PHYSICAL REVIEW E VOLUME 57, NUMBER 5 MAY 1998

Probability distribution of m-branch subsets in diffusion-limited aggregation

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(Received 2 June 1997; revised manuscript received 21 November 1997)

This is an attempt to redefine m-branch subsets in off-lattice two-dimensional diffusion-limited aggregation simulations, where m is the number of particles of a branch which lacks a hierarchy of order. In our simulations, the total number of aggregated particles N behaves as $N=(2R)^D$, where R is the radius of gyration of the cluster and D is the fractal dimension. The number of m-branch subsets $M_m(R)$ depends on R as $M_m(R)=A_mR^D$ and the subsets are D-dimensional self-similar fractals. These results show that the probability distribution of the subsets is stable, and has a peak at $m=2$, and that the subset at $m=2$ is the most observable of all the subsets independent of time. [S1063-651X(98)04705-9]

PACS number(s): 61.43.Hv, 05.45.+b

INTRODUCTION

Since the notation of a fractal was contrived, its beautiful characteristics have fascinated many scientists [1]. Not only mathematical and geometrical models, but also many objects in nature such as clouds, mountains, lightning, and galaxies, reveal their fractals. An understanding of the physical origin and the mechanism of fractals, however, is not so simple in many cases despite their clear appearance. This is owing to their complicated systems.

Among those systems, DLA (diffusion-limited aggregation) is relatively simple because the only thing that counts is its diffusion field. Since the simulation by Witten and Sander [2], DLA has been vigorously investigated by means of computer simulations, theoretical analysis, and experiments [3]. Many investigations have been reported relating to the fractal dimension, generalized dimension (f-α spectrum), anisotropy of the simulated lattice, irregularly branched structures, and morphological transitions among the other observable clusters in the diffusion field. An understanding of these has revealed the physical mechanism of the long ranged self-similarity and the determination of the fractal dimension. Several theoretical approaches have been introduced, for example, mean-field approaches, field theories, real-space renormalization group, fixed-scale transformation, and dynamical analysis between branches [4].

In spite of the achievement of such approaches, many problems remain. We focus on the branching structures of DLA. Studies of these structures have usually been based on a hierarchy of branch orders relating to the Horton-Strahler ordering [5,6]. It has been reported that the bifurcation ratio and the length ratio are constants, and that the similarity dimension estimated from the two ratios is nearly identical with the fractal dimension of the DLA cluster itself [7–9]. Other ordered branching structures have been recently reported, and it is argued that the maximum entropy formalism in equilibrium statistical physics derives from the branching distribution [10].

On the other hand, the branching structures are not limited to ordered branches. Dynamical branching structures without any ordered hierarchy have been studied about self-similar fractal patterns created by iterated contraction map with multiscaling factors [11]. Each branch has the probability measure defined as its length to the total length of the pattern. The probability decays exponentially with iteration time, and the subset which has the same decay exponent is a self-similar fractal. The maximum value of the fractal dimensions of all the subsets coincides with the similarity dimension of the pattern. Furthermore, by considering the increasing exponent of the number of branches in the subset, topological entropy has been calculated. Then an entropy spectrum from the above two exponents has been obtained; but that of DLA has not yet been reported on. In order to study the dynamical branching structures of DLA such as the entropy spectrum, we report in this paper on branching structures of DLA which lack any ordered hierarchy.

SIMULATIONS

The algorithms in our off-lattice two-dimensional DLA simulations are similar to those in Ref. [12], except for the flight distance of a random walker $d=d_{\min}-kl$, where $d_{\min}$ is

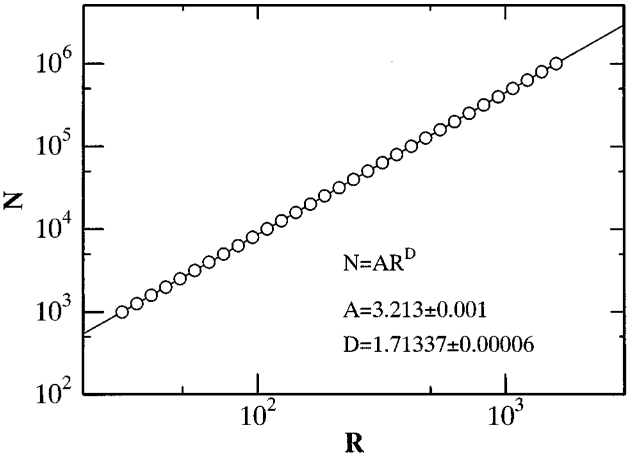

FIG. 1. Radius of gyration R vs particle number N. The relation $N=AR^D$ is written as $N=(2R)^D$; $A=3.213\pm0.001$ and $D=1.713\,37\pm0.000\,06$.

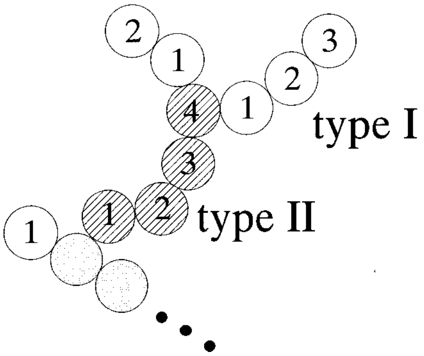

FIG. 2. Definition of the m branch. The numbering begins from a bifurcated particle. Type I (open circles) has a tip, and type II (hatched circles) has no tip.

the distance from a random walker to the closest aggregated particle, k representing some factor, and l being the diameter of the particle. The simulation can be carried out exactly when k is unity, although it takes much time. This occurs very rarely, however, because it is a point contact. In the simulations of Ref. [12], k is chosen as 0.8, and the aggregated particles are permitted to overlap. In their simulations, overlapped portions decrease as the cluster size increases. We use k as 0.995, and modify the positions of the newly aggregated particles so that they do not overlap. When k goes from 0.8 to unity, the fractal dimension D shows little change but the coefficient A ($N=AR^D$, where N is the total number of aggregated particles and R is the radius of gyration) changes slightly and approaches some value.

RESULTS AND DISCUSSION

We simulated $N_{\rm av}$ off-lattice two-dimensional DLA clusters of N particles at $k=0.995$, where $N_{\rm av}=1.2\times10^6$ for $N=10^3$, $N_{\rm av}=2\times10^5$ for $1259\leq N\leq10^4$, $N_{\rm av}=2\times10^4$ for $12\,589\leq N\leq10^5$, and $N_{\rm av}=2\times10^3$ for $125\,893\leq N\leq10^6$. We used 31 different values of N from 10^3 to 10^6.

In Fig. 1, we show the relation $N=AR^D$. Since these data are from $N_{\rm av}$ clusters for fixed N particles, R is the average value. To the best of our knowledge, the value $D=1.713\,37\pm0.000\,06$ coincides with the reported results [13], though we know of no reports about the value of A. The result of $A=3.213\pm0.001$ implies that we can put $N=(2R)^D$ because $2^D=3.279\cong A$. Strictly speaking, the line in Fig. 1 is slightly curved. Then, for larger R, the values of A and D become larger and smaller, respectively. We believe that for a larger DLA cluster at $k=1$, the above relation might hold exactly. The relation represents the definition of the self-similar fractal, and the value $2R$ is recognized as the size of the cluster measured with the minimum scale (the particle diameter is equal to 1). However, $2R$ does not correspond to, and in fact is less than, the DLA size. In general, the radius of gyration of the D_c-dimensional homogeneous fractal cluster is smaller than the radius of the cluster, and the ratio is $1/\sqrt{1+2/D_c}$ in two-dimensional space. Furthermore, the outer region of the DLA cluster (an active zone) does not complete D-dimensional self-similar formation [4–16]. Considering that the dimension of the active zone is about 0.9 [15], and that of the frozen zone is about 1.6 [16], the ratio is larger than the homogeneous case. Thus the mechanism of the above relation is an open question at present. It is clear, however, that the value $2R$ corresponds to the cluster size if N particles form a complete self-similar fractal cluster whose dimension is D.

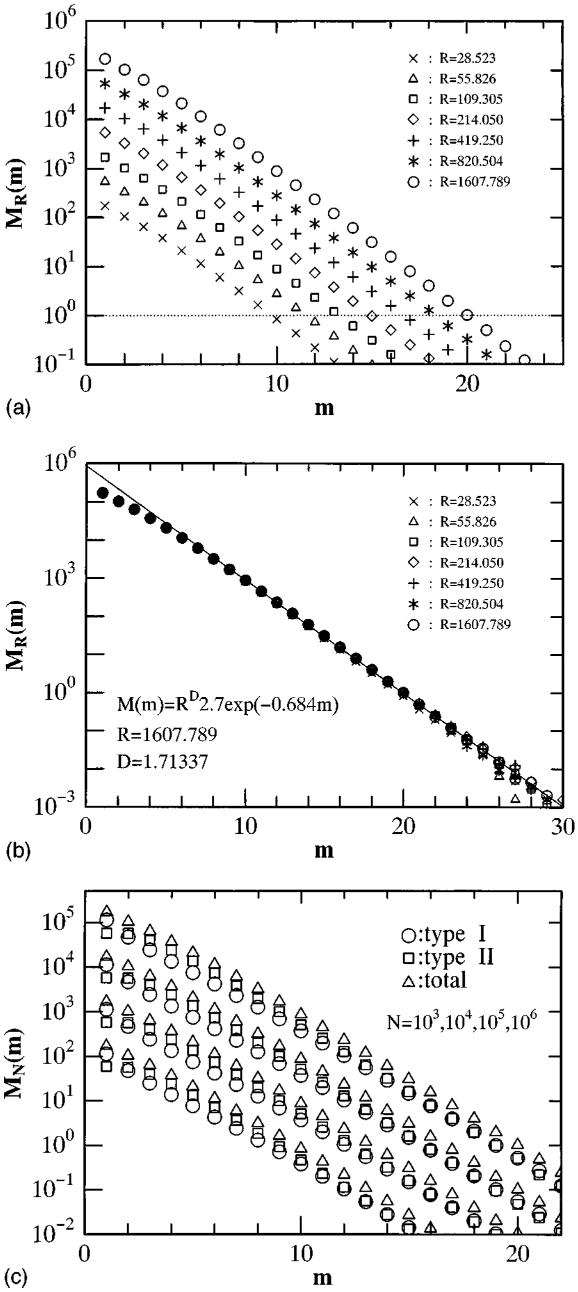

FIG. 3. (a) Branching distributions for seven cluster sizes. $M_R(m)$ is averaged and can be smaller than unity [the dashed line is $M_R(m)=1$]. (b) Scaled $M_R(m)$ to cluster size $R=1607.789$. $M_R(m)$ decays exponentially for larger m. (c) Detailed branching distributions for various N. The distribution of types I and II is also scaled.

Now we have divided the DLA cluster into m-branch subsets $S_R(m)$. We characterize a branch as m, the particle number of the branch (Fig. 2). There are two types of branches; branches with a tip (type I), and branches without

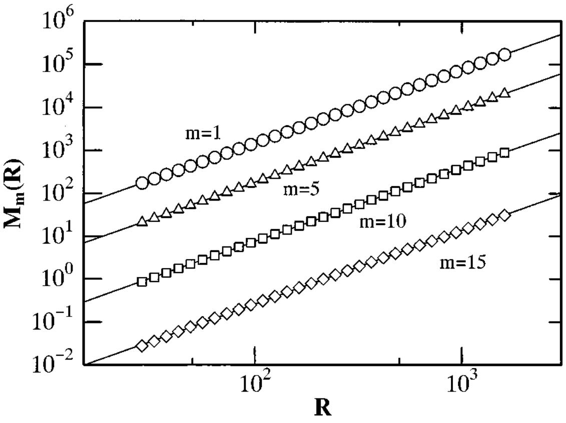

FIG. 4. The increase of some m-branch subsets. All of the subsets are D- dimensional fractals.

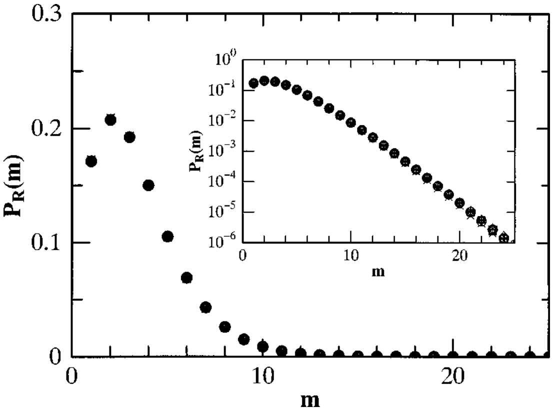

FIG. 5. Probability distribution of m-branch subsets. Seven kinds of symbols used in Fig. 3(a) are overlapped. The inset is for semilog plots. The distribution is almost stable.

a tip (type II), as shown in Fig. 2. Branches of type I can grow longer, but those of type II split (bifurcate) only.

In Fig. 3(a), we show the number of m-branch subsets $M_R(m)$ for various values of R. Since the data are for N_{av} clusters, $M_R(m)$ is the average value and can be smaller than unity. The branching of DLA consists mainly of one-particle branches, and $M_R(m)$ decreases as m becomes larger. As the cluster grows larger, longer branches appear in turn. This behavior suggests that plural contraction rates exist in DLA in the sense of a contraction map. In the case of a contraction map with a fixed contraction rate, only one new size appears when the pattern grows. In contraction maps with plural contraction rates, both the number of m branches and the kind of branches exponentially increase to the iteration time [11]. In the case of DLA, however, the number of m branches increases exponentially, but the appearance rate of the kind of m branch is smaller if we suppose that the DLA time is ln(R). This difference may yield a delicate correspondence between the contraction map and DLA. The branching distributions are scaled, and we show the scaled plots in the case of $R=1607.789$ ($N=10^6$) in Fig. 3(b); $M_R(m) = (N_R/N_{R_i})M_{R_i}(m) = (R/R_i)^D M_{R_i}(m)$, where R_i is for other clusters. For larger m ($m \geqslant 10$) $M_R(m)$ decays exponentially [the line in Fig. 3(b)], whereas for smaller m its behavior is not so simple. In Fig. 3(c), we also show $M(m)$'s of types I and II, and total branches for $N=10^3$, 10^4, 10^5, and 10^6 clusters. The distributions of type-I and -II branches are also scaled. In the case of $m=1$, the number of branches of type I is larger than that of type II. The opposite is true if m is from 2 to about 16. Both are almost the same for $m \geqslant 16$. This complicated behavior might be understood in the light of the branching dynamics of DLA. By considering the sticking probability of a random walker at the l (integer)th aggregated particle in an m branch $P(l;m)$, we can discuss the branching dynamics. $M_R(m)$ can be represented by $P(l;m)$. For example, $M_R(m)$ for a type-I branch excluding $m=1$ has increasing terms and decreasing terms. The increasing terms are related to tip-growing behavior $P(m-1;m-1)$, and branch-splitting behaviors $P(m;m+k)$ and $P(k;m+k)$ ($k=1,2,\ldots$). On the other hand, the decreasing terms are related to $P(k;m)$ ($k=1,2,\ldots,m$). We have simulated $P(l;m)$, and our results indicate that decreasing terms are nearly compensated for by the tip growing behavior. We will report on the detailed branching dynamics related to $P(l;m)$ elsewhere.

In Fig. 4, we show the R dependence of the number of the m-branch subset $M_m(R)$, which increases with $R^{D(m)}$. As the value of $D(m)$ is limited from 1.712 ($m=1$) to 1.733 ($m=20$), we can conclude that $D(m)$ is equal to D. Then we can put $M_m(R)=A_m R^D$. This result indicates that the DLA cluster is composed of m-branch self-similar subsets whose dimension is the same as that of the DLA itself. As mentioned above, in studies with a hierarchy of order, there are some scaling results. Note, however, that our m-branch subset is defined without such an ordering, and indicates that the scaling exponent is D.

This result also implies that the probability distribution of m-branch subsets $P_R(m)$ is stable because $P_R(m) = mM_R(m)/N_R = mA_m R^D/AR^D = mA_m/A$. In order to confirm the result, we show the probability distribution $P_R(m)$ for seven different cluster sizes in Fig. 5. The cluster sizes and the symbols are the same as those in Fig. 3(a), and the inset is for semilog plots. The data are almost coincident. In this distribution, there appears smaller $P_R(m)$ of larger m with increasing R. Strictly speaking, $P_R(m)$ of a smaller m changes in the presence of $P_R(m)$ of a new larger m. However, $P_R(m)$ of a smaller m is hardly influenced, because $P_R(m)$ of a larger m is much smaller. Indeed, $P(2)$ is 0.207 435 and $P(20)$ is 2.03×10^{-5} at $R=1607.789$. $P_R(m)$ has its maximum value at $m=2$. From this result it appears that there might exist a ''characteristic length $m=2$'' contrary to fractal DLA. However, $P_R(m)$ corresponds to the probability of an m-branch subset, and the maximum $P_R(m)$ means the most observable (or remarkable) m-branch subset in the cluster. In the case of a contraction map [11], such a subset is obtained for fixed k/n, where n is iteration time and k is some integer: $0 \leqslant k \leqslant n$. This implies that the most observable branch in real space changes in time, and that only such a subset remains when the time is infinity. Such a subset of DLA, though, does not depend on time. We will report in a future thesis on the most observable subset ($m=2$) focusing on entropy spectrum of DLA.

CONCLUSION

In conclusion, from the two-dimensional off-lattice DLA simulation at $k=0.995$, we have found the following. (i) The relation $N=(2R)^D$ holds. (ii) We can redefine an m-branch subset without a hierarchy of order. A DLA cluster is composed of many self-similar m-branch subsets whose dimensions have the same values as the DLA cluster. (iii) In such subsets, the most observable subset arises when $m=2$ independently of the cluster size, and their probability distribution is stable.

ACKNOWLEDGMENTS

We would like to thank Professor K. Honda and Professor M. Sano for many suggestive discussions. One of us (H.H.) is also indebted to Professor T. Vicsek and Dr. Z. Csahók for their useful comments and instructive discussions. We are also thankful to Professor P. Rawlings and Professor Y. Suzuki for their suggestions on the style of the present paper.

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