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A Toy Model for the Diffusion-Limited Aggregation

M. Wolf

Cardinal Stefan Wyszynski University
Faculty of Mathematics and Natural Sciences
ul. Wóycickiego 1/3, PL-01-938 Warsaw, Poland
E-mail: m.wolf@uksw.edu.pl

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Abstract: We consider the deterministic Vicsek fractal with the aim to understand the multifractal properties of the Diffusion-Limited Aggregation.
Key words: Diffusion-Limited Aggregation, multifractality

I. INTRODUCTION

In the past there was great interest in the study of irreversible kinetic processes leading to the formation of fractal objects. A simple stochastic model for the formation of clusters of particles in two-dimensional space was proposed by Witten and Sander [1]. In their model called Diffusion-Limited Aggregation (DLA), a Brownian particle is launched from a random position far away from the "seed" (usually located in the center of the lattice). In the strict formulation the walking particles are starting from infinity. If the particle reaches another particle ("seed") then it sticks and the occupied perimeter site is incorporated into the cluster. Then, a new particle initiates its random walk. If the particle contacts the cluster (now built of two particles) it stops and the cluster grows. This process is repeated many times (10^3–10^6) and leads to ramified structures possessing remarkable scaling properties, see Fig. 1. The growth appears mainly at outer parts of the cluster: the "fjords" and "gulfs" are hardly accessible to random walkers as the probabilities to "catch" particles are very small in these regions. The present world record for on lattice DLA seems to be [2] with the cluster made of 145 199 976 particles. The fractality manifests itself for example in behavior of the number $N(R)$ of particles contained inside a circle of radius R:

$$N(R) \sim R^{D_f} \ , \qquad (1)$$

where $D_f \approx 1.6 \div 1.7$ is the fractal dimension.

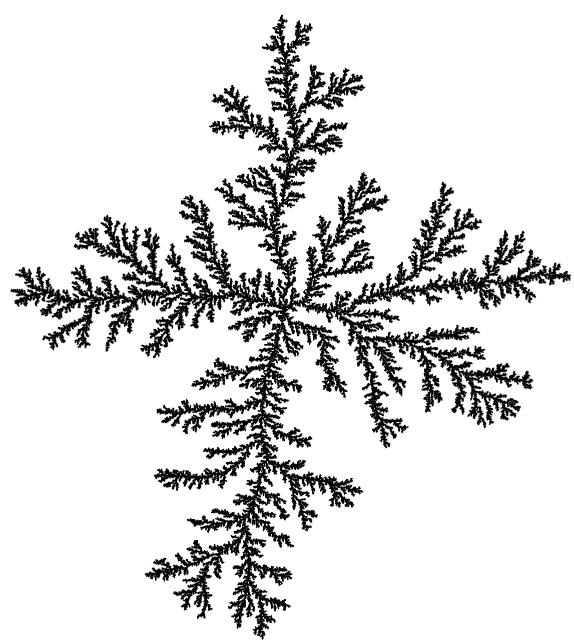

Fig. 1. The DLA cluster built from 480 000 particles on the square lattice

To our knowledge a satisfactory theory of the general growth processes, and of DLA in particular, is still missing. In our opinion the full theory should provide the formula for the behavior of the number of particles $N(R)$ averaged over all possible realizations of DLA clusters as a function of the radius R:

$$\langle N(R)\rangle \sim R^{D_f} \ , \tag{2}$$

with the value of D_f close to computer estimations $D \approx \approx 1.6 \div 1.7$. There were no analytical attempts to calculate the moments of the growth site probability distribution (GSPD) for DLA except the papers by Lee and *et al* [2], but these papers tackled the rather different model. In this paper we are going to present the results of the numerical calculations of moments of hitting probabilities GSPD for a Vicsek fractal, which we treat as a zero$^{\rm th}$ order approximation to the DLA clusters. The idea is to develop a kind of the perturbation theory by analogy with quantum mechanics, where information about unsolvable Hamiltonians which can be written as the sum of solvable H_0 and perturbing parts H_I, $H = H_0 + H_I$, is obtained via the perturbation theory.

In Sec. 2 we present the main properties of the GSPD for DLA which we attempt to model by the GSPD of deterministic Vicsek fractal. In Sec. 3 we present the main facts about Vicsek fractal. In Sec. 4 the methods of obtaining GSPD are discussed. In Sec. 5 the multifractal analysis of GSPD for Vicsek snowflake is presented. In Sec. 6 the reader will find the discussion and summary.

II. PROPERTIES OF THE GROWTH PROBABILITIES FOR DLA

In 1985, Scher and Turkevich [3] recognized in the DLA the role played by the set of the growth probabilities $\{p_i\}_{i=1\ldots P}$, 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. Therefore, this paper has focused on GSPD as an effective way to characterize these fractal growth processes. The customary way of studying the properties of the set of probabilities is by means of the moments averaged over different realizations of the growth process:

$$\langle Z_q(P)\rangle = \frac{1}{\sharp clusters}\sum_{n=1}^{\sharp clusters}\sum_{i=1}^{P_n}\left(p_i^{(n)}\right)^q \ , \tag{3}$$

where q is a real number $q \in \mathbb{R}$ and P_n is the number of perimeter sites in the $n^{\rm th}$ cluster and its averaged value $\langle P\rangle$ is linked to linear size (radius of gyration) R by the scaling $\langle P\rangle \sim R^{D_f}$ [4] of the DLA cluster.

In early investigations performed on small clusters [5] a powerlike dependence of the moments on R was found:

$$\langle Z_q(R)\rangle \sim R^{-\tau(q)}. \tag{4}$$

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,

$$\alpha(q) = \frac{d\tau}{dq}, \qquad f(\alpha) = q\alpha(q) - \tau(q) \ , \tag{5}$$

is called the multifractal spectrum [5, 6]. For linear $\tau(q)$ the function $f(\alpha)$ degenerates to just one point.

Simulations of larger clusters [7–9] have revealed that in fact for negative q's there is a breakdown of scaling and moments display the following behavior:

$$\langle Z_q(P)\rangle \sim \begin{cases} e^{-Bq(\ln P)^{2.15}} & q < 0, \\ P^{-\tau(q)} & q > 0. \end{cases} \tag{6}$$

This behavior is intimately connected with the following behavior of averaged over different realizations of the DLA process minimal growth probability $p_{\min}$ and maximal $p_{\max}$ in the set $\{p_i\}_{i=1\ldots P}$:

$$\langle p_{\max}\rangle \sim P^{-b} \ , \tag{7}$$

$$\langle p_{\min}\rangle \sim e^{-c(\ln P)^{2.15}} \ . \tag{8}$$

The last property of GSPD that we would like to mention consists in a very broad shape of the histogram of $\ln p_i$, see e.g. Fig. 2 in [9].

The set of probabilities possessing the properties listed above is very unique and it is not so easy to present a different than DLA mechanism leading to the set $\{p_i\}_{i=1\ldots P}$ reproducing relations (6).

III. DETERMINISTIC VICSEK SNOWFLAKE

In 1983, T. Vicsek [10] introduced the deterministic fractal. Surprisingly, this abstract construct has found practical applications as compact antennas in cellular phones, see [11, 12].

The construction of the deterministic Vicsek snowflake (DVS) is given by the recursive procedure. At the starting stage ($n = 0$) we simply have a single site. Next ($n = 1$), this site is reproduced four times at the "edges" of the original "seed" and a symmetric cross built of five particles is obtained. These procedure is repeated: the configuration at the $n^{\rm th}$ stage is obtained by adding to the four corners of the $(n-1)^{\rm th}$ stage configuration four copies of the cluster corresponding to the $(n-1)^{\rm th}$ stage of the growth, see Fig. 2, where a snowflake corresponding to $n = 5$ is given. This cluster is a possible, but very improbable, outcome of the usual DLA process and it should be compared with the DLA cluster shown on the right of Fig. 2 consisting of the same number (625) of particles.

For deterministic Vicsek snowflake the sizes R and the number of particles $N(R)$ increases with the stage n of the recursion process as $R = 3^n$ and $N(R) = 5^n$ respectively.

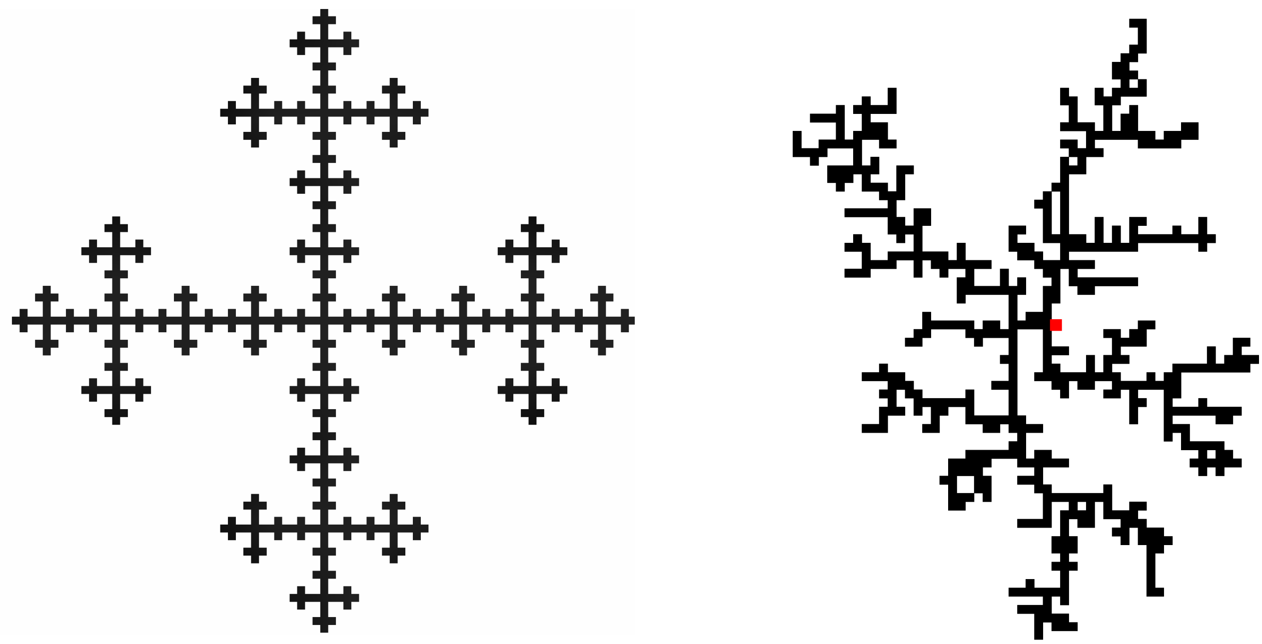

Fig. 2. Deterministic Vicsek snowflake corresponding to the 4^{th} stage of growth consisting of 625 particles with linear size equal to 243 lattice spacings. For comparison, on the right the usual cluster built of 625 particles is presented. The "seed" is marked in red – i.e. the first particle placed in the center of the lattice

From these two relations it follows that the fractal dimension of the DVS is given by $D_f = \ln 5/\ln 3 = 1.465...$ It is much smaller than the fractal dimension of the DLA clusters, which equals $\sim 1.6 \div 1.7$, see Eq. (1), but it became known that the very large ($N \sim 10^6$) on-lattice DLA clusters possess smaller fractal dimension – see [13]. We would like to point out that the ratio of the number of active (i.e. with $p_i \neq 0$) perimeter sites P_{active} to the number of *all* perimeter sites P is almost the same as for DLA [4] and we believe this ratio is responsible for main properties of the multifractal spectrum for DLA, because this ratio is smaller – more lakes or deep fjords are present with extremely small p_i and the scaling of negative moments breaks down. There are "dead" sites which cannot be reached by the random walker because they are screened in "fjords" and hence the probability to reach them is zero. Indeed, the number of all perimeter sites P for DVS is equal to $P = 6 \times 5^{n-1} + 2$ and the number of active perimeter sites (i.e. not "dead") is $P_{\text{active}} = 5^{n-2} \times 18 + 2$, which leads to the conclusion that $P_{\text{active}} = 0.6 \times P$ – for DLA this ratio saturates at $N \sim 500$ and remains constant up to $N = 10^5$ for large clusters at 0.635 [4]. Hence the number of "dead" sites is $P_{\text{dead}} = P - P_{\text{active}} = 12 \times 5^{n-2}$. In the Fig. 3 we present for the DVS with $R = 81$ and $N = 625$ the "dead" sites on the perimeter – the walker cannot reach these sites, and it will be stopped at earlier sites. In the next Section we are going to present methods for obtaining GSPD which we will apply in Sec. 4 to the perimeter sites of the Vicsek fractal.

IV. THE GROWTH PROBABILITIES OF DLA CLUSTERS

To calculate growth probabilities we will use a method based on the Spitzer theorem [14]. In the past the method based on the Monte Carlo simulations was used as well as the so called "DBM" prescription [11], but it is known now that these methods give rather inaccurate values of $\{p_i\}$, especially deeply inside the fjords (small p_i); for a discussion on this point see [8, 15]. We shall use the Spitzer formula [14] expressing the hitting probabilities of 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 in a two-dimensional lattice we will describe here the Spitzer recipe for calculating the hitting probabilities of a simple random walk by points belonging to a finite set B containing at least two sites. For the simple random walk the transition probability $P(x, y)$ is of the form

$$P(x,y) = \begin{cases} \frac{1}{4} & \text{if } x \text{ and } y \text{ are nearest-neighbor sites,} \\ 0 & \text{in other cases.} \end{cases} \tag{9}$$

As it is well known, this random walk is symmetric, aperiodic and recurrent (let us remind that in more than two dimensions the symmetric random walk is not recurrent, i.e. the probability to hit the given fixed point by a walker is less than 1). 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:

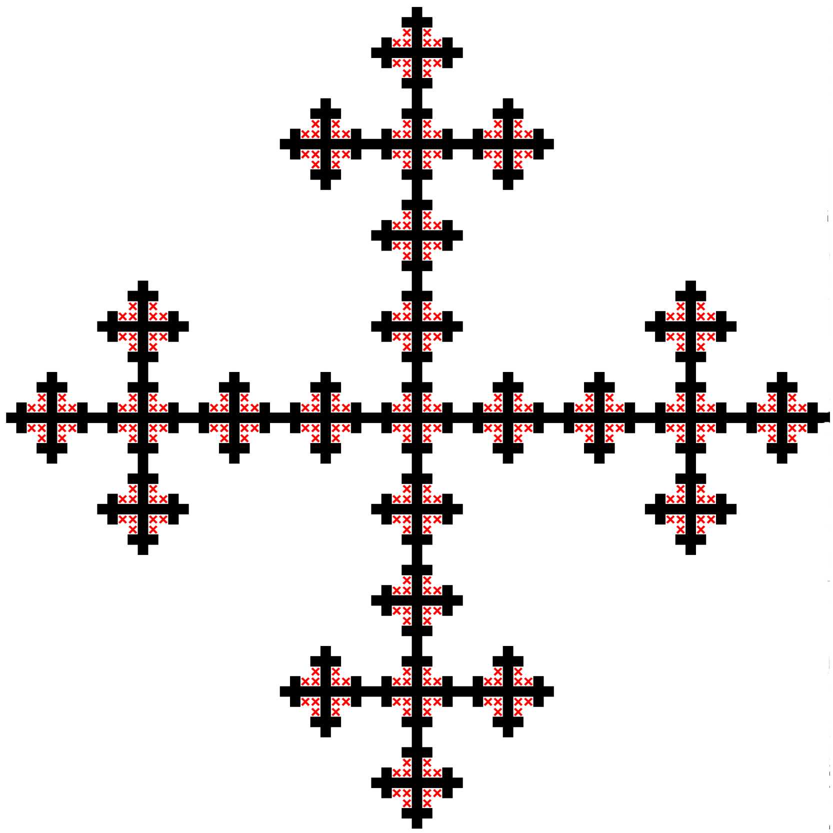

Fig. 3. The "dead" sites on the perimeter of the Vicsek snowflake for $n = 4$, i.e. $R = 81 = 3^4$ and $N = 625 = 5^4$

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

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:

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

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

$$A_n(x,y) = G_n(0,0) - G_n(x,y). \tag{10}$$

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

$$A(x,y) = \lim_{n\to\infty} A_n(x,y). \tag{11}$$

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:

$$\sum_{t\in B} A(x,t)K_b(t,y) = \delta(x,y) \qquad \text{for } \ x,y \in B. \tag{12}$$

Next, let us introduce the notation

$$K_B(x) = \sum_{t\in B} K_B(x,t), \tag{13}$$

$$K_B = \sum_{t\in B} K_B(t). \tag{14}$$

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

$$H_B(x,y) = \frac{K_B(y)}{K_B} + \sum_{t\in B} A(x,t)\Big(K_B - \frac{K_B(t)K_B(y)}{K_B}\Big). \tag{15}$$

In the DLA it is assumed that the particle starts from infinity: $|x| \to \infty$. For such a case it can be shown that the formula (15) reduces to a simpler expression [14, Theorem 14.1]:

$$H_B(\infty,y) \equiv p_B(y) = \frac{K_B(y)}{K_B}. \tag{16}$$

This function $p_B(y)$ provides the so called harmonic measure of the set $B : \sum_y p_B(y) = 1$. Now the prescription how to calculate the potential kernel (15) efficiently is needed. First of all, due to the translational symmetry of the simple random walk, we have

$$A(x,y) = a(x-y), \tag{17}$$

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

$$a(x) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{1-\cos(m\theta_1 + n\theta_2)}{1-\frac{1}{2}(\cos\theta_1 + \cos\theta_2)} d\theta_1 d\theta_2. \tag{18}$$

Here the notation $x = (m, n)$ was introduced. The symmetry properties of the above integral show that

$$\begin{aligned} a(m,n) &= a(-m,-n) = a(m,-n) = a(-m,n) = \\ &= a(-n,m) = a(n,-m) = a(n,m) = a(-n,-m). \end{aligned} \tag{19}$$

The integral (18) can be calculated exactly only for points lying on the "diagonal" $x = (n, n)$; it can be shown that [12, p.149]

$$a(n,n) = \frac{4}{\pi} \sum_{k=1}^{n} \frac{1}{(2k-1)}, \qquad a(0,0) = 0. \tag{20}$$

Because the double integral (18) cannot be calculated in the closed form for the points outside the diagonal, the following method of the determination of $a(x)$ for arbitrary x is used. From the definition (11) the recurrence relation can be shown to hold:

$$\begin{aligned} &4a(m,n) = \\ &= a(n-1,m) + a(n+1,m) + a(n,m-1) + a(n,m+1). \end{aligned} \tag{21}$$

By proper use of (13) and (15) the values (14) suffice to calculate the values of $a(x)$ for arbitrary x. Suppose the values of $a(k, m)$ for $0 \le m \le k \le n$ are known. Then, one can get $a(n+1, n)$ since $a(n, n)$ is the average of $a(n+ +1, n), a(n-1, n), a(n, n+1)$ and $a(n, n-1) = a(n, n+1)$. Next, $a(n+1, n+1)$ is found, the site $(n+1, n+1)$ being the only neighbor of $(n, n+1)$ where the value of $a(x)$ is unknown. In this way the values of $a(x)$ in the $(n+1)^{\text{th}}$ "column" can be determined, and then with the help of (19) the values of $a(x)$ for the remaining edges of the square can be obtained.

For large $x = (m, n)$ it can be shown that

$$a(x) = \frac{1}{\pi}\{2\gamma + \ln[8(m^2+n^2)]\}, \tag{22}$$

where the Euler constant is defined by the following limit:

$$\gamma = \lim_{n\to\infty} \left(\sum_{k=1}^{n} \frac{1}{k} - \log(n) \right) = 0.577215664902\ldots \tag{23}$$

The above method can be applied only to the clusters of the moderate size of about a few hundreds of particles – for really large systems there are problems with inversion of the matrices and storing them in the computer memory. For such big clusters we have used the method based on the solution of the discrete Laplace equation. The probability p_i that a particle occupies a lattice site $i = (m, n)$ is obtained from the field ϕ satisfying the discrete Laplace equation [16]:

$$\nabla^2 \phi(m,n) = 0. \tag{24}$$

Tab. 1. Comparison of probabilities obtained for DVS with 752 sites on the perimeter by two methods: Spitzer theorem and Laplace equation. Only a part of the data is presented. In the first columns coordinates of the sites are given (center is in $(0,0)$) and in next two columns values of p_i. The "dead" sites have $p_i = 0$

(x,y)	Laplace eq.	Spitzer th.
0, 41	2.35737E−2	0.235839360E−1
1, 40	1.05531E−2	0.105580294E−1
1, 42	1.05532E−2	0.105580294E−1
2, 39	8.72431E−3	0.872795544E−2
2, 43	8.72420E−3	0.872795544E−2
3, 38	7.87495E−3	0.787778836E−2
3, 40	6.16402E−8	0.000000000E+0
3, 42	0.00000E+0	0.000000000E+0
3, 44	7.87510E−3	0.787778836E−2
4, 37	7.57388E−3	0.757605406E−2
4, 39	0.00000E+0	0.000000000E+0
4, 40	6.71308E−8	0.000000000E+0
4, 42	0.00000E+0	0.000000000E+0
4, 43	0.00000E+0	0.000000000E+0
4, 45	7.57419E−3	0.757605406E−2
5, 36	1.02709E−2	0.102727763E−1
5, 46	1.02710E−2	0.102727763E−1
6, 37	2.03638E−3	0.203615884E−2
6, 39	0.00000E+0	0.000000000E+0
6, 40	8.53695E−8	0.000000000E+0
6, 42	1.32880E−7	0.000000000E+0
6, 43	5.42305E−8	0.000000000E+0
6, 45	2.03600E−3	0.203615884E−2
7, 38	8.58725E−4	0.858808258E−3
7, 40	1.70730E−7	0.000000000E+0
7, 42	0.00000E+0	0.000000000E+0
7, 44	8.58578E−4	0.858808258E−3
8, 39	3.53153E−4	0.353500276E−3
8, 43	3.53391E−4	0.353500276E−3
9, 32	9.41480E−3	0.941471286E−2
9, 40	9.56218E−5	0.957810423E−4
9, 42	9.58805E−5	0.957810423E−4
9, 50	9.41487E−3	0.941471286E−2
10, 31	6.35143E−3	0.635073634E−2
10, 33	1.99014E−3	0.199016921E−2
10, 40	8.16383E−5	0.817169480E−4
10, 42	8.17177E−5	0.817169480E−4
10, 49	1.99013E−3	0.199016921E−2
10, 51	6.35161E−3	0.635073634E−2
11, 30	6.10324E−3	0.610189526E−2
11, 34	8.50681E−4	0.850918822E−3

The boundary conditions are $\phi = 0$ on the cluster and its *perimeter* and $\phi = 1$ far away from the cluster; such a choice is called the DLA boundary conditions. The probability $p_{(m,n)}$ that a particle will hit the site (m,n) is given by the formula

$$p_{(m,n)} = \frac{1}{4}(\phi_{m-1,n} + \phi_{m+1,n} + \phi_{m,n+1} + \phi_{m,n-1}). \quad (25)$$

We have checked for the Vicsek fractals up to $N = 625$ that both methods give *exactly* the same values for p_i, see Tab. 1, and GSPD for $N = 3125$ and $N = 15\,625$ (for this cluster the perimeter has 56 252 sites and the size of matrix $K_B(x,y)$ is $56\,252 \times 56\,252$ and it would occupy many gigabytes of RAM, not to mention the problem of numerical stability of the computer program) was obtained only via the Laplace equation. We solved this equation numerically using the over-relaxation method, see e.g. [17, 18]. The iterations were performed until two consecutive iterations of the field differed by less than 10^{-12} on the whole lattice.

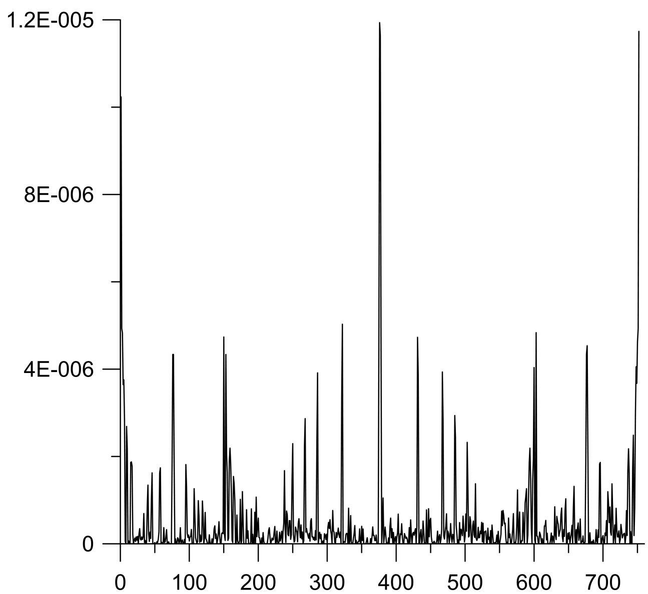

Fig. 4. The absolute values of the differences between probabilities obtained by two methods plotted as the function of the number of the perimeter site: there are 752 such sites

In the Fig. 4 the differences between probabilities obtained by the Spitzer theorem and from the Laplace equation are shown.

V. MULTIFRACTALITY OF THE GSPD FOR VICSEK FRACTAL

Because DLA is very hard to tackle analytically, it is worth having a simpler "toy" model solution which can provide insights into the full problem. Our idea is to try to solve some fractal which can be regarded as the "zero$^{\mathrm{th}}$" approximation to the real DLA clusters. Next, this solution can be perturbed in some way. It resembles quantum mechanics, where the hydrogen atom or the harmonic oscillator can be solved analytically and these solutions are perturbed to obtain more realistic models.

We have calculated GSPD for a series of DVS up to $n = 7$, i.e. for $N = 5, 25, ..., 78\,125$, which corresponds to $P = 8, 32, ..., 93\,752$ and linear sizes ranging from 3 to 2187. For $n = 1, ..., 4$ we have calculated p_i both via the Spitzer Theorem and Laplace equation. It allowed for checking that the DLA boundary conditions perfectly reproduces numbers obtained via Spitzer theorem. For $n = 5, 6$ and 7 we were able to use only the Laplace equation method.

For $n = 7$ we have calculated GSPD on the lattice 2501×2501 in double precision and on the lattice $3501 \times$ $\times 3501$ in single precision to compare the differences in p_i and to look for possible instabilities. Obtained results were the same.

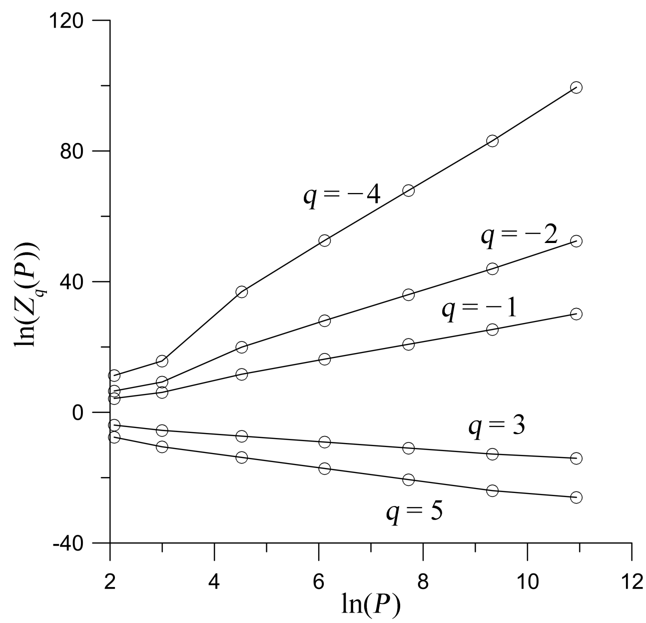

Fig. 5. The plot of and $\ln(Z_q(P))$ vs $\ln(P)$ in for $q = -4, -2, -1, 3, 5$ to test scaling law. Because the points are lying on the perfect straight line, there is no need for generating GSPD for larger Vicsek snowflakes

In Fig. 5 the plots of $\ln Z_q(P)$ vs $\ln P$ are presented and we see that DVS provides a model with perfect scaling law. Also the quantities $p_{\min}$ and $p_{\max}$ displays a strict power law behavior. It means that the multifractal formalism is applicable here in full extent and the function $\tau(q)$ is well defined. We calculated this function $\tau(q)$ from fitting to $\ln(Z_q(P)$ vs $\ln(P)$ straight line via the least square method. The plot of $\tau(q)$ is presented in Fig. 6. As it is seen, there are two regimes: for $q < 0$ and $q > 0$ where $\tau(q)$ is strictly linear, hence there is no multifractality present for DVS.

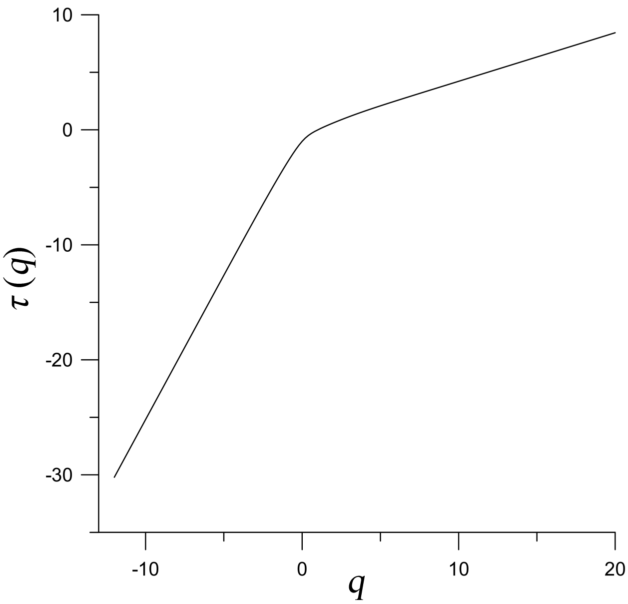

Fig. 6. Dependence of $\tau(q)$ on q. There is a phase transition at $q = 0$

VI. CONCLUSIONS

We have shown that the exact moments of the growth probabilities for a Vicsek fractal display a strict power scaling. In contrast with the moments averaged over usual DLA clusters, and despite the fact that this DVS has a DLA-aggregate like structure, it does not manifest the multifractal behavior. It suggests that the mechanism leading to the formation of the DLA clusters is generic and very complicated, and cannot be substituted by a different prescription. We tried to somehow "perturb" probabilities obtained for DVS but we were not able to obtain nonlinear $\tau(q)$. We are going to continue search for the proper "deformation" of the set p_i for DVS that will display full multifractal spectrum.

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Marek Wolf obtained his PhD degree in Physics (1982) and habilitation (1993) at the Wroclaw University, where he was employed till 2011. Since 1984 he has been doing computer experiments in physics and mathematics. In 1991 and 1993 he was a research fellow at the Center for Polymer Studies at Boston University. Now he is a member of the Faculty of Mathematics and Natural Sciences, College of Sciences at the Cardinal Stefan Wyszynski University in Warsaw. His hobby is photography: he owes a few camera bodies, 15 lenses and 6 flashes. Photography by Marta Wolf.

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