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Distribution of growth probabilities for off-lattice diffusion-limited aggregation

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We study the distribution $n(\alpha,M)$ of growth probabilities $\{p_i\}$ for *off-lattice* diffusion-limited aggregation (DLA) for cluster sizes up to mass $M=20000$, where $\alpha_i \equiv -\log p_i/\log M$. We find that for large α, $\log n(\alpha,M) \propto -\alpha^\gamma/\log^\delta M$, with $\gamma=2\pm0.3$ and $\delta=1.3\pm0.3$. One consequence of this form is that the minimum growth probability $p_{\min}(M)$ obeys the asymptotic relation $\log p_{\min}(M) \sim -(\log M)^{(\gamma+1+\delta)/\gamma}$. We find evidence for the existence of a well-defined crossover value α^* such that only the rare configurations of DLA contribute to $n(\alpha,M)$ for $\alpha>\alpha^*$, while both rare and typical DLA configurations contribute for $\alpha<\alpha^*$.

Diffusion-limited aggregation (DLA) was introduced in 1981 by Witten and Sander[1] as a simple computer algorithm for particle aggregation. Since then, it has served as a model for a variety of growth phenomena controlled by a scalar field Φ that satisfies the Laplace equation, $\nabla^2\Phi=0$, everywhere except on the surface of the growing aggregate and on the system boundary, where $\Phi=\Phi_1$ and $\Phi=\Phi_2$, respectively.[2] Growth occurs on each perimeter site i with a probability p_i proportional to $\nabla\Phi$.

The most detailed description of the cluster growth process is provided by the growth probabilities $\{p_i\}$ at each of the perimeter sites i.[3,4] In this work, we report results for the normalized distribution function $n(\alpha,M)$ for a sequence of off-lattice clusters up to mass 20000. Here $n(\alpha,M)d\alpha$ is the number of growth sites with α values in the interval $[\alpha,\alpha+d\alpha]$, with $\alpha_i \equiv -\log p_i/\log M$. The normalization is chosen such that the area is unity for each M. We find that for large α (small p_i), the distribution function can be described by the expression

$$n(\alpha,M) \sim n_0 \exp[-A(\alpha^\gamma-\alpha_0^\gamma)/\log^\delta M],\quad \alpha>\alpha_0, \tag{1}$$

where n_0 and α_0 are functions of M.[5] We also demonstrate that Eq. (1) is consistent with a specific functional form for the asymptotic behavior of the *typical* minimum growth probability[6]

$$\log p_{\min}(M) \sim -(\log M)^{(\gamma+1+\delta)/\gamma}. \tag{2}$$

Our calculations are for DLA grown with an *off-lattice* algorithm, since *on-lattice* DLA displays anisotropy, especially for large mass.[2] We assign to each cluster particle the closest grid coordinates on a square lattice with mesh size equal to the particle diameter.[7]

For each cluster, we solve the Laplace equation by standard relaxation methods; our maximum error in each p_i is $10^{-3}p_i$. We used "DLA-boundary conditions," requiring that $\Phi=0$ on all sites on the surface of the aggregate and $\Phi=1$ on a circle of radius $R=1.5R_c$ where $2R_c$ is the spanning diameter of the cluster; we found that p_i depends on R_c, but that this dependence is within the error bars of our calculation of the p_i for $R>1.5R_c$.

Figure 1 is a semi-log plot of $\langle n(\alpha,M)\rangle$ vs $\alpha^\gamma/\log_{10}^\delta M$ using the values $\gamma=2$ and $\delta=1.3$. The brackets $\langle\,\rangle$ denote the average over the number of clusters studied for a given mass, ranging from 90 clusters for $M\le3000$ to 10 clusters for $M=20000$. The data display linear behavior in the region $\alpha>\alpha_0(M)$, supporting the form (1); $\alpha_0(M)$ denotes the location of the maximum of $n(\alpha,M)$, and $n_0(M)$ is the value of $n(\alpha,M)$ at $\alpha=\alpha_0(M)$.[8]

We find that $\gamma=2\pm0.3$ by requiring straight-line behavior of the large α region in Fig. 1, and $\delta=1.3\pm0.3$ by requiring parallel lines. We also study ensembles of 56 and 79 clusters on the square and triangular lattices, with masses $M\le5000$, and find the same values of γ and δ within the error bars.

Up to now, we have only described the properties of the *averaged* distribution $\langle n(\alpha,M)\rangle$ over clusters of mass M. It is also interesting to study *fluctuations* of the $n(\alpha,M)$.

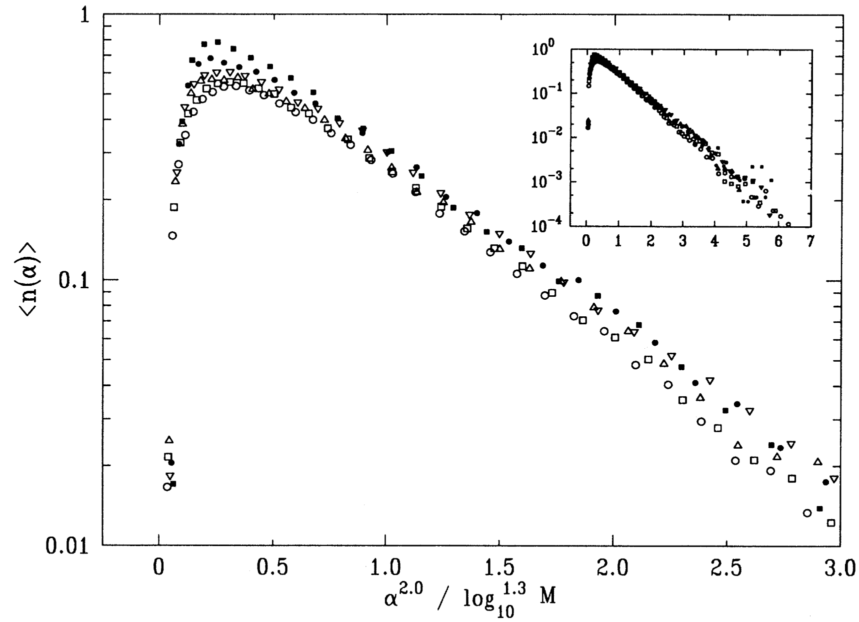

FIG. 1. $\langle n(\alpha,M)\rangle$ vs $\alpha^{\gamma}/\log_{10}^{\delta+1}M$ with $\gamma=2$, $\delta=1.3$. The main part of the figure shows the portion of $n(\alpha,M)$ close to the maximum; note that in order to obtain a relation $n(\alpha)\sim\exp(-A\alpha^{\gamma}/\log^{\delta}M)$ for the tail, we only require the lines to be parallel. The inset of the figure shows the same data, but over the complete range of α values. Data for six cluster masses are shown: (■), $M=753$ [90]; (●), 1471 [90]; (▽), 3000 [90]; (△), 5000 [10]; (□), 10000 [10]; and (○), $M=20000$ [10]. The numbers in square brackets are the number of off-lattice clusters which have been averaged to obtain the point shown.

To this end, we consider the moments

$$\mathcal{M}(\alpha,q)\equiv\langle[n_k(\alpha,M)]^q\rangle\equiv\sum_k[n_k(\alpha,M)]^q/N_{\text{clusters}}\,. \quad (3)$$

Here $n_k(\alpha,M)d\alpha$ is the normalized number of growth sites of cluster k and α values in the interval $[\alpha,\alpha+d\alpha]$, and N_{clusters} is the total number of clusters of mass M used in the average.

In Fig. 2(a), we plot $[\mathcal{M}(\alpha,q)]^{1/q}$ as a function of scaled α, $\tilde{\alpha}\equiv\alpha/(\log_{10}M)^{(\delta+1)/\gamma}$. Below a characteristic crossover value $\tilde{\alpha}^*$, we find that DLA is self-averaging in the sense that $[\mathcal{M}(\alpha,q)]^{1/q}$ is independent of q—which implies that for $\tilde{\alpha}<\tilde{\alpha}^*$ there is not much sample-to-sample fluctuation of $n_k(\alpha,M)$. On the other hand, we find that above $\tilde{\alpha}^*$, $[\mathcal{M}(\alpha,q)]^{1/q}$ depends strongly on q and the system ceases to be self-averaging—which implies large sample-to-sample fluctuations.

In Fig. 2(b) we plot the relative number of configurations contributing to the average $\langle n(\alpha,M)\rangle$. We find evidence for a similar sharp crossover—which occurs at roughly the same value of $\tilde{\alpha}$. Hence, from Figs. 2(a) and 2(b), we conclude that (a) the part of the distribution function with $\tilde{\alpha}<\tilde{\alpha}^*$ is common to the majority of DLA clusters. For $\tilde{\alpha}>\tilde{\alpha}^*$, the distribution function is dominated by rarely occurring configurations, (b) that even with many more realizations, the behavior shown in Fig. 2 would *not* change—due to the lack of self-averaging. These properties can be used as a definition of a typical cluster, namely a cluster for which the maximum of $\tilde{\alpha}$ is smaller than $\tilde{\alpha}^*$.

Figure 2(b) can equally well be interpreted as a probability distribution for $\tilde{\alpha}_{\max}^{\text{typ}}$, giving the probability $P(\tilde{\alpha}_{\max}^{\text{typ}}>\tilde{\alpha})$ to find in one given cluster a value $\tilde{\alpha}_{\max}^{\text{typ}}$ exceeding a given $\tilde{\alpha}$.[9] The data collapse observed in Fig. 2 and the definition of $\tilde{\alpha}$ imply that for "typical" DLA configurations, $\alpha_{\max}^{\text{typ}}(M)/(\log M)^{(\delta+1)/\gamma}$ is a constant. Hence $\alpha_{\max}^{\text{typ}}(M)\sim(\log M)^{(\delta+1)/\gamma}$, thereby providing direct evidence in support of Eq. (2). Figure 2(b) is also consistent with the inset of Fig. 1 which shows that there is no evidence of self-averaging for large α.

The above finding is related to the fact, discussed in Ref. 6, that the properties of a typical DLA cluster must be distinguished from the properties of a complete ensemble containing *every* possible DLA of mass M. For example, in the complete ensemble the smallest growth probability $p_{\min}^{\text{ens}}(M)$ is found in a cluster with a spiral-like structure. In order to penetrate, the field Φ has to explore a deep slit of length proportional to M. Hence, $p_{\min}^{\text{ens}}(M)\sim\exp(-M)$ and $\alpha_{\max}^{\text{ens}}(M)\equiv-\log p_{\min}/\log M\sim M/\log M$. Such a configuration has a remarkably small statistical weight[10] that we cannot expect to find it in the usual process of statistical sampling. Hence for a typical cluster, we expect to find the largest value of α, $\alpha_{\max}^{\text{typ}}(M)$, which is smaller than $\alpha_{\max}^{\text{ens}}(M)$.

Assuming (1) to hold for values $\alpha\gg\alpha_{\max}^{\text{typ}}(M)$ but at most up to $\alpha\le\alpha_{\max}^{\text{ens}}(M)$, we can calculate a typical value for $\alpha_{\max}^{\text{typ}}(M)$. We require, that—on the average—this value of $\alpha_{\max}^{\text{typ}}(M)$ shall be realized at least on one site of every cluster. The number of growth sites of a cluster of mass M is proportional to M, the constant of proportionality larger, but of order one. Thus we are led to the condition

$$\frac{1}{N_g}\approx\frac{1}{M}\approx\int_{\alpha_{\max}^{\text{typ}}(M)}^{\alpha_{\max}^{\text{ens}}(M)}n(\alpha,M)d\alpha\,, \quad (4)$$

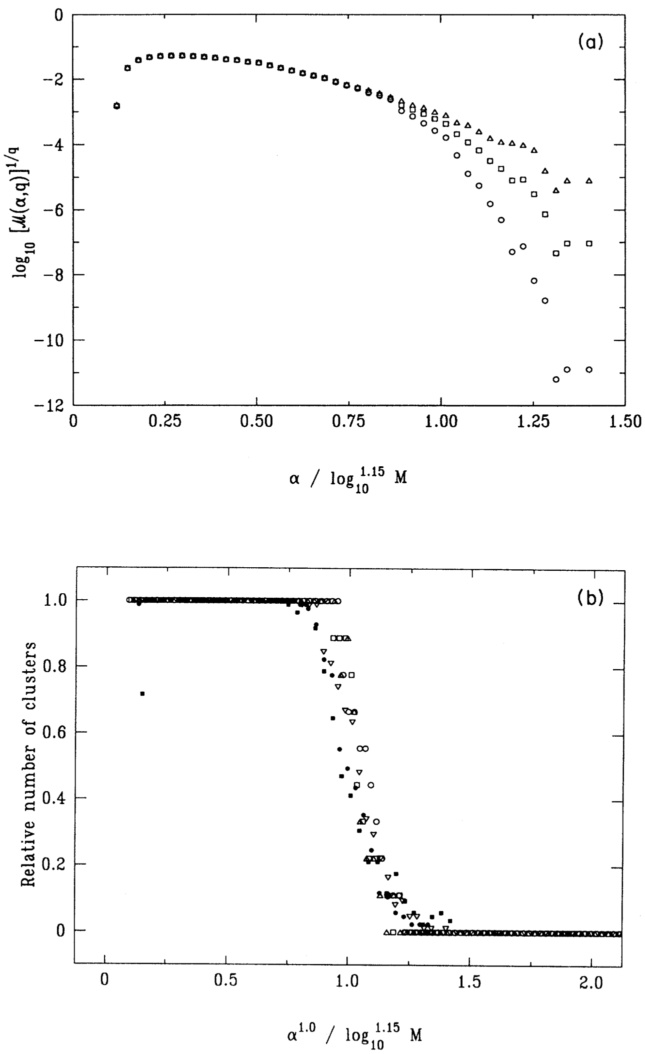

FIG. 2. (a) Dependence on $\tilde{\alpha}\equiv\alpha/(\log_{10}M)^{(\delta+1)/\gamma}$ (scaled α) of $[\mathcal{M}(\alpha,q)]^{1/q}$, for three values of q: (○), $q=0.25$; (□), 0.5; and (△), 1.0. Each curve represents an average over 90 off-lattice clusters of mass $M=3000$. (b) The relative number of clusters contributing to $\langle n(\alpha,M)\rangle$ is plotted against $\tilde{\alpha}$, with $\gamma=2$, $\delta=1.3$. The precipitous drop to zero appears roughly in the same range of values of the argument for all values of M. This plot can be interpreted as the accumulated probability distribution of the largest $\tilde{\alpha}$ values in each configuration considered. The symbols used correspond to those in Fig. 1.

where N_g is the number of growth sites. Hence,

$$\frac{1}{M}\approx n_0(M)\left[\int_{\alpha_{\max}^{\rm typ}(M)}^{\infty}\exp\{-A[\alpha^{\gamma}-\alpha_0(M)^{\gamma}]/\log^{\delta}M\}d\alpha-\int_{\alpha_{\max}^{\rm ens}(M)}^{\infty}\exp\{-A[\alpha^{\gamma}-\alpha_0(M)^{\gamma}]/\log^{\delta}M\}d\alpha\right]. \tag{5}$$

We use an asymptotic series expansion for the integrals, neglect nonleading powers, and under the assumption that $\alpha_{\max}^{\rm ens}(M)\gg\alpha_{\max}^{\rm typ}(M)$, we arrive at a scaling relation for $\alpha_{\max}^{\rm typ}$,

$$\alpha_{\max}^{\rm typ}\sim(\log M)^{(\delta+1)/\gamma}, \tag{6}$$

giving the typical value of $p_{\min}$ of Eq. (1).

A relation of this form has been found in Ref. 6 for the behavior of the quantity $\langle\log p_{\min}(M)\rangle$. We argue that averaging the logarithm of $p_{\min}$ in this relation is an alternative approach to define typical averages. The smallest growth probabilities are quantities which differ by orders of magnitude from one configuration to another. Taking the logarithm reduces the influence of single deviating values significantly and stresses values around the most likely one. In Ref. 6 the exponent $(\delta+\gamma+1)/\gamma$ has been observed to be approximately two, matching the value $(\delta+\gamma+1)/\gamma=2.15\pm0.22$ within the error bars.

In conclusion, we find an analytical form for the distribution function of growth probabilities [Eq. (1)]. This leads to a specific prediction [Eq. (2)] for how the smallest growth probability $p_{\min}$ depends on cluster mass. This work provides additional evidence favoring the possible phase transition in DLA (Ref. 11) since it supports the possibility that for a typical DLA configuration, $p_{\min}$ decreases faster than a power law. Also, we find evidence for the existence of a well-defined crossover value α^* with the property that only the rare configurations of DLA contribute to $n(\alpha,M)$ for $\alpha>\alpha^*$, while both rare and typical DLA configurations contribute for $\alpha<\alpha^*$. The reader should not confuse our crossover at α^* with the possible crossover[12] as a function of the distance from the origin, which is based on the observation that DLA cluster sites fall into two spatial regions, a "finished" or "semifrozen" region and an "unfinished" or "growing" region.

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