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LETTER TO THE EDITOR

Evidence for the first-order phase transition in the multifractal spectrum for diffusion-limited aggregation

Marek Wolf

Institute of Theoretical Physics, University of Wrocław, 50-205 Wrocław, Cybulskiego 36, Poland

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Abstract. A new method of calculating the growth probabilities of the DLA clusters based on the Spitzer theorem is presented. It allows very accurate determination of the probabilities of hitting the random walkers by the perimeter of the cluster, even deep in the 'fjords' where the probabilities are small. The evidence for the first-order phase transition in the plots of $f(q)$ are found. The large fluctuations of the minimal growth probabilities between different clusters are also discussed.

Recently there has been a growing interest in understanding the mechanism leading to formation of the 'fjords' in the diffusion-limited aggregation (DLA) clusters (see Ball and Blunt 1989, 1990) and the related phase transition in the multifractal spectrum $f(q)$ (Blumenfeld and Aharony 1989, Lee and Stanley 1988, Lee *et al* 1989) as well as the breakdown of the scaling behaviour of the moments (Cohen and Harris 1990, Trunfio and Alstrom 1990). In this letter I present the results of very accurate computer calculations of the hitting probabilities of DLA clusters based on the Spitzer theorem (Spitzer 1964) which allow the firm detection of the first-order phase transition at $q = 0$.

Diffusion-limited aggregation is a simple stochastic process leading to the formation of fractal patterns. It was proposed by Witten and Sander (1981) and now a large amount of literature devoted to this topic exists (see e.g. Stanley and Ostrovsky 1985, Vicsek 1988). In this model a single particle walks randomly on the square lattice until it reaches another particle ('seed'), usually located in the centre of the lattice. Then, a new particle initiates its random walk. If the particle contacts the cluster (now consisting of two particles) it is incorporated into the cluster and the cluster grows. This process is repeated many times ($\sim 10^3$-10^6) and leads to the formation of the ramified fractal structure for which the relation between the number, $N(R)$, of particles inside the circle of radius R is of the form

$$N(R) \sim R^D \tag{1}$$

where $D \simeq 1.7$ is the fractal dimension.

A satisfactory theory of DLA is still missing. In particular, nobody has yet proved equation (1) although a few attempts were made (see Muthukumar 1984, Tokuyama and Kawasaki 1984 and Kolb 1987). The breakthrough occurred with the recognition of the role played by the set of the growth probabilities $\{p_s\}_{s\in\Gamma}$, where p_s is the probability that the perimeter site s is the next to grow and Γ is the set of the nodes on the perimeter of a given DLA cluster (Turkewich and Scher 1985). The customary

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way of studying the properties of the set of probabilities $\{p_s\}$ is by means of the moments (Halsey *et al* 1985, Amitrano *et al* 1986)

$$Z_q(R) = \sum_s p_s^q \tag{2}$$

where R is the linear size (radius of gyration) of the aggregate and $q \in \mathbb{R}$. In the early works, the power-like dependence of the moments on R was found:

$$Z_q(R) \sim R^{-\tau(q)}. \tag{3}$$

The fact that the function $\tau(q)$ is not linear is called *multifractality* (Halsey *et al* 1986) and the function $f(q)$

$$\alpha(q) = \frac{\mathrm{d}\tau}{\mathrm{d}q} \tag{4a}$$

$$f(q) = q\alpha(q) - \tau(q) \tag{4b}$$

is called the *multifractal spectrum.* Sometimes the relation (4*a*) is inverted and substituted into (4*b*) giving the Legendre transform $f(\alpha)$ of the function $\tau(q)$.

Blumenfeld and Aharony (1989) gave the theoretical arguments that the function $f(q)$ should display the first-order phase transition at $q_c = 0$. The detection of the phase transition is a problem of a numerical nature—it is linked to the sites with very small hitting probabilities, p_s, and to get reliable results the accuracy of the calculation of p_ss should be many orders smaller than $p_{\min}$. I have quite recently performed a numerical calculation using the Spitzer theorem and these results are reported here. This method is very accurate; for the completely screened sites (for which $p_s = 0$ and which do not contribute to the moments) I have sometimes obtained p_s of the order 10^{-20} instead of p_s. There is also another check of the accuracy; for pairs (or triplets) of the sites, which by symmetry arguments should possess the same p_s, I have obtained probabilities whose first 18 digits coincide.

The Spitzer formula gives the hitting probabilities of the arbitrary finite set for the *arbitrary aperiodic recurrent random walk in two dimensions.* Because in the usual DLA the particles perform the symmetric random walk on a two-dimensional lattice $\mathbb{Z}_2$, I will describe here the Spitzer recipe for calculating the hitting probabilities of a *simple* random walk by points belonging to a finite set B. For the simple random walk the transition probability $P(x, y)$ is of the form

$$P(x, y) = \begin{cases} \frac{1}{4} & \textit{if } x \textit{ and } y \textit{ are nearest-neighbour sites} \\ 0 & \textit{in other cases.} \end{cases} \tag{5}$$

Let $P_n(x, y)$ denote the probability that a particle executing a random walk and starting at the point x will reach the point y after n steps:

$$P_n(x, y) = \sum_{x_i \in \mathbb{Z}_2, i = 1, \ldots, n-1} P(x, x_1)P(x_1, x_2) \ldots P(x_{n-1}, y). \tag{6}$$

Let $G_n(x, y)$ denote the expected number of visits of the random walk starting at x to the point y within n steps:

$$G_n(x, y) = \sum_{k=1}^{n} P_k(x, y). \tag{7}$$

The crucial quantity in the Spitzer formula is the potential kernel defined as

$$A_n(x, y) = G_n(0, 0) - G_n(x, y). \tag{8}$$

Let $A(x, y)$ denote the limit

$$A(x, y) = \lim_{n \to \infty} A_n(x, y). \tag{9}$$

It can be proved that the operator $A(x, y)$ is symmetric and, if restricted to any finite subset B of $\mathbb{Z}_2$, invertible. Let $K_B(x, y)$ denote this inverse matrix

$$\sum_{t \in B} A(x, t) K_B(t, y) = \delta(x, y) \qquad \text{for } x, y \in B. \tag{10}$$

Next let us introduce the notation

$$K_B(x) = \sum_{t \in B} K_B(x, t) \tag{11a}$$

$$K_B = \sum_{t \in B} K_B(t). \tag{11b}$$

Let $H_B(x, y)$ denote the probability of first hitting the set B at the point y when starting point $x \notin B$. If the set $B \in \mathbb{Z}_2$ consists of at least two points then the following formula holds

$$H_B(x, y) = \frac{K_B(y)}{K_B} - \sum_{t \in B} A(x, t)\left(K_B(t, y) - \frac{K_B(t) K_B(y)}{K_B}\right). \tag{12}$$

In the diffusion-limited aggregation it is assumed that the particle starts from infinity; $|x| \to \infty$. For such a case it can be shown that (12) reduces to a simpler expression (see Spitzer 1964, theorem 14.1)

$$H_B(\infty, y) \equiv p_B(y) = \frac{K_B(y)}{K_B}. \tag{13}$$

Due to the translational symmetry of the simple random walk we have

$$A(x, y) = a(x - y)$$

where the function $a(x)$ is given by the following integral:

$$a(x) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{\pi}^{\pi} \frac{1 - \cos(m\theta_1 + n\theta_2)}{1 - \frac{1}{2}(\cos\theta_1 + \cos\theta_2)} \, d\theta_1 \, d\theta_2. \tag{14}$$

Here the notation $x = (m, n)$ was introduced. The integral (14) can be calculated exactly only for points lying on the 'diagonal' $x = (n, n)$, but it suffices by proper use of the symmetry properties of the double integral (14) to obtain values of $a(n, m)$ for arbitrary points on the plane (see Spitzer 1964).

In this approach the natural parameter describing the size of the clusters is the number of perimeter sites, which I will denote as P. I have checked that there is a power-like dependence between P and N (or R): $P \sim N^{\gamma}$ with $\gamma \simeq 0.92$ and it justifies the use of P instead of R or N.

I have generated 400 clusters consisting of up to $P = 79$, which corresponds to about 60 particles. At five stages of the growth process, $P = 60 \ldots 61$, $64 \ldots 65, \ldots$, $78 \ldots 79$ (it should be remarked that the perimeter can also change by two sites), the actual p_s were calculated by means of the Spitzer theorem and recorded. The moments were averaged over clusters:

$$Z_q(P) = \frac{1}{\#\text{clusters}} \sum_{i=1}^{\#\text{cluster}} \sum_{s=1}^{P} (p_s^{(i)})^q \tag{15}$$

where $p_s^{(i)}$ is the probability of the sth perimeter site in the ith cluster. Next the functions $f(q, P)$ were calculated according to

$$\tau(q, P) \equiv -\ln Z_q(P)/\ln P \tag{16}$$

$$\alpha(q, P) \equiv \frac{\mathrm{d}\tau(q, P)}{\mathrm{d}q} \qquad f(\alpha, P) \equiv q\alpha(q, P) - \tau(q, P). \tag{17}$$

In figure 1 the functions $f(q, P)$ are plotted. The values taken by fs are rather unusual. This is caused by looking for the scaling of the moments with respect to the number of perimeter sites P, and not N or R. It is seen from figure 1 that exactly at $q_c = 0$ all fs have the first derivative equal to zero meaning that at this point the phase transition occurs. For larger P (thermodynamic limit) the maximum is becoming sharper and for $P \to \infty$ the first derivative $f'(q, P)$ should become non-analytical at $q_c = 0$. It turns out that there is no shift of the critical point with the size of the clusters (i.e. $q_c(P)$ do not depend on P) so, despite the small clusters I was able to simulate, they provide the reliable information about the point of phase transition. This situation can be contrasted with, for example, the Ising model, where the point of the maximum (in the thermodynamic limit the point of phase transition) specific heat shifts with the size of the lattice, see e.g. (Stosic *et al* 1990, figure 5). Because of the small number of clusters my results confirm the suspicion that the phase transition should also occur for *typical* clusters (Blumenfeld and Aharony 1989).

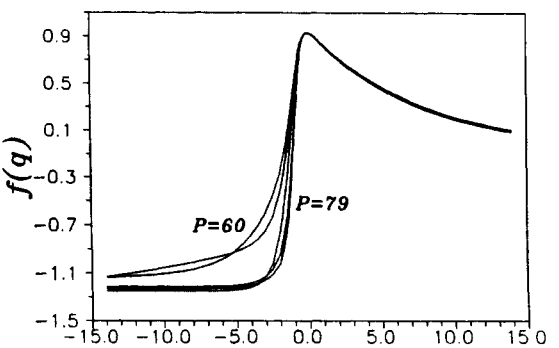

Figure 1. The dependence of $f(q, P)$ on q. Exactly at $q_c = 0$ all fs have the first derivative equal to zero—for larger P (thermodynamic limit) the maximum is becoming sharper.

My data does not allow a firm conclusion about the dependence of the typical minimum growth probabilities $p_{\min}(N)$ with the size of the cluster. Three dependencies were proposed in the past. Blumenfeld and Aharony (1989) based their reasoning on the assumption that $p_{\min}$ decreases exponentially with cluster mass:

$$p_{\min}(N) \sim \exp(AN^x). \tag{18}$$

Harris and Cohen (1990) proposed the power-like behaviour

$$p_{\min}(N) \sim N^{-\alpha_{\max}/D}. \tag{19}$$

Quite recently Schwarzer *et al* performed numerical simulations suggesting surprising dependence:

$$-\ln p_{\min}(N) \sim (\ln N)^y \qquad (y \approx 2). \tag{20}$$

Unfortunately the sizes of the clusters I have generated are too small to allow the distinction between the relations (18)-(20); points plotted in the appropriate way to

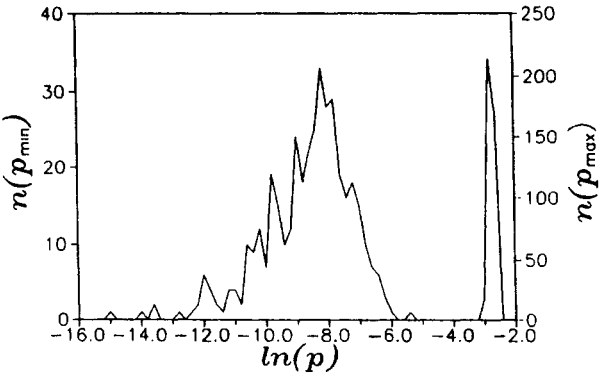

Figure 2. The histogram showing the number of clusters with $P = 78$ or 79 having p_{min} contained in the interval of length 0.2 around $\ln p_{min}$; the histogram for p_{max} is shown on the right (note different scales on the left and right axis).

test these dependencies lie exactly on straight lines for all these cases. However I would like to point out another phenomenon which was detectable due to the high accuracy of my method; namely there are large fluctuations between p_{min} belonging to different clusters. The absolute minimum growth probability among 400 clusters was 2.96×10^{-7} and the largest was 4.11×10^{-3}, see figure 2. As these fluctuations will increase with the sizes of the clusters, the validity of this observation is not restricted by small numbers of particles in the clusters I was able to generate. Even if the p_{min} decreases in the power-like way, these large fluctuations can lead to the scaling violation because they prevent the steepest-descent estimation of the moments for negative qs. It should be stressed that practically all p^i_{max} $(i = 1, \ldots, 400)$ are equal and they lie in the narrow interval $(4.4 \times 10^{-2}, 7.6 \times 10^{-2})$, see figure 2.

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