Entropy spectrum for distribution of history probabilities in growth models

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Based on the multifractal formalism, we introduce a multifractal spectrum associated with entropy of clusters in growth models by calculating probability distributions of histories from an initial seed to a resultant cluster. The entropy spectrum is shown in a ballistic growth model producing fanlike clusters and Eden growth as examples. Numerical calculations of the models give results that suggest the existence of phase transitions in the spectrum. [S1063-651X(97)09506-8]

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Considerable theoretical and experimental efforts have been undertaken to investigate scaling properties of fractal clusters and rough surfaces of compact clusters in the past few years [1]. Although our understanding of geometrical features of clusters is advanced by these efforts, most of them study only resultant patterns as snapshots at a moment rather than growth itself. For instance, the $f(\alpha)$ spectrum [2] of diffusion-limited aggregation (DLA) [3] gives us some information about the distribution of active or unscreened sites at the surface, but one could hardly predict how the pattern evolves. In such an analysis, one assumes that patterns should be self-similar in every time step and the fractal clusters are most probable. However, in what sense could we confirm that our observing patterns are so generic and most probable? To understand that, one has to take into account a huge number of possible ways of growth and those probabilities. Recently, Elezgaray *et al.* have introduced the ''history probability,'' that is, the probability of finding a history from a seed particle to a resultant cluster, and studied morphology selection mechanism of Laplacian growth [4]. If the distribution of history probabilities is given in some invariant form independent of the number of particles, one can know how often a cluster to be examined is observed in all possible patterns. To our knowledge, there is no formulation to characterize such statistics of clusters, except for a few studies on entropy [4–6]. Our primary purpose in this Brief Report is to give a general formalism of the distribution of history probabilities for stochastic growth models in a similar way to the analysis of chaotic orbits in dynamical systems, i.e., the multifractal spectrum of entropy [7,8]. In addition, we would like to show a few examples for the formulation in well-known models.

Let us consider a growth model starting with a single seed particle on a lattice. Let σ_m be a cluster consisting of m particles and $p(\{\sigma_m\})$ be the probability of finding a history set $\{\sigma_m\}$. Assuming that the conditional probability that σ_m becomes σ_{m+1} is proportional to its mass m at the some power γ, the history probability takes the form

$$p(\{\sigma_1,\sigma_2,\ldots,\sigma_{m+1}\}) \sim C^{-m}(m!)^{-\gamma}, \tag{1}$$

where $m!$ denotes the factorial of m and C is a constant depending on the details of the growth rules and lattice structure. We have checked numerically the validity of this assumption for Eden clusters [9] and DLA clusters on a two-dimensional square lattice. The dependence of history probabilities on m obtained numerically is shown in Fig. 1. In these plots, only one typical growth process was sampled and we did not make any averaging. However, the scaling in

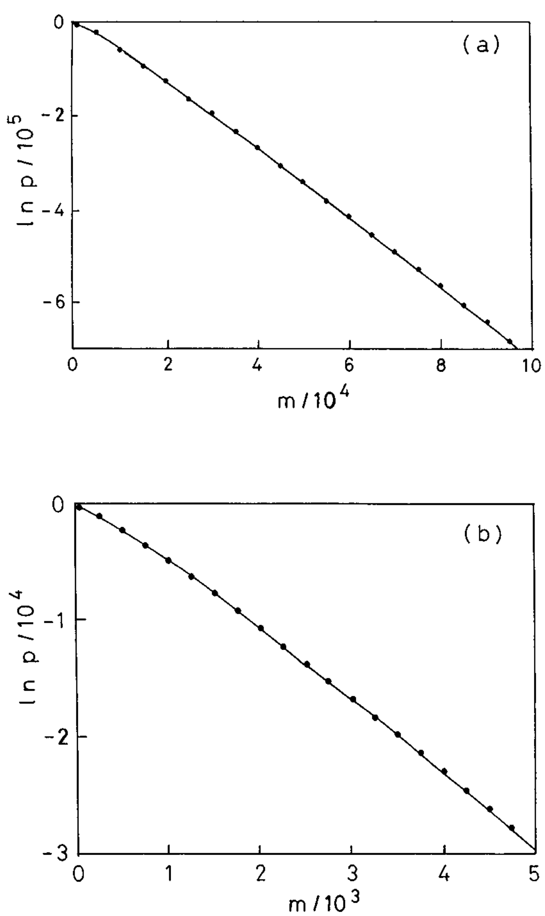

FIG. 1. Dependence of ln$p$ on m for (a) an Eden cluster and (b) a DLA cluster. The numerical data denoted by the solid circle are in an excellent agreement with the solid line based on Eq. (1).

Eq. (1) seems to hold very nicely. The fitting parameters are $C=6.70$ and $\gamma=0.509$ for an Eden cluster and $C=3.54$ and $\gamma=0.608$ for a DLA cluster using a least-squares method.

When the history probability is proportional to $(m!)^{-\gamma}$, the number N_γ of histories that have the same index γ will be also scaled as $(m!)^{h(\gamma)}$. We write a partition function as

$$Z_m(q)=\sum_{\{\sigma_n\}} p(\{\sigma_1,\ldots,\sigma_m\})^q, \tag{2}$$

where the sum is taken over all possible histories from σ_1 to σ_m. The entropy of the qth order K_q is defined by

$$K_q=\lim_{m\to\infty} -\frac{1}{q-1}\frac{\ln Z_{m+1}(q)}{\ln m!}. \tag{3}$$

One can easily obtain h and γ via the Legendre transform

$$\gamma(q)=\frac{d}{dq}\tau_q, \quad h(q)=q\gamma(q)-\tau_q, \tag{4}$$

with $\tau_q=(q-1)K_q$. The most natural definition of entropy may be given from an ensemble average of $\ln p(\sigma_m)$ taken over equal-size clusters, where $p(\sigma_m)$ is the probability of finding σ_m [5]. However, it is difficult to estimate $p(\sigma_m)$ accurately because there is a huge number of paths from an initial seed to σ_m. By contrast, the history probability $p(\{\sigma_1,\ldots,\sigma_m\})$ can be estimated accurately even for large m when the transition probability to the next cluster is given.

Let p_γ be the history probability scaled as $(m!)^{-\gamma}$. Then the probability of finding the index γ is given by $N_\gamma p_\gamma$, which is scaled as $(m!)^{-\nu}$ with $\nu=\gamma-h(\gamma)$. The exponent ν is not negative because the probability cannot exceed unity. All history probabilities except $\nu=0$ will decay, which implies that only the history with $\gamma=\gamma(1)$ will be observed in the limit $m\to\infty$.

We apply the method to a few examples. We first consider a ballistic aggregate growth model on a two-dimensional square lattice. A seed particle is put into the origin of the lattice and the rest of the particles move parallel to the y axis with random x coordinates until they either escape from or stick to the cluster [10]. The particles cannot stick on the $y=0$ line except at the origin. This process leads to a fanlike structure. Let L_m be the horizontal size of a cluster σ_m. Then the particles stick to the cluster at one of L_m+2 sites of the surface. The history probability from σ_1 to σ_m is determined from a set of horizontal sizes $\{L_1,L_2,\ldots,L_m\}$. Considering histories whose resultant cluster has the horizontal size L and mass m, the history probability p and the number of histories N are of the forms

$$p(\{L_1,\ldots,L_m\})=3^{-n_1}4^{-n_2}\cdots(L+2)^{-n_L}, \tag{5}$$

$$N(\{L_1,\ldots,L_m\})=1^{n_1-1}\times 2\times 2^{n_2-1}\times 2\cdots(L-1)^{n_{L-1}-1}\times 2\times L^{n_L}, \tag{6}$$

where n_k is the number of particles that stick to the cluster with horizontal size k. Here the conditions $n_1+n_2+\cdots+n_L=m-1$, $1\leqslant n_1,\ldots,n_{L-1}$, and $0\leqslant n_L$ hold in Eqs. (5) and (6). We consider the history satisfying the relation $L_m\sim m^\gamma$ for $0<\gamma\leqslant 1$. This relation leads to $n_k\sim k^{(1-\gamma)/\gamma}$ in Eqs. (5) and (6). Replacing the sum of k by an integral for $\ln N(\{L_i\})p(\{L_i\})$, one has

$$\ln N(\{L_i\})p(\{L_i\})^q\sim\gamma(1-q)m\ln m[1+O(m^{\gamma-1})], \tag{7}$$

where $O(m^{\gamma-1})$ denotes the terms vanishing as m goes to infinity. For $\gamma=0$, the horizontal size remains a finite value L and the cluster is shaped like a rod. Then the contribution of the history to the partition function is of the order of $L^{-q(m-L)}$. Using Starling's formula, the partition function $Z_{m+1}(q)$ can be written as

$$Z_{m+1}(q)\sim\sum_L L^{-q(m-L)}+\sum_{0<\gamma\leqslant 1}(m!)^{(1-q)\gamma}, \tag{8}$$

where the first sum is taken over the histories whose horizontal size is finite in the large-m limit. The first sum is of the order of L^{-qm} and the second sum vanishes for $q>1$ in the limit $m\to\infty$. One can therefore see that $\ln Z_{m+1}(q)/\ln(m!)$ vanishes in the limit, which leads to $h(q)=\gamma(q)=0$ for $q>1$. In the case of $q<1$, the contribution of the first sum to $Z_{m+1}(q)$ is negligible. Then one can rewrite Eq. (8) for $q<1$ as

$$Z_{m+1}(q)\sim(m!)^{1-q}\left(1+\sum_{0<\gamma<1}(m!)^{(1-q)(\gamma-1)}\right). \tag{9}$$

Equation (9) shows that $h(q)=\gamma(q)=1$ since the sum of γ vanishes as m goes to infinity.

For $q=1$, h and γ cannot be derived from Eqs. (8) and (9). However, the asymptotic behavior of L_m can be obtained from simple consideration. Let δL be an increment of L_m between m and $m+\delta m$. The averaged value of δL is estimated as $\delta L\sim 2\delta m/(L_m+2)$ because the probability of increasing L_m is given by $2/(L_m+2)$. Approximating the relation by a differential equation, one has

$$\frac{dL_m}{dm}=\frac{2}{L_m+2}. \tag{10}$$

The solution of this equation leads to the asymptotic behavior $L_m\sim m^{1/2}$, which implies $\gamma(1)=\frac{1}{2}$.

From the above calculations, one can see that the spectrum consists of three phases as shown in Fig. 2, that is, $(h,\gamma)=(0,0)$ for $q>1$, $(\frac{1}{2},\frac{1}{2})$ for $q=1$, and (1,1) for $q<1$. We also calculated the spectrum numerically as follows. We first generate a sequence of horizontal size $\{L_n\}$ randomly. If $L_n=L$, then L_{n+1} is set equal to $L+1$ with the probability $p^*=an^{1-\gamma}$ and L with the probability $1-p^*$, where a and γ are chosen randomly between 0 and 1. We next calculate the history probability p_γ and the number N_γ of such histories and add $N_\gamma p_\gamma^q$ to the partition function. This procedure is repeated 10^5 times. In order to satisfy the equality $Z_m(1)=1$, $Z_m(q)$ is divided by the sum of $N_\gamma p_\gamma$. The numerical results suggest that $h(\gamma)$ converges to the line $h=\gamma$ as shown in Fig. 2, which is in agreement with Eq. (7). It should be noted that γ parametrizes all possible clusters and tells us the ways of growth of the clusters.

Another nontrivial example is the Eden model. The transition probability from an Eden cluster σ_m to σ_{m+1} is deter-

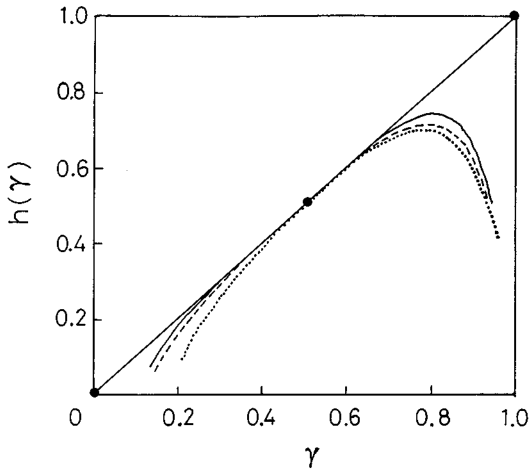

FIG. 2. Entropy spectrum of the ballistic aggregate model whose trajectories of particles are parallel to the vertical axis. The solid circles are obtained from the theoretical estimation of the partition function and the three lines are obtained numerically. The dotted line is for $m=950$, the dashed line is for $m=9500$, and the solid line is for $m=90\,000$.

mined from its perimeter size L_m because the cluster grows in the way that a new particle is added to one of the adjacent empty sites with the probability $1/L_m$. We have calculated the entropy spectrum of Eden clusters on a two-dimensional square lattice numerically as shown in Fig. 3. The distribution of history probabilities is computed by summing over all the histories up to $m=15$. To remove influence of the factor C in Eq. (1), K_q is determined from the ratio of partition functions $Z_{m+1}(q)Z_{m-1}(q)/Z_m(q)^2 \sim [m/(m-1)]^{-\tau(q)}$. For higher values of m, we are faced with computational limitations due to the increasing number of histories. So we adopt an alternative definition of $Z_m(q)$. Replacing the sum

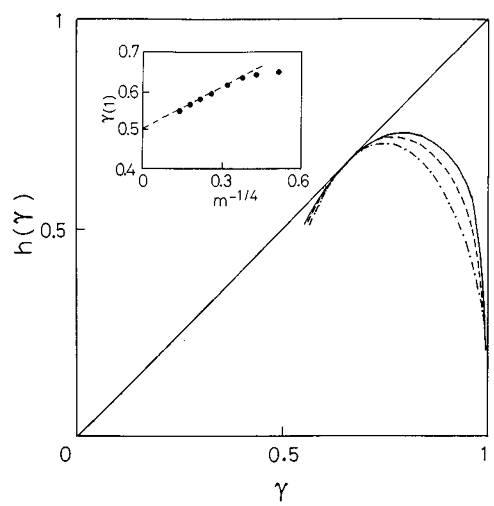

FIG. 3. Effect of mass m on the entropy spectrum in Eden growth. The dash-dotted line is for $m=7$, the dashed line is for $m=10$, and the solid line is for $m=15$. The spectrum for only $q<0.9$ is plotted. It is difficult to estimate the spectrum accurately for $q>1$ from small clusters because a phase transition occurs at $q=1$. The inset shows the dependence of $\gamma(1)$ on $m^{-1/4}$. The dashed line is drawn as a guide for the eye.

of histories in Eq. (2) by an ensemble average [7], one can write the partition function as

$$Z_m(q) = \langle\langle p(\{\sigma_n\})^{q-1}\rangle\rangle, \tag{11}$$

where a pair of double angular brackets refers to the ensemble average taken over possible histories from σ_1 to σ_m. As m increases, the history probability whose scaling index is given by $\gamma \sim \gamma(1)$ still remains large since it has a small escape rate. Equation (11) is useful for obtaining the spectrum near $q=1$.

The minimum scaling index $\gamma(\infty)$ is expected to be $\frac{1}{2}$ because of the requirement that σ_m has the smallest perimeter size leads to a circular object. If the cluster is compact and has the index γ, then L_m is scaled as $R^{2\gamma}$ with a linear size R of the cluster. The surface of the cluster is self-similar, except $\gamma=\frac{1}{2}$, and has the fractal dimension 2γ. On the other hand, if the cluster is self-similar like a DLA cluster, most of sites of the cluster belong to its perimeter and L_m is scaled as $L_m \sim m$. Thus γ is directly related to the morphology of Eden clusters and distributed between $\frac{1}{2}$ and 1. In the case that $\gamma(1)$ is equal to some value between $\frac{1}{2}$ and 1, the cluster must have a complicated surface such as a fractal curve.

We have found that $\gamma(1)$ is about 0.66 for $m=12$ and checked the dependence of $\gamma(1)$ on m. In the inset of Fig. 3, $\gamma(1)$ calculated from the ensemble average of 10^4 clusters is plotted versus $m^{-1/4}$. It is known that the interface width w in Eden growth starting from an initially flat surface with a linear size R is scaled with m and height l as $w(R,l) = R^{\alpha} f(l/R^z)$, where the exponents $\alpha=\frac{1}{2}$ and $z=\frac{3}{2}$correspond to the stationary and dynamic scaling [11]. The scaling function $f(x)$ is such that $f(x) \sim x^{\beta}$ for $x \ll 1$ and $f(x) \sim$ const for $x \gg 1$ with $\beta = \alpha/z$. One can also take the alternative form $w(R,l) = l^{\beta} f(R^z/l)$, which is useful for Eden clusters starting from a single seed. Assuming that $l \sim R \sim m^{1/2}$ for Eden clusters starting from a single seed, the scaling form is rewritten by $w(m) = m^{1/6} f(m^{1/4})$. The asymptotic behavior of physical quantities for $m \to \infty$ can be represented well by using a function of $m^{1/4}$. The inset of Fig. 3 shows that $\gamma(1)$ converges to $\frac{1}{2}$ as m goes to infinity, which is consistent with the fact that Eden growth leads to compact and spherical clusters. The equality $K_1 = K_\infty$ implies that K_q is constant for $q \geq 1$ because K_q must decrease monotonical as q increases. Our numerical calculations suggest that the generalized entropy varies continuously for $q<1$. We therefore expect that a phase transition occurs at the critical point $q=1$.

We next consider DLA clusters on a two-dimensional square lattice. DLA growth is intrinsically different from the above two examples with respect to growth rules. The transition probability from a DLA cluster σ_m to σ_{m+1} is equal to the growth probability at the interface proportional to the gradient of Laplacian field, while it is determined from the perimeter size or linear size in ballistic aggregates. Nevertheless, the assumption of Eq. (1) is still effective for Laplacian growth as already shown in Fig. 1(b). Let R_m be a linear size of σ_m and D_m be the fractal dimension of σ_m. Using the dimension spectrum $f(\alpha)$, the transition probability from σ_m to σ_{m+1} can be estimated by $R_m^{-\alpha_m}$, where α_m is the singularity of growth probability at the interface of σ_m. Then the history probability takes the form

$$p(\{\sigma_1,\sigma_2,\ldots,\sigma_m\}) \sim \prod_{n=1}^{m-1} n^{-\alpha_n/D_n}. \qquad (12)$$

Considering a history of a growing cluster whose fractal dimension is independent of mass, the probability is scaled by $m!$. The factorial of m again appears and the scaling assumption of Eq. (1) is now justified.

We point out a relation connecting the entropy K_1 to the fractal dimension D. The fractal dimension of typical DLA clusters is independent of m and the statistically averaged singularity of the growth probability can be given by $\alpha(1)$, where $\alpha(1)$ is the singularity for $q=1$ in the dimension spectrum. We therefore conjecture the relation

$$K_1 = \alpha(1)/D. \qquad (13)$$

We checked this relation numerically for the same data in Fig. 1(b). The fractal dimension calculated from the radius of gyration is 1.69 ± 0.02 and the information dimension for the harmonic measure of two-dimensional DLA clusters is unity [12]. Substituting these values into Eq. (13), the entropy $K_1 = 0.608$ is well approximated by $1/D$.

In summary, we have introduced an invariant that is obtained from the history probabilities in growth models. Here ''invariant'' means that it does not depend on the lattice structure and extrinsic details of growth rules. The entropy obtained from history probabilities and the multifractal spectrum $h(\gamma)$ are directly related to statistics of growing clusters and the escape rate $\gamma - h(\gamma)$ tells us how often the cluster will be observed in growth models. The history probability has the advantage of numerical estimation in comparison to the probability of finding a cluster among equal-size clusters. To demonstrate the application of the method to growth models, we have calculated the entropy spectrum of the ballistic aggregate growth producing fanlike clusters as a solvable example. An analytical estimation of the spectrum and numerical results show the existence of a phase transition at $q=1$. We have also applied the method to Eden clusters starting from a single seed. Numerical calculations of $h(\gamma)$ suggest that a phase transition occurs at the critical point $q=1$. The index γ in Eden growth is related to the fractal dimension of the surface and the spectrum shows that the cluster with a fractal surface will not be observed for large m. To study the statistics of clusters generated in stochastic growth models, it is not sufficient that one considers only geometrical quantities such as the fractal dimension. We believe that the entropy spectrum is useful to study statistical physics of growth models.

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