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1983 J. Phys. A: Math. Gen. 16 L647

(http://iopscience.iop.org/0305-4470/16/17/003)

J. Phys. A: Math. Gen. **16** (1983) L647–L652. Printed in Great Britain

LETTER TO THE EDITOR

Fractal models for diffusion controlled aggregation

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Received 8 September 1983

Abstract. A two-dimensional fractal model is constructed for diffusion controlled deposition on a surface. The fractal geometry of the deposit and the power law behaviour of the quantities characterising the non-equilibrium cluster size distribution are shown to be consequences of the competition generally present in a nonlinear growth process. A qualitative agreement with previous numerical results is found and the scaling laws for the critical exponents of the problem are shown to be satisfied exactly.

The study of the geometry and statistics of clusters in an equilibrium system belongs to the standard approaches of statistical physics. Properties of correlated and random equilibrium clusters have been reviewed in Müller-Krumbhaar (1979), Essam (1980), Stauffer (1979) and Stanley *et al* (1982).

Recently interest has grown in the investigation of clusters formed as a result of an irreversible kinetic process. These non-equilibrium clusters appear in a wide variety of problems such as coagulation of smoke particles (Witten and Sander 1981), the early stage of nucleation (Klein 1981), sol–gel transition (Herrmann *et al* 1982) and red blood cell aggregation (Wiegel and Perelson 1982). A characteristic feature of these irreversible processes is a nonlinear competition between the neighbouring parts of a large growing cluster or among clusters growing simultaneously in the system. Here the term nonlinear competition corresponds to a process in which at first two or several clusters (or branches of a cluster) grow relatively independently, but at a later stage all but one of these clusters stop growing, being almost entirely suppressed by the largest cluster (branch). This usually happens when the range of interaction or screening length of the clusters (branches) becomes comparable to the distance between two clusters (branches). The aim of this letter is to show how fractal geometry and scaling properties are generated by competitive growth processes of this kind.

Recently a growth model called diffusion controlled aggregation was introduced by Witten and Sander (1981, 1983) in which an unstable growth of branches within one large cluster was observed. The rules of this model are quite simple. The process is started with an initial seed particle at a lattice point. Another particle is allowed to walk at random (i.e. diffuse) from far away until it arrives at one of the lattice sites adjacent to the occupied site. Then it is stopped; another particle is launched and halted when adjacent to the two occupied sites, and so forth.

In their Monte Carlo simulations Witten and Sander (1981, 1983) found that in large clusters formed in this way the density correlations decay algebraically. In the further computer experiments of Meakin (1983a) the fractal dimension (Mandelbrot 1977) of such aggregates was also determined in dimensions $d = 2$ to 6. Results of

the recent mean field (Muthukumar 1983) and renormalisation group calculations (Gould *et al* 1983) agree well with the simulations.

In order to have a qualitative insight into the events going on during the diffusion controlled deposition we build up a regular model reflecting the two main features of the process: growth and freezing in (stopping further growth) of the clusters or branches of a cluster. In addition, a regular model has the advantage that we can obtain explicit expressions for the quantities of interest.

For our purposes a two-dimensional version of the original model is more suitable, in which instead of having one seed particle we have at the beginning a whole straight line of occupied sites (seed particles) playing the role of a surface (figure 1). This model has very recently been investigated by Meakin (1983b), who determined the root-mean-square thickness exponent of the deposit, and was independently proposed by Rácz and Vicsek (1983) in order to study non-equilibrium cluster distribution. The clusters are generated in this process in a natural way. A particle sticking to the surface forms a basis for a new, tree-like cluster growing as more particles are launched. During the growth process two such clusters are very unlikely to join; nevertheless, if it happens, they are regarded as one new cluster.

Figure 1. Clusters generated in a small scale Monte Carlo simulation. As the number of particles M added by a diffusion controlled aggregation process is increased, the relatively small clusters stop growing since they become suppressed by the neighbouring larger clusters. In this figure M denotes the number of particles in the deposit normalised by the length of the substrate.

In figure 1, configurations of a small scale Monte Carlo simulation of this model are shown for four increasing values of the number of particles added by the diffusion controlled rule. This diagram demonstrates the growth and the following freezing in of the small clusters during the process. Now we try to imitate this kind of aggregation with the help of a regular construction. Let us imagine that the first particles fill every third site nearest to the surface (figure 2), each of them forming a basis for a new tree. If one of these sites starts growing it suppresses the growth of the nearest neighbouring sites. Therefore, we allow the growth of every third site in the first row. These clusters continue growing until the screening length l_{sc} of the trees (clusters) becomes comparable to the distance between them. As l_{sc} and the height of the clusters

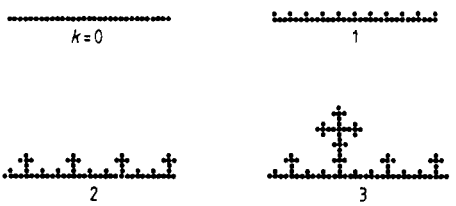

Figure 2. Subsequent steps made in the process of constructing a regular model for the diffusion controlled deposition on a one-dimensional surface.

h are of the same order, we suppose that when h becomes equal to half of the distance between the trees, a new stage of the growth process is started. Every third cluster continues growing and the neighbours will be suppressed. (Branches of the clusters grow according to the same principle.) As a result a system of ramified clusters, some of which grow infinitely large, is obtained.

The most striking feature of the configuration produced in this way is that it has essentially the same structure as one of the simplest fractals, shown in figure 3. In both fractals the basic cell has the shape of a square divided into nine equal parts, but only five out of these nine parts are retained when in the process of generating the fractal further steps are made. The only difference is that in the first case (figure 2) the fractal is obtained in the $L \to \infty$ limit (where L is the linear size of the regular cluster measured in the lattice units), while in the case of the division of a square (figure 3) the $\varepsilon \to 0$ limit must be taken (where ε denotes the linear size of the squares after subsequent divisions). In other words, a fractal imitating the diffusion controlled aggregation process is produced by repeating firstly the original cell (consisting of five particles) according to the configuration of particles within this cell, then repeating this new cell according to the configuration of the original unit cell and doing so *ad infinitum*. This process results in a fractal corresponding to an aggregate grown from one seed particle. Properties of the deposits can be derived from this model. This is discussed later in the paper.

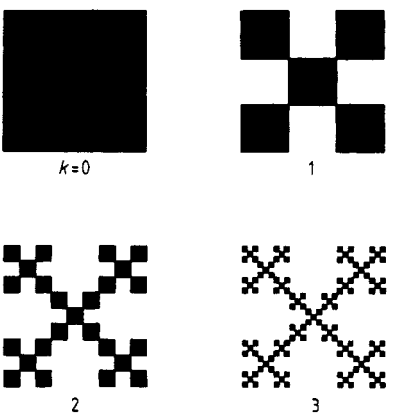

Figure 3. Successive stages of generating a fractal having essentially the same geometry as the regular model shown in figure 2.

Now it is possible to calculate the fractal dimension D of our regular aggregate. D is defined by the expression

$$D = \lim_{L\to\infty} (\ln M(L)/\ln L), \tag{1}$$

where $M(L)$ is the number of particles in a model aggregate of linear size equal to L. If the size of the unit cell of a fractal is denoted by l and the number of sites in this cell is equal to m, then, as the subsequent stages are generated, L and $M(L)$ increase according to $L = l^k$ and $M(L) = m^k$, where k is the number of steps made in the process of producing the fractal.

Substitution into (1) gives

$$D = \ln m/\ln l \tag{2}$$

and for the fractal dimension of our model we get $D = \ln 5/\ln 3 = 1.465\ldots$. The corresponding Monte Carlo result $D \sim 1.67$ (Meakin 1983a) is somewhat higher. However, better agreement can be achieved by choosing larger, less simplified unit cells. Fractals generated using the unit cells shown in figure 4 have fractal dimension $D = 1.561\ldots$, $D = 1.654\ldots$ and $D = 1.672\ldots$ respectively, and have an aggregate like structure at the same time.

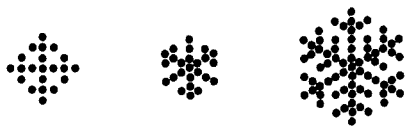

Figure 4. Unit cells defining aggregate-like regular fractals of dimension (*a*) $D = 1.561\ldots$, (*b*) $D = 1.654\ldots$, (*c*) $D = 1.672\ldots$.

The most important feature of the fractal model described above (figure 2) is that it is possible to get explicit expressions for the quantities characterising the statistics of clusters defined in the deposition model. In order to treat the statistics of clusters on a surface we define n_s as the number of clusters consisting of s sites divided by the length of the substrate and the quantity $S = \Sigma_s s^2 n_s/\Sigma_s s n_s$ which we shall call the mean cluster size. These quantities are analogous to those used in percolation theory for the description of the statistics of random equilibrium clusters. There are only a few works on non-equilibrium cluster distribution. Binder and Stauffer (1976) in an Ising system and Jan *et al* (1983) in a kinetic gelation simulation observed a qualitative difference between the equilibrium and the non-equilibrium cluster size distributions.

From the construction of figure 2 it follows that in the subsequent stages of the growth process clusters consisting of $s(k) = \Sigma_{j=1}^{k} 5^{j-1} = (5^k - 1)/4 \sim 5^k$ sites are generated, where k denotes the number of iterations completed. The number of clusters $n_{s(k)}$ consisting of $s(k)$ sites is proportional to $(\frac{1}{3})^k$. In the random deposition model Monte Carlo simulations indicate that for large s values the expression $n_s \sim s^{-\tau}$ applies. The exponent τ in our system can be calculated from

$$\tau = -\ln(n_{s(k)}/\Delta s(k))/\ln s(k) = -\ln((\tfrac{1}{3})^k/5^k)/\ln 5^k = 1.682\ldots \tag{3}$$

where the cluster numbers $n_{s(k)}$ have been normalised by the factor $\Delta s(k) \sim 5^k$ proportional to the difference of two subsequent cluster sizes $s(k)$, since in (3) $n_{s(k)}$ is regarded

as the number of $s(k)$ clusters in a given interval of the cluster sizes. The value $\tau = 1.682\ldots$ is in qualitative agreement with the simulation result $\tau \approx 1.4$ (Rácz and Vicsek 1983) and is definitely less than 2, which is the smallest value of τ allowed in an equilibrium system. For $S(k)$ we obtain

$$S(k) = \sum_{j=1}^{k} s^2(j) n_{s(j)} \Big/ \sum_{j=1}^{k} s(j) n_{s(j)} \sim 5^k.$$

Writing $S(k)$ in the form $S(k) \sim N^{\gamma}$ (where the control parameter $N \sim (\frac{5}{3})^k$ is the number of sites in the clusters) we get for the exponent γ

$$\gamma = \ln 5/(\ln 5 - \ln 3) = 3.150\ldots. \tag{4}$$

Finally, we introduce an exponent denoted by σ in percolation theory and defined by the expression $s_\xi \sim N^{1/\sigma}$, where s_ξ is the typical cluster size giving the main contribution to the singular sums such as $S(k)$. In our model $s_\xi \sim 5^k$ since the cluster sizes diverge as a geometrical progression and the sums are always determined by the last term of the series. From here

$$\sigma = \ln N/\ln s_\xi = (\ln 5 - \ln 3)/\ln 5 = 0.317\ldots. \tag{5}$$

Assuming a scaling ansatz of the form $n_s \sim s^{-\tau} f(s^\sigma/N)$ for the cluster distribution in the random deposition model, Rácz and Vicsek (1983) obtain the following scaling laws for the exponents γ, τ and σ:

$$\gamma = 1/\sigma \qquad \text{and} \qquad 2 - \tau = \sigma. \tag{6}$$

Substitution of (3), (4) and (5) into (6) results in identities, demonstrating the internal consistence of our fractal model and its relevance to the description of non-equilibrium cluster distribution.

In conclusion, a regular construction of clusters using rules which simulate the competitive growth process present in the two-dimensional diffusion controlled deposition model has been shown to result in a fractal and in a non-equilibrium cluster distribution with scaling properties. Due to the simple assumptions of the aggregation process a wide variety of competitive growth models is expected to exhibit analogous behaviour.

The author thanks Z Rácz for useful discussions.

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