Size dependence of the minimum-growth probabilities of typical diffusion-limited-aggregation clusters

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The results of the numerical calculations of the growth probabilities of diffusion-limited-aggregation clusters based on the Spitzer theorem are presented. They support the recent results of Schwarzer *et al.* [Phys. Rev. Lett. **65**, 603 (1990)] on the non-power-like size dependence of minimum-growth probabilities and the resulting phase transition in the multifractal spectrum.

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In a series of recent papers [1–3] the problem of the phase transition in the multifractal spectrum of diffusion-limited aggregation (DLA) was discussed. Diffusion-limited aggregation was introduced by Witten and Sander [4] and a large literature devoted to this topic now exists [5]. In this model a single particle walks randomly on the square lattice until it reaches another particle (the "seed"), usually located in the center of the lattice (there are many variants of this simple rule, also off-lattice). A new particle then initiates its random walk. If this particle contacts the cluster (now consisting of two particles) it is incorporated into it and the cluster grows. This process is repeated many times (10^3–10^6) and leads to the formation of ramified fractal patterns. The growth process is governed by the set $\{p_i\}_{i=1,\ldots,P}$ where p_i is the probability for perimeter site i to be the next to grow and P denotes a total number of perimeter sites. The customary way of studying the properties of the set of probabilities $\{p_i\}$ is by means of the moments

$$Z_q(R)=\sum_i p_i^q \;, \tag{1}$$

where R is the linear size (radius of gyration) of the DLA cluster and q is a real number. In early works [6] a powerlike dependence of the moments on R was found, i.e.,

$$Z_q(R)\sim R^{-\tau(q)} \;. \tag{2}$$

The fact that the function $\tau(q)$ is not linear is called multifractality and the function $f(\alpha)$ obtained by means of the Legendre transform of $\tau(q)$ with respect to the variable q,

$$\alpha(q)=\frac{d\tau}{dq},\quad f(\alpha)=q\alpha(q)-\tau(q) \tag{3}$$

is called the multifractal spectrum [7].

It was argued in the past [2] that a function $f(q)$ should display the first-order phase transition at $q_c=0$. This phase transition was linked with a breakdown of the scaling law (2) of the moments $Z_q(R)$ for negative q (see Ref. [1–3]). Because for negative q moments are dominated by smallest p_i, this fact is in turn connected with the dependence of $p_{\min}$ on the size of the clusters. Three types of the dependence of $p_{\min}$ on the size of clusters were proposed in the past: Blumenfeld and Aharony [2] based their reasoning on the assumption that $p_{\min}$ decreases exponentially:

$$p_{\min}(R)\sim \exp(-AR^x) \;. \tag{4a}$$

Such a dependence is characteristic for "tunnel-like" configurations and Harris and Cohen [3] claimed that such special clusters are so rare that they cannot influence the formula (2) and that a typical ("typical" means averaged over samples) $p_{\min}$ decreases in a powerlike manner:

$$p_{\min}(R)\sim R^{-b} \;. \tag{4b}$$

The above formulas (4a) and (4b) were in fact conjectured and the first results of the computer simulations appeared in Ref. [8]. Surprisingly, the authors of Ref. [8] found yet a different dependence, intermediate between (4a) and (4b):

$$\ln p_{\min}(R)\sim -(\ln R)^y,\quad y\sim 2.15 \;. \tag{4c}$$

The detection of the phase transition is a problem of a numerical nature—to get reliable results the accuracy of the calculation of p_i should be many orders of magnitude smaller than $p_{\min}$, which even for a moderate cluster of the size of about 200 particles can be of the order 10^{-10}. In a paper [9] I presented the results of a numerical calculation of the probability p_i for a perimeter site i to be next to grow based on the Spitzer theorem. This theorem provides exceedingly accurate information on the p_i, but the application of it is limited by the size of present-day computers to small clusters only. In Ref. [9] I presented in detail the Spitzer theorem as well as results of a numerical analysis done for clusters consisting of only ~70 particles. This size was sufficient to confirm suggested [2] nonanalycity of $f(q)$ at $q_c=0$ but the data did not allow for a firm discrimination between the possible dependencies (4a)–(4c). In this report I present the results of the simulations of a larger cluster.

In the method based on the Spitzer theorem the natural parameter characterizing the growth of the clusters is P, the number of sites on the perimeter. I was able to generate clusters consisting of $P=250$ perimeter sites, corresponding to about 220 particles. The use of P instead of the number of particles N or radius R is justified in view of the scaling relations between these characteristics (see Ref. [10]). I have generated 500 clusters and hitting probabilities were recorded at five stages of the growth process: when $P=50$, 100, 150, 200 and 250. In Figs. 1(a)–1(c) the fittings of these results to Eqs.(4a–4c), respectively, are presented. It is clear from these figures that Eq. (4c) is confirmed and the dependencies (a) and (b) are ruled out. To trust results obtained from clusters of the rather small size I have generated I would like to point out that the ratio of inaccessible perimeter sites to total number of perimeter sites for $P=250$ was 0.36, and in Ref. [10] it was found that the value of this ratio saturates at 0.365 for $N\sim500$ and remains constant up to $N=10^5$ (although the fractal dimension for square-lattice DLA decreases slowly with mass). Using the argument that the upper end of the considered mass range is close

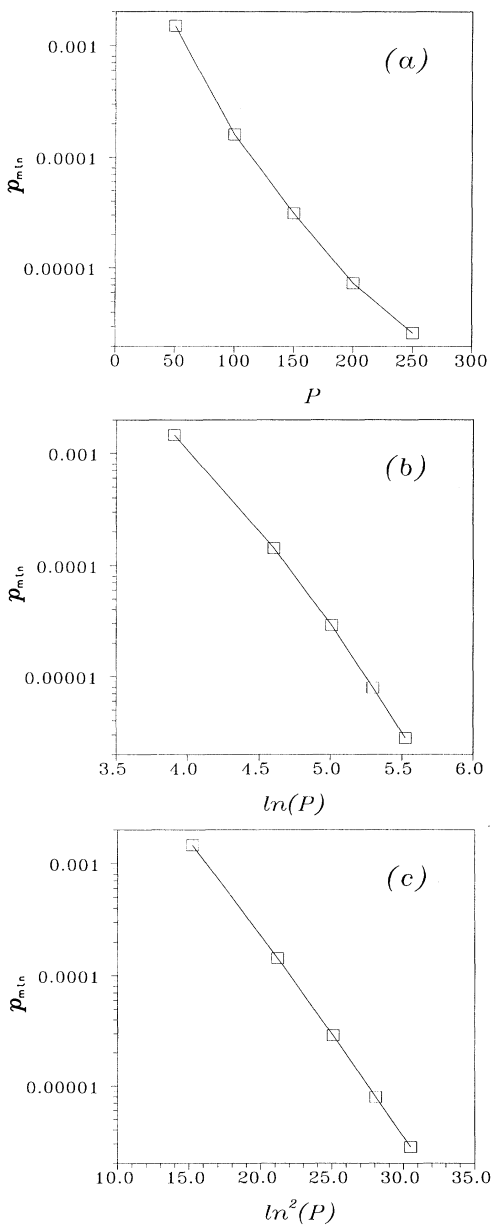

FIG. 1. The plots of the average values of $\ln(p_{\min})$ vs P in (a), vs $\ln(P)$ in (b) and vs $\ln^2(P)$ in (c).

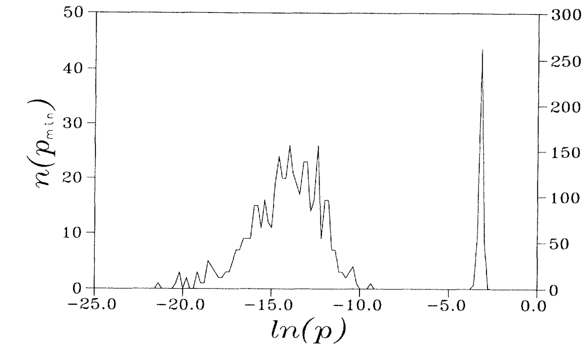

FIG. 2. A histogram showing the number of clusters with $P=250$ or 251 having $\ln p_{\min}$ contained in the interval of length 0.2 around $\ln p_{\min}$ ($\ln p_{\max}$ on the right). The left scale is for $n(\ln p_{\max})$.

to the beginning of the "asymptotic regime" does not support the behavior of $p_{\min}$ for masses smaller than 250, but nevertheless my results obtained by means of the independent very precise method confirm the numerical data of Schwarzer *et al.* [8] in a mass range which has not been examined. Because of the large fluctuations of $p_{\min}$ between different clusters (five orders of magnitude among 500 clusters, see below) instead of $p_{\min}$ I have averaged $\ln p_{\min}$ over clusters—nevertheless I would like to stress that the usual arithmetic averaging does not lead to significantly changed plots.

In Fig. 2 I have plotted a histogram of $n(p_{\min})$ showing the number of clusters ($P=250$) with growth possibilities in the range $\ln p_{\min}\pm0.1$. The smallest and largest $p_{\min}^{(n)}$ among 500 clusters were 1.49×10^{-10} and 4.8×10^{-5} (see Fig. 3), so the difference in magnitude was five orders! These large sample-to-sample fluctuations of $p_{\min}^{(n)}$ are consistent with the multifractality of the set p_i. Random multiplicative processes can give rise to multifractality Ref. [11(a)] and have been investigated in the context of DLA in Ref. [11(b)]. In contrast the $p_{\max}^{(n)}$ are almost equal; see Fig. 2, where a histogram of $p_{\max}^{(n)}$ is also given.

The non-power-like behavior of $p_{\min}$ should lead to the violation of scaling (2) moments for negative q [12]. I have calculated the "annealed" moments according to the formula

$$\langle Z_q(P)\rangle=\frac{1}{N_{\rm cl}}\sum_{n=1}^{N_{\rm cl}}\sum_{i=1}^{P}(p_i^{(n)})^q\,, \tag{5}$$

where $p_i^{(n)}$ is the probability of the ith site to grow in the nth cluster and $N_{\rm cl}$ is the number of clusters. In Fig. 4(a)

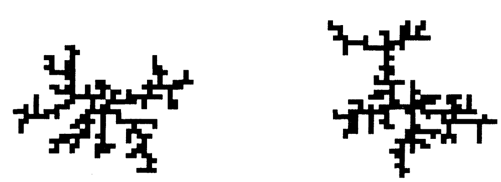

FIG. 3. Shapes of the clusters with the smallest $p_{\min}$ (left) and largest $p_{\min}$ (right). The site with the smallest $p_{\min}$ is deeply inside the stairlike fjord on the left cluster and on the right cluster there is a lot of screened sites and one completely closed large gulf ("lake") right below the seed.

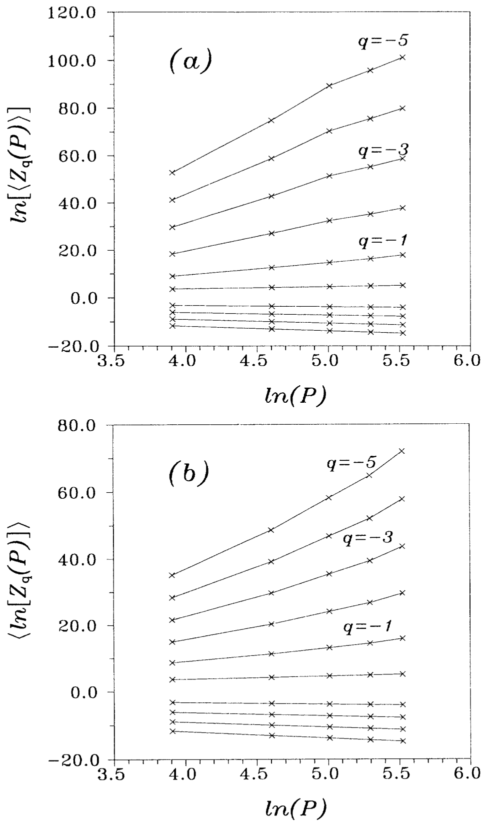

FIG. 4. The plots of $\ln\langle Z_q(P)\rangle$ vs $\ln(P)$ in (a) and $\langle\ln[Z_q(P)]\rangle$ vs $\ln(P)$ in (b) for $q=-5,-4,\ldots,5$ with the exception of $q=1$ $[Z_1(P)\equiv 1]$ to test scaling law (2).

the plots of $\ln\langle Z_q(P)\rangle$ vs $\ln P$ for a few values of q are shown. In spite of the violation of power dependence (4b) there is no upward curvature in this plot for negative q, which should reflect the non-power-like dependence of $p_{\min}$. Because the magnitudes of p_i differ considerably, for sufficiently large negative q's only a few smallest probabilities are contributing to the sum (5), i.e., a kind of floating point truncation can occur. To avoid such cases

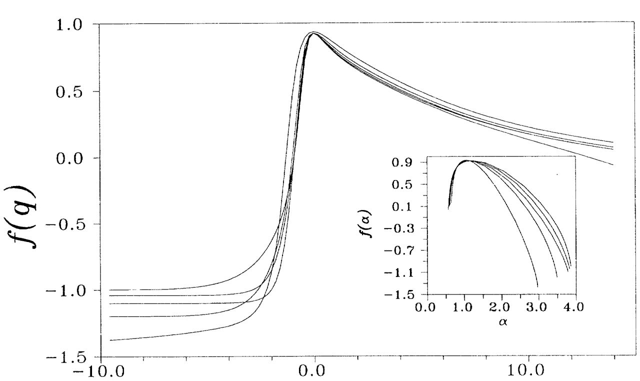

FIG. 5. The dependence of $f(\alpha,P)$ on q and plot of f vs α in inset for different P calculated from "annealed" moments. The values of $\alpha_{\max}$ and $f_-(P)$ shift to larger values with increasing P (see Table I).

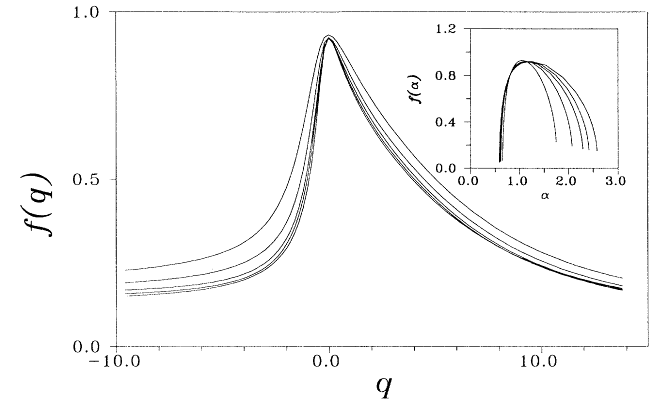

FIG. 6. The dependence of $f(\alpha,P)$ on q and plot of f vs α in inset for different P calculated from "quenched" moments. Here also the values of $\alpha_{\max}$ and $f_-(P)$ increase with P (see Tables II and III).

it is common to use the "quenched averages" for Z_q, defined as follows:

$$\langle \ln Z_q(P)\rangle = \frac{1}{N_{\rm cl}}\sum_{n=1}^{N_{\rm cl}} \ln\left[\sum_{i=1}^{P}(p_i^{(n)})^q\right] . \tag{6}$$

The plots of these quenched moments are shown in Fig. 4(b) and indeed in contrast to Fig. 4(a) there is an upward inclination in the plots supporting the conjecture made in Refs. [1,2] that there is a phase transition at $q=0$ from the powerlike dependence of moments to non-power-like behavior. The values of quenched moments are systematically smaller than corresponding values of the annealed Z_q computed according to Eq. (4). To show this let us rewrite the right-hand side of (6) in terms of the geometrical average:

$$\langle \ln Z_q(P)\rangle = \frac{1}{N_{\rm cl}}\sum_{n=1}^{N_{\rm cl}} \ln\left[\sum_{i=1}^{P}(p_i^{(n)})^q\right] = \ln\prod_{n=1}^{N_{\rm cl}}\left[\sum_{i=1}^{P}(p_i^{(n)})^q\right]^{1/N_{\rm cl}} .$$

But the geometrical averages are smaller than arithmetical ones and we get finally

$$\langle \ln Z_q(P)\rangle = \ln\prod_{n=1}^{N_{\rm cl}}\left[\sum_{i=1}^{P}(p_i^{(n)})^q\right]^{1/N_{\rm cl}} \le \ln\left[\frac{1}{N_{\rm cl}}\sum_{n=1}^{N_{\rm cl}}\sum_{i=1}^{P}(p_i^{(n)})^q\right] = \ln\langle Z_q(P)\rangle . \tag{7}$$

TABLE I. Comparison of the values of $f_-(P)$ predicted by Eq. (11) with the results of simulations.

	$f_-(P)$ annealed	
P	Eq. (11)	Simulations
50	−1.411	−1.376
100	−1.199	−1.199
150	−1.102	−1.102
200	−1.042	−1.042
250	−1.000	−0.999

TABLE II. Comparison of the values of $f_{-}(P)$ predicted by Eq. (12) with the results of simulations.

	$f_{-}(P)$ quenched	
P	Eq. (12)	Simulations
50	0.177	0.226
100	0.151	0.188
150	0.138	0.167
200	0.131	0.156
250	0.126	0.149

TABLE III. Comparison of the values of $\alpha_{\max}$ predicted by Eq. (13) with the results of simulations.

	$\alpha_{\max}$	
P	Eq. (13)	Simulations
50	1.751	1.748
100	2.075	2.073
150	2.291	2.290
200	2.414	2.413
250	2.575	2.573

From moments $Z_q(P)$ I have calculated the functions $f(q,P)$ and $f(\alpha,P)$ according to the formulas

$$\tau(q,P) \equiv -\ln Z_q(P)/\ln P \;, \tag{8}$$

$$\alpha(q,P) \equiv \frac{d\tau(q,P)}{dq} \;, \tag{9}$$

$$f(q,P) \equiv q\alpha(q,P) - \tau(q,P) \;. \tag{10}$$

In Fig. 5 the plots of functions defined in this way are shown. Figure 5 supports the conjecture that at $q_c=0$ there is a phase transition in the multifractal spectrum, see Refs. [1,2]. In Fig. 6 I have plotted $f(q)$ and $f(\alpha)$ obtained from the "quenched" moments (6), i.e., $\tau_{\rm qu}(q,P) = -\langle \ln Z_q(P) \rangle / \ln P$. The values of multifractal spectra obtained in these two ways differ considerably: for moments obtained according to Eq. (5) there are values of f which are negative, while for moments obtained according to Eq. (6) they are only positive. It is caused by the way in which averaging is done and it turns out that the number of samples enters explicitly the formula for limiting values of $f_{\pm}(P) = \lim_{q\to\pm\infty} f(q,P)$. For the annealed moments an easy calculation gives

$$f_{\pm}^{\rm ann}(P) = [\ln(a_{\pm}) - \ln(N_{\rm cl})]/\ln(P) \;. \tag{11}$$

Here $a_{\pm}$ is the number of sites with the same smallest and largest probability among *all* numbers $\{p_i^{(n)}\}_{i=1,\ldots,P;n=1,\ldots,N_{\rm cl}}$. For the quenched moments we get the explicitly positive values.

$$f_{\pm}^{\rm qu}(P) = \frac{1}{N_{\rm cl}\ln(P)} \sum_{n=1}^{N_{\rm cl}} \ln(a_{\pm}^{(n)}) \;, \tag{12}$$

where now $(a_{\pm}^{(n)})$ denotes the number of sites with the smallest and largest probability among sites of the nth cluster. Setting $a_{-}=2$ in Eq. (11) reproduces very well the limit values of the function f for $q=-\infty$ (see Table I), while setting $a_{\pm}^{(n)}=2$ in Eq. (12) gives values a little bit smaller than in Fig. 6 (see Table II), which suggests that sometimes values of $a_{\pm}^{(n)}$ are larger than 2. In these tables I have given only values corresponding to $q=-\infty$; for positive q the contribution to the sums comes from many values of $p_{\max}$, which are almost the same for each cluster (see Fig. 2). Because of the explicit dependence on $N_{\rm cl}$ in (11) the plots of annealed $f(\alpha)$ are in some sense artificial. On the other hand for quenched $f(\alpha)$ from (12) there is a chance that it will not depend on $N_{\rm cl}$ because the sum appearing in (12) can be proportional to $N_{\rm cl}$ and the dependence on it can cancel out. Similarly for limiting values of α for quenched averaging we get the formula

$$\alpha_{\substack{\max\\ \min}} = -\frac{1}{N_{\rm cl}\ln(P)} \sum_{n=1}^{N_{\rm cl}} \ln p_{\substack{\min\\ \max}}^{(n)} \;, \tag{13}$$

which reproduces quite well values of $\alpha_{\max}$ obtained in simulations (see Table III).

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