Z. Phys. B – Condensed Matter 70, 213–217 (1988)

Condensed
Zeitschrift für Physik B Matter

A Percolation Model with Disaggregation and Aggregation

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Received July 17, 1987

A model of percolation with disaggregation and aggregation (PDA) is proposed and studied by means of the Monte Carlo simulation on the square lattice. The critical concentration (ϕ_c), the correlation length exponent and the fractal and spreading dimensions of the largest cluster at ϕ_c have been computed. The obtained results suggest that the PDA model belongs to the same universality class than the standard percolation model. Nevertheless, the critical concentration ($\phi_c = 0.464 \pm 0.005$) of the former is quite different from the critical probability ($p_c = 0.5927$) of the later model.

I. Introduction

During the last years, the "static" percolation theory has concentrated considerable attention (see for example the reviews [1, 2]). This interest has recently been renewed due to the fractal properties of incipient percolation clusters. On the other hand a huge effort has been dedicated to the study of irreversible kinetic growth models, such as diffusion-limited aggregation [3] and clustering of clusters [4] (for a review see [5]). From the theoretical point of view, the main interest on these models arise from the fact that the kinetic effects are relevant in the sense that they determine to which universality class belongs each model. Also, in order to study the "dynamic" effects in percolation, some models such as the invasion percolation [6], and the percolation with diffusion of particles with non-additive lateral interactions [7], have been introduced.

On the other hand, variants of the static standard percolation model (henceforth SP) have also been investigated. For example, the so called "Bootstrap Percolation" [8] (henceforth BP), in which lattice sites are randomly occupied with probability p, but all sites, with less than a fixed number m of nearest-neighbour $(n-n)$ occupied sites are culled until a stable configuration is attained. The study of the BP model has been focused to the dependence of both, the class of the percolation transition and the critical exponents on m [8–10]. The BP model involves some kind of disaggregation (or evaporation) of occupied sites and consequently the number of particles on the lattice changes due to the culling process. In other context, a model of diffusion limited aggregation with disaggregation (henceforth DLAD) has been analized [11] (for models of clustering of clusters with disaggregation, see [12]). In the DLAD model, a single bonded particle may scape from a loopless cluster undergoing a random walk until it reaches the cluster again. If, for example, one starts with a loopless diffusion-limited aggregation cluster, this dynamic disaggregation-aggregation process changes the fractal dimension of the cluster, and in the steady state regime the fractal dimension is independent of the type of the initial cluster.

In the present work, a new model of percolation with disaggregation and aggregation (henceforth PDA) is introduced and discussed (for the definition see Sect. II). The PDA model can be thought of as some kind of "dynamic" $m=2$ BP where the culling process is replaced by a dynamic disaggregation-aggregation process and the total number of particles is conserved. It should be noted that the rigid rules which dominate the culling process in BP do not allow any possible restructuration and/or relaxation of the clusters. This limitation is raised in the PDA model where the disaggregation and diffusion of weakly bonded particles is allowed. Also, the main differences

* Financially supported by the Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) de la República Argentina

between the present model and the DLDA merit a brief comment. In the DLDA the disaggregation-agregation procedure is a particle by particle process since during each time step only one particle disaggregated from a single loopless cluster is allowed to diffuse until it becomes attached again. On the other hand, the initial configuration for the PDA model, which is a SP distribution, involves many (and not necessarily loopless) clusters. Furthermore, in the PDA model the number of diffusing particles depends on the time.

The aim of this work is to study the effect of the disaggregation-aggregation process on some critical and structural properties of SP clusters. For this purpose the critical concentration, the correlation length exponent and the fractal and spreading dimensions have been evaluated using the Monte Carlo simulation in two dimensions. These results are presented and discussed in Sect. III, and the conclusions are stated in Sect. IV.

II. The PDA Model

The starting configuration corresponds to the classic SP model, i.e. it is obtained by filling the lattice with probability ϕ (each site can be either occupied by only one particle or empty). Let us only consider $n-n$ bonds between adjacent particles. In order to account for the disaggregation of weakly bonded particles only, the movement of particles linked by more than one bond is forbidden (in other words, a single movement of one particle could break at most only one bond). Then mobile particles (MP), which could participate in the diffusion process, are monomers (which have empty all their $n-n$ sites) and particles with only one $n-n$ occupied site. Note that disaggregation could also generate MPs and therefore the disaggregation-aggregation process involves more particles than those which were present in the starting configuration. Once the lattice has been filled the disaggregation-aggregation process is simulated as follow. At each Monte Carlo time step, a MP and one of its $n-n$ sites are chosed at random. If this site is unoccupied, the selected MP jumps to it. Otherwise, the MP remains fixed. The diffusion finishes when all the MPs have been exhausted. Then, in the final "static" configuration all the particles are linked by at least two bonds.

The Monte Carlo simulation has been carried out on $L\times L$ square lattices ($L\leqslant 201$) with periodic boundary conditions. For $\phi\cong 0.46$ and $L=201$ the final configuration is typically reached after 6×10^4 Monte Carlo time steps. For $L=201$ and for all values of ϕ, the statistic was made starting with about of 200–600 different initial configurations.

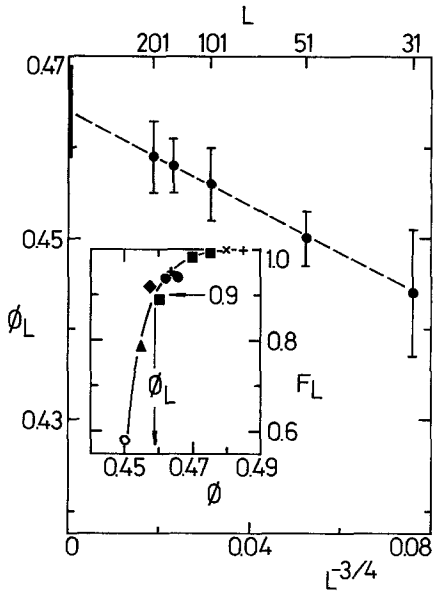

Fig. 1. Plot of the L-dependent threshold ϕ_L (see (2)) versus $L^{-3/4}$. The error bars take the uncertainties in the determination of each ϕ_L into account. The thick line on the left ordinate axis represents the extrapolated value of $\phi_c=0.464\pm 0.005$. The method employed in the determination of ϕ_L (see (1)) is shown in the inset for $L=201$. The points ○, ●, ◆, ■, ×, ▲, +, have been obtained averaging over 50, 100, 150, 200, 300, 500 and 750 samples respectively

III. Results

III.1. The Critical Concentration and the Correlation Length Exponent

Let us briefly explain the method employed to evaluate the critical concentration [7]. On a $L\times L$ lattice with periodic boundary conditions a percolating cluster is a cluster which has either its length or its width (or both) equal to L. Let F_L be the fraction of percolating clusters (see the inset of Fig. 1) and ϕ_L be the L-dependent threshold defined by

$$F_L(\phi_L)=0.9. \tag{1}$$

Now, using the finite-size scaling argument, one has [13]

$$\phi_c=\phi_L+AL^{-1/\nu}, \tag{2}$$

where ϕ_c is the critical concentration in the thermodynamic limit ($L=\infty$), A is a constant and ν is the correlation length exponent (viz. the correlation length ξ in the infinite system behaves as $\xi\propto(\phi-\phi_c)^{-\nu}$). Figure 1 shows a plot of ϕ_L against $L^{-3/4}$. The straight line obtained suggest that (see (2))

$$\nu=4/3, \tag{3}$$

that is, the same value than for SP. The discussion of the universality class of the PAD model will be

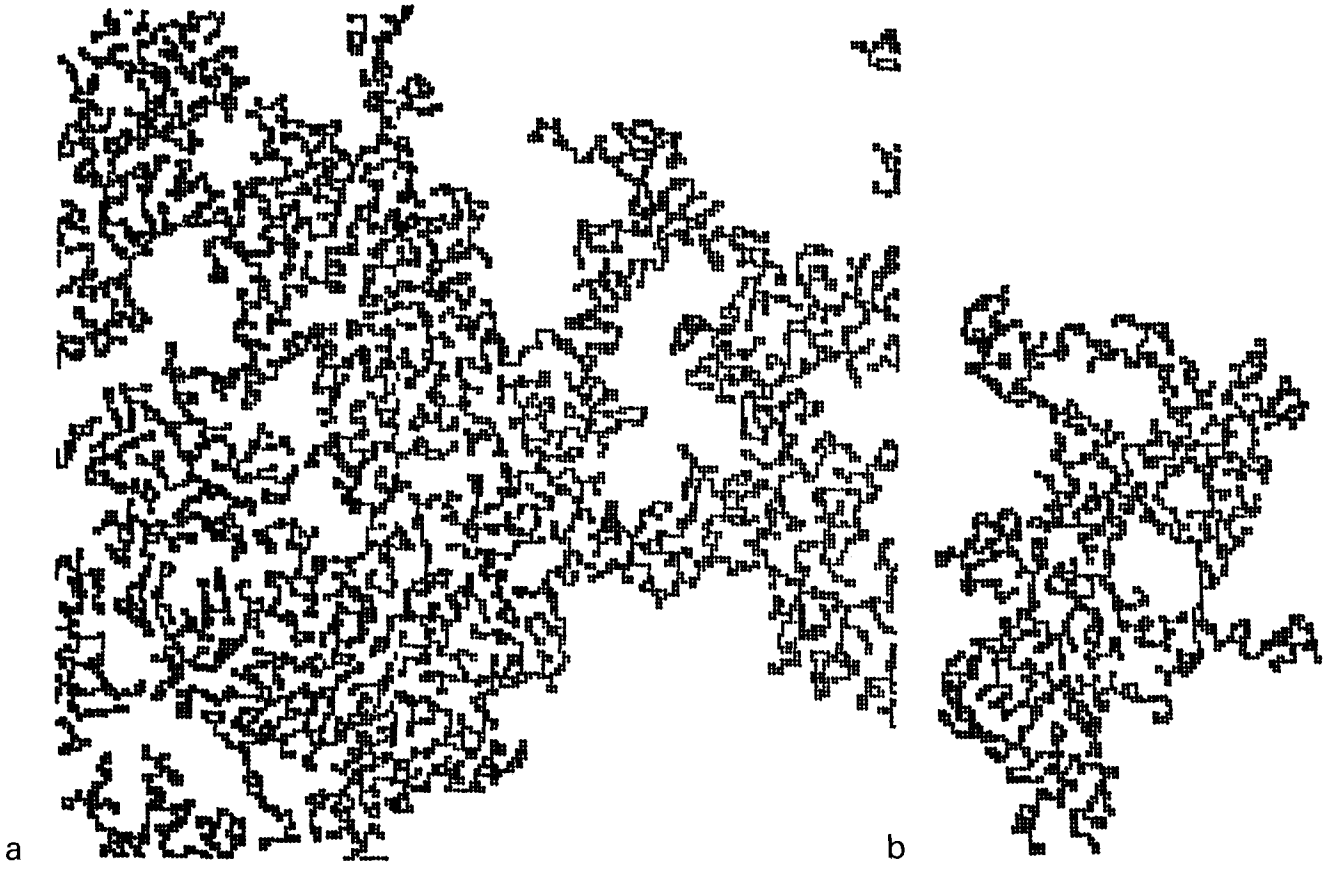

Fig. 2a and b. The final configuration of two largest clusters obtained working with $\phi=0.455$ and $L=201$ and starting with two different initial configurations. The cluster of **a** (**b**) has $S_a=11606$ ($S_b=3064$) particles respectively

presented later on. Also from Fig. 1 (and (2)) one obtains

$$\phi_c=0.464\pm0.005, \tag{4}$$

where the large error bar takes the possible correction to (2) due to finite-size effects into account. Let us stress that ϕ_c is appreciably smaller than the best available value of the critical probability $p_c=0.5927\pm0.0001$ (see for example [14] and references cited therein) for the SP model on the square lattice. The change in the critical concentration is a consequence of the disaggregation-aggregation process. In fact, a single diffusing particle can sticks together two (and sometime three) adjacent clusters. Furthermore, as the particles which can be disaggregated have at most one bond, the number of particles constituing a cluster can not be decreased by more than one at each Monte Carlo step. For these reasons, the aggregation process prevails over the disaggregation one, and the final static configuration of the PAD model is characterized by a considerable increment of the mean cluster size as compared to the cluster size distribution of the SP model at the same concentration. Note that the aggregation of monomers $(\phi_c(1-\phi_c)^4\cong0.04$, i.e. about of 4% of the total amount of particles of the starting configuration) is not relevant.

Figure 2 shows the largest clusters at $\phi=0.455$ ($L=201$) of two final configurations obtained by starting with different initial configurations. One of them is a percolating cluster which has $S_a=11606$ particles and the other has $S_b=3064$ particles. These values may be compared with the average number $S=8394$ (averaged over 500 samples) of particles of the largest cluster at the same concentration and lattice size. It should be mentioned that the fluctuation in the number of particles of the largest cluster at ϕ_c is about of the same order of magnitude than for SP at p_c. The configurations shown in Fig. 2 have been selected in order to point out that, even when S_a and S_b are quite different, the clusters have some structure similarity after a view inspection.

III.2. The Fractal Structure of the Incipient Percolating Cluster

In order to analyze the fractal structure of the largest cluster close to ϕ_c, its spreading and fractal dimensions have been evaluated.

III.2.1. The Spreading Dimension. Considering the infinite cluster at the critical concentration, let A_N be the average number of occupied sites connected by at most $N\,n-n$ bonds to a given origen in the cluster (N is the so called chemical distance). Then, for large N, A_N behaves as

$$A_N \sim N^{\hat{d}}, \tag{5}$$

where $\hat{d}$ is the spreading (or chemical) dimension (see for example [15]) which is an intrinsic exponent of the cluster.

In Fig. 3 a plot of A_N/N for the largest cluster against N is shown for the SP model at $p_c=0.5927$ and for the PDA model at $\phi_c=0.464$. Note that for the results of Fig. 3, $N \lesssim L/2$ in order to avoid boundary effects. The full straigth line in the figure corresponds to one of the best available values of $\hat{d}=1.675$ [16, 17] for the SP model. Although in the present work the lattice size is smaller than the one used in previous works for the determination of $\hat{d}$ for ordinary percolation, from Fig. 3 one clearly sees that for the PDA model the slope of A_N/N vs N asymptotically approach to that of ordinary percolation. This behaviour strongly suggests that both models have the same spreading dimension, at least within the accuracy of the Monte Carlo method.

III.2.2. The Fractal Dimension. For a fractal infinite cluster on the square lattice, the number M of particles inside a square of linear size l (centred in one point belonging to the cluster) scales as

$$M \sim l^D, \tag{6}$$

where D is the fractal dimension of that cluster (see for example [5]). Figure 4 shows the ln−ln plot of M/l^2 versus l for both, the SP and the PDA models, evaluated for the largest cluster at probability p and concentration ϕ slightly below to the critical values p_c and ϕ_c, respectively (this is an appropriate procedure for obtaining the fractal dimension [7]). For ordinary percolation a good straight line is obtained whose slope corresponds to

$$D=1.90\pm0.02, \tag{7}$$

which agrees with the exact and well known result $D=91/48\cong 1.896$ for this model.

For the PDA model the points do not show a well defined straight-line behaviour, as for the SP model. This result is a consequence of the change of the linear scale. In fact, for the SP model the smallest clusters are the monomers, while for the PDA model the smallest clusters, on the square lattice, are squares constituted by four particles. This means that the linear scale has been increased by a factor 2. Although this change of scale is not the same for different clusters, one could expect, at least in average, some kind of dilatation of the linear scale. Also, note that in Fig. 3 the asymptotic regime (full line) for the PDA model is reached for a larger value of N than that for the SP model. Following this point of view, the square lattice of size $L=201$ could be small in order to allow an accurate determination of the frac-

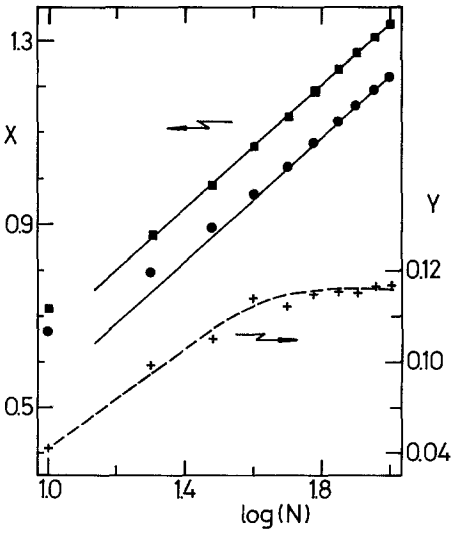

Fig. 3. The double logarithmic plot of $X=A_N/N$ versus N for the largest clusters of the SP model (■) and the PDA model (●) working with $p_c=0.5927$ and $\phi_c=0.464$, respectively. Results obtained on a square lattice of size 201×201 by averaging each point over 600 samples. The full straight line corresponds to the best available value of $\hat{d}=1.675$ for the SP model on the square lattice [16]. In the lower part of the figure the ratio $Y(+)$ between A_N for the SP model and A_N for the PDA model, is plotted against N in a double logarithmic scale. The dashed line has been drawn to guide the eyes. The behaviour of this line for large values of N strongly suggests that the incipient infinite clusters of both models have the same spreading dimension

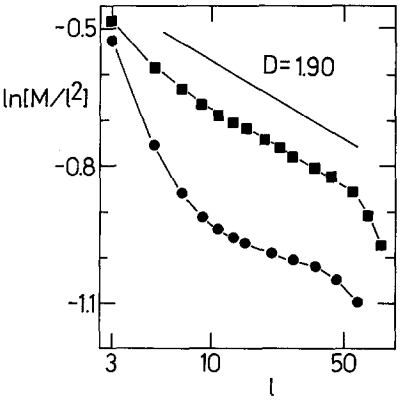

Fig. 4. The ln−ln plot of M/l^2 against l, using $L=201$, for the SP model (■), (averaged over 400 samples) and the PDA model (●), (averaged over 500 samples), working with $p=0.583$ and $\phi=0.455$ respectively. These figures have been taken slightly smaller than the respective critical values ($p_c=0.5927$, $\phi_c=0.464$). The full line with slope $D=1.9$ has been drawn to guide the eyes

tal dimension. For further details see that the M/l^2 vs l line for the SP model has three well defined regions: the first one for small values of l which has a large slope, an intermediate region where the slope corresponds to $D=1.90$, and a curved region due to boundary effects (the lattice is finite and $p<p_c$). In the PDA model the first region becomes enlarged with respect to that of the SP model and as the boundary effects are also present, it is very difficult to obtain a precise value of D. Unfortunately, to work with larger lattices is beyond our computational capacity. In spite of this difficulty, from Fig. 3 one obtains

$$D=1.90\pm0.06 \tag{8}$$

which agrees within the error bars with the value of the SP model.

IV. Summary

A new model of percolation is introduced and studied by means of the Monte Carlo simulation on the square lattice. In this model (called the percolation with disaggregation and aggregation (PDA) model), a transient dynamic disaggregation and diffusion process of single bonded particles, which also involves the monomers, leads to the formation of statics aggregates. The proposed model can be thought of as a certain kind of $m=2$ BP model with diffusion.

The results obtained for the correlation length exponent ν (see (3)), the spreading dimension $\hat{d}$ (see Fig. 3) and the fractal dimension D (see (8)), suggest that the new model belongs to the same universality class than the SP model. Also, this seems to be the case of the BP model with $m=2$ [10]. But, since the rules of these three models are quite different, this is not at all a trivial result.

The critical concentration ϕ_c for the PDA model on the square lattice $\phi_c=0.464$ (see (4)) is appreciably smaller than the critical probability $p_c=0.5927$ for the SP model on the same lattice. This fact is due to the disaggregation-aggregation process (see also below of (4)).

On the other hand, in both, the DLAD and the PDA models, only single bonded particles can be disaggregated form the clusters. Nevertheless, in contrast to the DPA model which belongs to the same universality class than the SP model, the DLAD model seems to have the same universality class than lattice animals [11, 12].

We would like to thank to L. Molinari for her precious help in the preparation of the graphics.

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