamming coverage reaches unity. This is a non-Markovian process and therefore mean-field theory cannot be used, except for very early times, when $\theta(t)\propto t$.

Experimental studies [2–7] include processes with relaxation times much longer than the formation time of deposites, e.g. adhesion of latexes [2], proteins [4] and colloidal particles [7] on homogeneous substrates. In theoretical studies of RSA, which include Monte Carlo simulations [11, 12], both continuous and discrete models were analysed. Analytical results are also available [13] for one-dimensional models. In such studies, it was shown that the late-stage deposition kinetics follows a power law for continuous models. For discrete models the late stage jamming coverage is approached exponentially [10–12], i.e.

$$\theta(t)=\theta(\infty)-A\exp\left(-\frac{t}{\sigma}\right)$$

where A and σ are parameters which may depend on the shape, size etc. of the adsorbing object, and this is in agreement with analytical results [13].

In the present work we study a single-layer random sequential deposition of line segments on a 1D lattice initially and randomly occupied with point-like quenched impurities at low concentration. The length of the line segment k-mers are integral multiples of the lattice unit $k=L/N$, where L is the length of the chain and N is the number of points. As $N \gg k$ we can neglect finite-size effects [10] and take periodic boundary conditions. The Monte Carlo procedure goes as follows: we take 1D lattice of size L with randomly quenched point-like impurities and line segments of length k (in lattice units), and randomly select one of the N lattice points. If the chosen site is already occupied, the attempt is abandoned and a new site is selected. If the site is unoccupied, we fix one end of the line and randomly pick one of two possible directions and search whether all successive k sites are unocuppied. If so, we occupy these k sites, deposit the segment and increase the number of occupied sites by k. If the attempt fails (it is irrelevant whether it was because some of the k sites were occupied by impurities or by an earlier deposited segment) a new site is selected. The time is counted for the number of attempts to select a lattice site and scaled by the total number of 1D lattice sites N. Simulation ends when each of the N sites are randomly selected once and no sites are unoccupied, except blocked ones.

Two results of these simulations are the focus of our interest. In the first place, we compare graphs drawn in the semi-log scale (Figures 2 and 3) for the purpose of investigation of the rate of late-stage deposition of dimers on a 1D lattice with impurities. The results shown in the figures confirm that relative area coverage $\theta(t)$ of the 1D discrete substrate with point-like impurities approaches the jamming limit $\theta(\infty)$ exponentially. Exponent factor multiplying scaled time is -1, as in the case of random sequential deposition of line segments on clean 1D lattices [10]. In figure 1 we present the results of simulation of deposition of dimers on a 1D lattice substrate, with 10% point-like impurities and without impurities. Results of the same simulations are shown in figure 2 in semi-log scale. It is obvious that the lines are parallel, with slope -1. It is also important to say that coverage includes deposited dimers and point-like impurities, and therefore, in the case of deposition with 10% of the substrate already occupied by impurities, coverage starts with value $\theta(0)=0.1$ (figure 1). Lines corresponding to simulations with 2%, 4%, 6% and 8% impurities lie between these two shown in figure 2. In figure 3. we present $\ln(\theta(\infty)-\theta(\tau))$ versus scaled time τ for deposition of line segments of length $k=2$, $k=3$ and $k=4$ on a 1D lattice with 2% point-like impurities. The exponent factor multiplying scaled time is -1 in all cases. This means that, in the presence of quenched impurities, the kinetics of RSA is not disturbed in the late-time regime.

The next parameter we are interested in is jamming coverage, depending on concentration of quenched impurities. Numerical results are shown in table 1 and figure 4. As the relative concentration of impurities p increase, $\theta_p(\infty)$ decrease and reach a minimum value for p between 0.13 and 0.14 (see solid curve on figure 4). For increased concentrations, jamming coverage grows and for $p=1$ reaches unity. This is

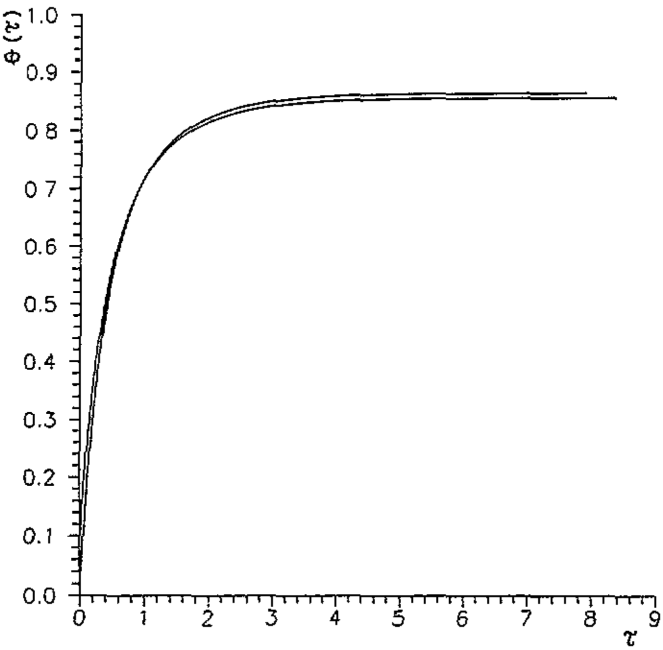

Figure 1. Relative coverage $\theta(\tau)$ versus scaled time τ for deposition of dimers on a 1D lattice. Line starts from $\theta(0) = 0$, which corresponds to deposition on a clean lattice. The other one, starting with $\theta(0) = 0.1$, corresponds to deposition on a 1D lattice with 10% point-like quenched impurities.

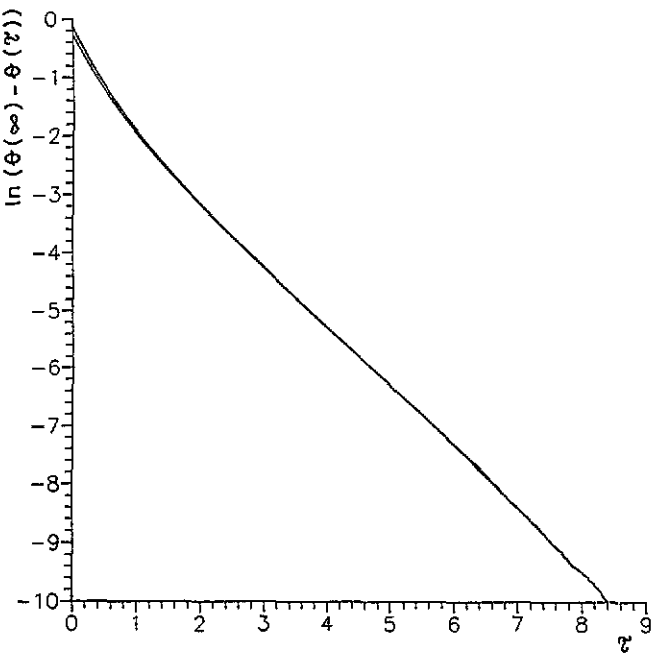

Figure 2. As figure 1 on semi-log scale.

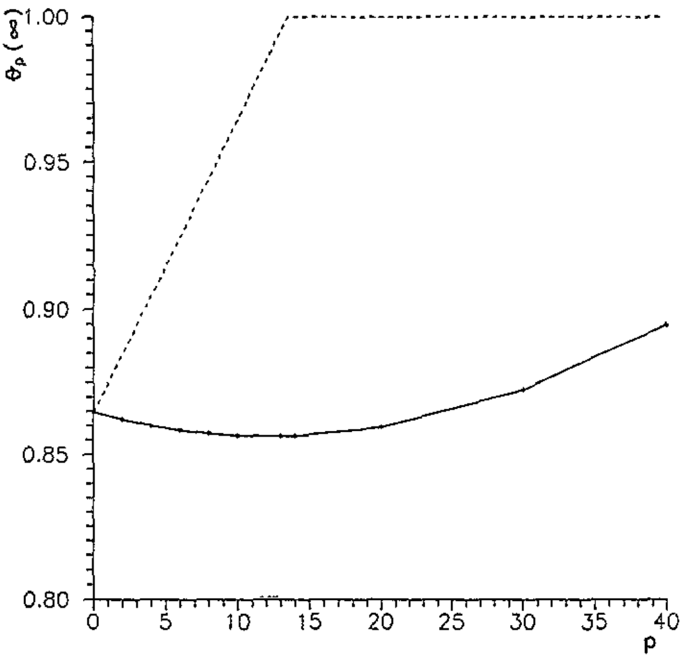

Figure 3. The plot of $\ln(\theta(-\theta(\tau))$ as a function of τ for deposition of line segments of length $k=2$, $k=3$ and $k=4$ (from top to bottom) on a 1D lattice with 2% of quenched point-like impurities.

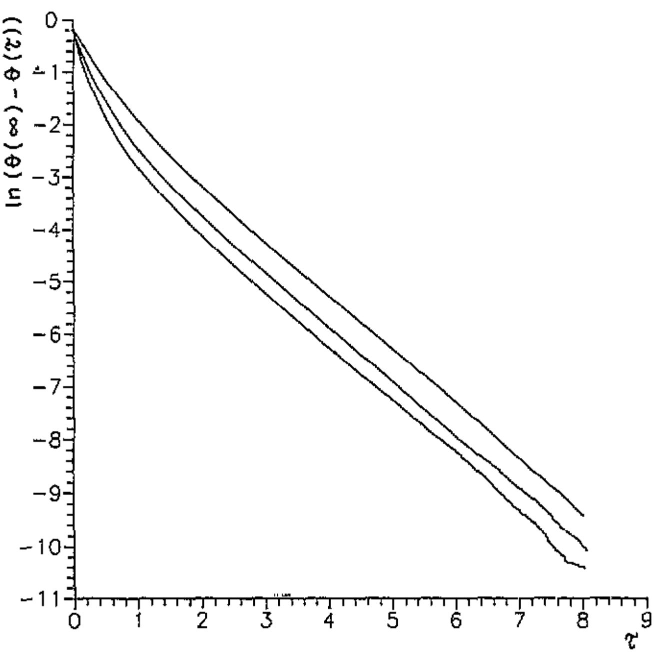

Figure 4. Jamming limit values $\theta_p(\infty)$ versus concentration of point-like impurities p on a 1D lattice. The solid line is for quenched point-like impurities and the dotted line corresponds with annealed ones.

Table 1. Jamming coverage values for deposition of dimers on a 1D lattice with different concentrations of quenched point-like impurities.

%	$\theta(\infty)$
0	0.8647
2	0.8622
4	0.8600
6	0.8585
8	0.8573
10	0.8565
13	0.8564
14	0.8564
20	0.8595
30	0.8726
40	0.8948

a trivial result because all sites are occupied by impurities. It will be interesting to compare these results with jamming coverage values for different concentrations of annealed point-like impurities (dotted curve on figure 4.) Systems with annealed impurities are trivial, because constant drifting of impurities enables deposition of the same number of dimers as in the case of a clean substrate, but a larger number of attempts are expected. Therefore, for annealed point-like impurities $\theta_p(\infty)=\theta_0(\infty)+p$ for $p<0.1354$ and $\theta_p(\infty)=1$ for $p>0.1354$.

An interesting result of these simulations is that the value of the relative concentration p of quenched impurities, where jamming coverage has a minimum value, is probably the same as the value of relative concentration of annealed impurities where jamming coverage reaches unity. That value is equal to the number of blocked sites in the case of RSA of dimers on a clean substrate. In the numerical results shown in table 1 the fourth decimal point is relevant. We repeated the simulations with a different random number generator and $\Delta\theta(\infty)=0.0001$.

Some efforts to find an analytical solution for RSA in 1D with impurities have been made [9, 10], but they fail in predicting minimum values of $\theta_p(\infty)$ as a function of relative concentration of impurities. Generally, the presence of impurities (both quenched and annealed) change initial conditions in such a way that numerical methods of solving rate equations [9, 10] are probably the only ones possible. In summary, we performed a Monte Carlo simulation of RSA of line segments on the 1D lattice, with some sites previously occupied by quenched point-like impurities. An exponential approach to the jamming limit is obtained, with the same exponential factor -1 multiplying the scaled time in all cases. The jamming coverage value is calculated for various concentrations of point-like impurities. The minimum value is obtained for the relative concentration of quenched impurities that corresponds with the number of blocked empty sites in random sequential deposition of dimers on a clean substrate.

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