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Pascal Préa. Fractal Self-Avoiding Walks. GASCom, 2012, Bordeaux, France. hal-02435803

HAL Id: hal-02435803 https://hal.science/hal-02435803

Submitted on 11 Jan2020

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Fractal Self-Avoiding Walks

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Abstract

For any odd integer K > 1, we define \mathcal{F}_K , a new family of self-avoiding walks (SAW) on the square lattice $Z \times Z$, called *K*-fractal walks. These families have a simple and natural characterization and they seem to all have a critical exponent ν for mean-square displacement in]0.5, 1[. For small values of K at least, these families are easy to count and it is also very easy to randomly generate a K-fractal walk. In addition, $\lim_{K\to\infty} \mathcal{F}_K$ is the set of all SAWs on $Z \times Z$. We present also some variants of fractal SAWs, e.g. fractal SAWs on the *d*-dimensional grid Z^d .

Key Words: Self Avoiding Walks, Fractal Structures, Enumeration, Random Generation.

1 Introduction

A walk on a lattice is *self-avoiding* if it never passes twice through the same vertex. Self-avoiding walks (SAWs) appeared as a model for polymers [10]. They also have applications in statistical physics [11] and in probability theory [13]. Given a lattice (for instance, the hexagonal lattice on plane or the cubic one $\mathbb{Z} \times \mathbb{Z} \times \mathbb{Z}$ in space), the two main questions concerning SAWs on that lattice are:

• What is the number c_n of SAWs of length n?

• Given a distribution on the SAWs (for instance the uniform distribution on the SAWs of length n), what is the average distance d_n between the two extremities of a SAW of length n?

It is conjectured [13] that:

- $c_n \sim \mu^n n^{\gamma-1}$
- $d_n \sim n^{\nu}$

It is strongly believed that the *critical exponents* γ and ν depend only on the dimension (and not on the lattice) while the *connective constant* μ also depends on the lattice.

Despite decades of efforts, these questions remain unsolved, especially in low dimensions. It has recently been shown [8] that the connective constant for the hexagonal lattice on plane is $\sqrt{2 + \sqrt{2}}$. Conversely, for the square lattice on plane, it is conjectured [12] that the connective constant is the unique positive root of $13x^4 - 7x^2 - 581 = 0$ (i.e. $\sqrt{\frac{7+\sqrt{30261}}{26}} \approx 2.64$). For two-dimensional lattices, it is conjectured that $\gamma = 43/32$ and that $\nu = 3/4$.

Until now, these conjectures have not been rigorously proved. It is thus natural [1] [2] [6] [7] to define and/or study classes of SAWs which:

- have a natural definition.
- can be easily counted or studied.

In this paper, we introduce new classes of SAWs which satisfy these goals. In Section 2, we give the definition of this new class, then we show how to count these SAWs. In Section 4, we show how to generate random such SAWs and we see that, for these SAWs, the critical exponent ν seems to be < 1. We end by presenting some variants of these SAWs.

2 Definitions

We consider the square grid $\mathbb{Z} \times \mathbb{Z}$ on plane. A *walk* is a sequence $A = (a_0 = (0, 0), a_1, \ldots, a_n)$ of vertices such that, for all i < n, a_i and a_{i+1} are neighbours (i.e. if $a_i = (x_i, y_i)$ and $a_{i+1} = (x_{i+1}, y_{i+1})$, then $(x_{i+1} = x_i \text{ and } y_{i+1} = y_i \pm 1)$ or $(y_{i+1} = y_i \text{ and } x_{i+1} = x_i \pm 1)$. The walk A is *self-avoiding* if $i \neq j \implies a_i \neq a_j$.

Let K be an odd integer > 1. For every positive integer p, we simultaneously partition $\mathbb{Z} \times \mathbb{Z}$ into squares of side K^p such that for every p > 0, every square of size K^{p+1} contains K^2 squares of size K^p (see figure 1). Throughout this paper, we will always consider such multi-partitions, and we we call *square* a part of one of the partitions (a square is of size $K^p \times K^p$).



Figure 1: Partition of $Z \times Z$ for K = 3

Let A be a SAW on $\mathbb{Z} \times \mathbb{Z}$, A is K-Fractal (we say it is an F_K SAW) if:

- 1. It does not pass twice through the same square (i.e., once it has left a square, it never comes back in it Before leaving a square, the walk can, of course, pass through many vertices of this square)
- 2. When it leaves a square, it is through the middle of a side.

These two conditions have to be verified for any square, of any size. We denote by \mathcal{F}_K the set of all these SAWs. We will suppose in addition that one of the two following properties is verified:

- For every k > 0, point (0,0) is at the center of a square of size K^k . Equivalently, there exists p > 0 and a square of size K^p such that the walk begins at the center of the square and stays inside this square. We will call these SAWs *centered*.
- There exists p > 0 and a square of size K^p such that the walk begins at the middle of the West side of the square and ends at the middle of the East side of it. The walk is entirely contained in this square. We will call these SAWs *directed*.

These two supplementary conditions do not change the fundamental nature of fractal SAWs. The first one yields nice drawings and the second one requires fewer computations to count the SAWs. Clearly, every SAW of length k is a centered 2k + 1-Fractal SAW. So:

Property 1. $\lim_{K\to\infty} \mathcal{F}_K$ is the set of all SAWs.

3 Counting Fractal SAW

We first show that, for every odd integer K, K-Fractal SAWs admit a connective constant μ_K . Then we will see that, at least for small values of K, the value of μ_K can be determined from an enumeration of SAWs in a $K \times K$ square.

Property 2. For every odd integer K > 1, K-Fractal SAWs admit a connective constant μ_K .

Proof. The proof is exactly the same that the one for general SAWs (see [13] p. 9-10); we will only give its sketch. Let $c_K(n)$ be the number of K-Fractal SAWs of length n. Every K-Fractal SAW of length n + m is the concatenation of a K-Fractal SAW of length n and of a K-Fractal SAW of length m. So, $c_K(n+m) \le c_K(n) \times c_K(m)$, thus $\log c_K(n+m) \le \log c_K(n) + \log c_K(m)$ and $\mu_K = \lim_{n \to \infty} (c_K(n))^{1/n}$ exists.

Actually, a Fractal SAW "considers" each square (of size $K^p \times K^p$) as a vertex (it does not pass through it twice). So, if we look at a F_K SAW in a $K^{p+1} \times K^{p+1}$ square without detailing how is the walk inside the $K^p \times K^p$ squares, it is like looking at a SAW inside a $K \times K$ square. If we look at directed SAW, we only have to consider two types of SAWs in a $K \times K$ square (see Figure 2):

Walks which cross the square from one side to the opposite side.

Walks which turn inside the square.

If we look at centered SAWs, we have to consider in addition the three following types (see Figure 2):

Walks which begin at the center of the square and leave it.

Walks which enter the square and do not leave it.

Walks which begin at the center of the square and stay inside it.



Figure 2: The five types of SAWs on a 3×3 square

We now detail the case K = 3. There are nine walks which cross a 3×3 square from one side to the opposite side (see Figure 3):



Figure 3: The nine walks crossing a 3×3 square

If we look at the rightmost walk of the first line, and consider it as a walk of length n in a $3^{k+1} \times 3^{k+1}$ square, then each vertex on the walk can be seen as a walk in a $3^k \times 3^k$ square. More precisely, a walk of length n is the concatenation of four walks which turn inside a $3^k \times 3^k$ square and one walk which crosses a $3^k \times 3^k$ square from one side to the opposite side. So, if we denote by $T_k(p)$ the number of F₃ SAWs of length p which turn inside a $3^k \times 3^k$ square from one side to the opposite side, the number of F₃ SAWs of length p which cross a $3^k \times 3^k$ square from one side to the opposite side, the number of walks which cross a $3^{k+1} \times 3^{k+1}$ square like the rightmost walk of Figure 3 is $\sum_{n_1+\ldots+n_5=n} S_k(n_1) \cdot T_k(n_2) \cdot T_k(n_3) \cdot T_k(n_4) \cdot T_k(n_5)$.

Using this method, we can get the total number of F₃ SAWs of length n which cross a $3^{k+1} \times 3^{k+1}$ square from one side to the opposite side:

$$S_{k+1}(n) = \sum_{n_1+n_2+n_3=n} S_k(n_1) \cdot S_k(n_2) \cdot S_k(n_3) + 2 \sum_{n_1+\ldots+n_7=n} S_k(n_1) \cdot T_k(n_2) \cdot T_k(n_3) \cdot T_k(n_4) \cdot T_k(n_5) \cdot T_k(n_6) \cdot T_k(n_7) + 6 \sum_{n_1+\ldots+n_5=n} S_k(n_1) \cdot T_k(n_2) \cdot T_k(n_3) \cdot T_k(n_4) \cdot T_k(n_5)$$

Using generating functions [9, 15] yields a more concise writing. If we set $s(z) = \sum_{n \in \mathbb{N}} S_k(n) z^n$, $t(z) = \sum_{n \in \mathbb{N}} T_k(n) z^n$ and $S(z) = \sum_{n \in \mathbb{N}} S_{k+1}(n) z^n$, the equation above rewrites as:

$$S = s^3 + 2st^6 + 6st^4 \tag{1}$$

Without taking symmetries into account, there are eight walks who turn inside a 3×3 square (see Figure 4):



Figure 4: The SAWs turning inside a 3×3 square

So, by setting $T(z) = \sum_{n \in \mathbb{N}} T_{k+1}(n) z^n$, we have:

$$T = t^3 + t^7 + s^2 t + 2s^2 t^3 + 3s^2 t^5$$
⁽²⁾

For the square 5×5 , we obtain the following:

$$\begin{split} S &= s^5 + 4s^{13}t^{10} + 6s^{13}t^{12} + 12s^{11}t^8 + 44s^{11}t^{10} + 56s^{11}t^{12} + 18s^{11}t^{14} + 4s^9t^6 + 56s^9t^8 + 168s^9t^{10} + 198s^9t^{12} + 80s^9t^{14} + 8s^9t^{16} + 32s^7t^6 + 134s^7t^8 + 306s^7t^{10} + 372s^7t^{12} + 222s^7t^{14} + 52s^7t^{16} + 4s^7t^{18} + 20s^5t^4 + 64s^5t^6 + 174s^5t^8 + 324s^5t^{10} + 368s^5t^{12} + 256s^5t^{14} + 98s^5t^{16} + 16s^5t^{18} + 2s^5t^{20} + 20s^3t^4 + 60s^3t^6 + 124s^3t^8 + 174s^3t^{10} + 164s^3t^{12} + 122s^3t^{14} + 60s^3t^{16} + 8s^3t^{18} + 30st^8 + 32st^{10} + 8st^{12} + 8st^{14} + 6st^{16} + T \\ &= 2s^{14}t^9 + 2s^{14}t^{11} + 4s^{12}t^7 + 14s^{12}t^9 + 14s^{12}t^{11} + 6s^{12}t^{13} + 16s^{10}t^7 + 46s^{10}t^9 + 76s^{10}t^{11} + 3t^{10}t^{10} + 16s^{10}t^{10} + 16s^{10}t^{10}$$

 $52s^{10}t^{13} + 12s^{10}t^{15} + 14s^8t^5 + 54s^8t^7 + 171s^8t^9 + 278s^8t^{11} + 228s^8t^{13} + 68s^8t^{15} + 6s^8t^{17} + 4s^6t^3 + 26s^6t^5 + 123s^6t^7 + 306s^6t^9 + 483s^6t^{11} + 406s^6t^{13} + 168s^6t^{15} + 26s^6t^{17} + s^4t + 4s^4t^3 + 22s^4t^5 + 86s^4t^7 + 239s^4t^9 + 370s^4t^{11} + 337s^4t^{13} + 194s^4t^{15} + 62s^4t^{17} + 14s^4t^{19} + 2s^4t^{21} + 4s^2t^3 + 10s^2t^5 + 19s^2t^7 + 54s^2t^9 + 85s^2t^{11} + 86s^2t^{13} + 45s^2t^{15} + 18s^2t^{17} + 6s^2t^{19} + t^5 + 3t^9 + 5t^{13}$

Theoretically, for any odd K, it is possible to generate all the SAWs crossing a $K \times K$ square and then to derive from this the formulas for S and T. But practically, for K > 7, the generation of all the SAWs crossing a $K \times K$ square requires a prohibitively large amount of memory.

In [5, 4], A.J. Guttmann and others counted the SAWs crossing a square up to size 19×19 without generating them, using what they called the *finite lattice method*. It is easy to adapt their method to our purpose (generating the expressions for S and T): instead of consider only the total number of SAW of length n between two points, we have to determine the number of SAWs of length n having k turns, for k in $\{0, \ldots, n\}$. It is thus possible, after intensive computation, to obtain S and T for K up to 11.

From such a formula, it is possible to get the value for the connective constant μ_K . The radius of convergence of the function $C(z) = \sum_{n \in N} c_K(n) z^n$ is equal to $1/\mu_K$. This radius of convergence can be easily estimated by dichotomy: starting with an arbitrary value x for s and t, we reiterate (for K = 3) equations 1 and 2. If the result tends to 0, then $|x| < 1/\mu_K$, and if it tends to the infinite, $|x| > 1/\mu_K$. We get the following values for μ_K :

 $\mathcal{F}_3: \mu_3 \approx 1.758; \mathcal{F}_5: \mu_5 \approx 2.035; \mathcal{F}_7: \mu_7 \approx 2.180; \mathcal{F}_9: \mu_9 \approx 2.269; \mathcal{F}_{11}: \mu_{11} \approx 2.330;$

4 Random Generation of Fractal SAW

It is very easy to randomly generate a K-fractal SAW:

- 1. Generate a random SAW in a $K \times K$ square.
- 2. Replace each vertex of the SAW by a random SAW in a $K \times K$ square.
- 3. Repeat step 2 until the SAW is long enough.

We can get drawings like those in Figure 5. With this generation method, we do not obtain an uniform



Figure 5: A 5-Fractal SAW of length 1434 and a 7-Fractal SAW of length 2745

distribution on the K-fractal SAW, since we can not fix the length of the SAW. But we have the following fact:

Let us Consider a randomly generated K-Fractal SAW for which Step 2 has been repeated p times. The distance between its two extremities is $\sim K^p$.

The shortest paths which go through a $K \times K$ square are of length K (we only consider paths which start at the middle of a side of a square and finish at the middle of another side). Let l_S (resp. l_T) be the average length of the SAWs crossing (resp. turning into) a $K \times K$ square. If we consider only paths which turn on each squares, the average length of such paths for which Step 2 has been repeated p times is l_S^p . Similarly, the average length of randomly generated K-Fractal SAWs for which Step 2 has been repeated ptimes is in $[\min(l_S, l_T)^p, \max(l_S, l_T)^p]$. We have $K^p = ((K')^p)^{\log_{K'} K}$ and $\log_{K'} K < 1$ for $K' = l_S$ or $K' = l_T$, so we conjecture the following:

The critical exponent ν for the K-Fractal SAW is < 1, i.e. the average distance between the two extremities of a K-Fractal SAW of length n is $\approx n^{\nu}$, with $\nu < 1$.

We conjecture that this is true for the uniform distribution. Actually, the random generation process can be seen as a decision tree. At each level, one uniformly choose a SAW in a $K \times K$ square. But a long SAW has more (and longer) descendants than a short one. So, with the distribution got with the generation process, the short paths are overrepresented.

5 Variants

One can imagine many variants of Fractal SAW. We present some of them in this section.

The first way of defining variants consists in taking other building blocks that the square.

For example, the same definition can be applied to the lattice Z^d for any $d \ge 2$, with hypercubes instead of squares and we can use the same technique to compute the connective constant. For instance, for 3 dimensional cubes $3 \times 3 \times 3$, we have $\mu = 2.799$.

It is also possible to use rectangles instead of squares, but one has to consider three types of SAWs crossing a rectangle: those which turn inside the rectangle, those which cross from a small side to the other one and those which cross from a long side to the other one.

We can also forbid some squares (of size $K^p \times K^p$) inside squares of size $K^{p+1} \times K^{p+1}$. For instance, if we forbid the central node in a 3×3 square, we can get a Fractal SAW on the Sierpiński carpet [14] (see Figure 6). For such SAWs, we have:

 $S = 2st^4$ $T = t^3 + s^2 t^5$ And thus $\mu = 1.207$

One can add some restrictive conditions, in order to obtain a family of SAWs which is easier to study. For instance, if we force to a Fractal SAW to always turn inside a square (of any size, including the nodes), we get a *Sinuous SAW* [3] for which only one parameter is necessary for counting. We get:

$$\begin{split} K &= 3: \ T = t^3 + t^7 \\ K &= 5: \ T = 3t^9 + 5t^{13} + t^5 \\ K &= 7: \ T = 6t^{11} + 28t^{19} + t^7 + 34t^{23} + 15t^{15} + 23t^{27} + 5t^{31} \\ \cdots \end{split}$$

From these expressions, we can get the Connective constant μ of Figure 7.



Figure 6: A 3-Fractal SAW of length 4880 on the Sierpiński Carpet

K	μ	K	μ
3	1.210	11	1.405
5	1.288	13	1.427
7	1.335	15	1.444
9	1.376	17	1.458

Figure 7: The connective constant μ for Sinuous SAWs

It is also possible to require the walk, inside a square, to belong to a well known family, as the prudent SAWs [7] or the up-side SAWs [16]. It is this possible to count the SAWs crossing a square without enumerate them, thus with no intensive computations. It is so possible to get the connective constants for this kind of SAWs for much larger squares that for the basic family. We will detail the up-side SAWs.

An *up-side* SAW is a SAW on the square lattice which never goes down. If a *K*-Fractal SAW is, up to a rotation, a up-side SAW inside each square (the smaller squares are considered as points), we say that it is a *K*-Fractal-UpSide SAW (see Figure 8). Equivalently, a SAW is Fractal-Upside if, inside every square, there is a forbidden direction (if the walk enters the square on the West side and goes out through the opposite side, the forbidden direction is West; if the walk enters the square on the West side and goes out through the South side, the forbidden direction can be West or North). One can notice that a *K*-Fractal-UpSide SAW is generally not Up-Side. The advantage of such Fractal SAW is that it is possible to get the number of SAWs into a $K \times K$ square without intensive computations:

There are two types of Up-Side SAWs: the ones whose last move was a North move, and the ones whose last move was an East or a West move. When last move is North, next move can be North, East or West; when last move is East (resp. West), next move can be North or East (resp. West). Since we consider moves inside a square, we have to take into account the "remaining place" into the square (see Figure 9). If we call U(d, r, s, t) (resp H(d, r, s, t)) the number of K-Fractal-UpSide SAWs starting at the middle of the South side, ending at distance d from the North side and r from the East side, whose last move is North (resp. East), with s straights and t turns, we have:



Figure 8: A 5-Fractal-UpSide SAW



Figure 9: The parameters to be considered to count K-Fractal-UpSide SAWs

$$\begin{split} U(d,r,s,t) &= U(d+1,r,s-1,t) + H(d+1,r,s,t-1) + H(d+1,K-r+1,s,t-1) \\ H(d,r,s,t) &= U(d,r+1,s,t-1) + H(d,r+1,s-1,r) \\ H(K,(K+1)/2,0,0) &= 1 \end{split}$$

In addition, if we call S(s,t) the number of K-Fractal-UpSide SAWs with s straights and t turns crossing a $K \times K$ square from one side to the opposite one, and T(s,t) the number of K-Fractal-UpSide SAWs with s straights and t turns turning into a square, we have:

S(s,t) = U(0, (K+1)/2, s, t)

 $T(s,t) = 2 \cdot H((K+1)/2, 0, s, t) - C(s, t)$

The 2 factor for T(s,t) is because there are two (symmetrical) types of K-Fractals-UpSide SAWs turning into a square (see Figure 10, left and middle); but SAWs which contains only North and East moves (see Figure 10, right) belong to the two categories. So we remove their number (that we call C(s,t)). It is thus



Figure 10: Three K-Fractal-UpSide SAWs turning into a square

possible to obtain the values for the connective constants μ shown in Figure 11.



Figure 11: The connective constant μ for K-Fractal-UpSide SAWs

The last way of defining variants of fractal SAWs consists in loosen the definition. We will remove Condition 1¹. So we now consider SAWs which always enter into (or go out of) a square through the middle of a side (see Figure 12). These SAWs can come back into an already visited square. We cell such SAWs K-QuasiFractal SAWs and we denote by QF_K the sets of K-QuasiFractal SAWs. As for K-Fractal SAWs, we have:

Property 3. $\lim_{K\to\infty} Q\mathcal{F}_K$ is the set of all SAWs.

For every K, QF_K has a connective constant.

Similarly, in order to count K-QuasiFractal SAWs, we only have to enumerate walks in a $K \times K$ square. As for K-Fractal SAWs, we will count directed SAWs, but we have now to consider three types of walks (see Figure 13):

- The ones who go from one side of a square to the opposite side.
- The ones which turn inside a square.
- The ones which "crosses" in a square, i.e. which are made of two independent SAWs. We have to notice that this type of SAW does not concern vertices and that, since we count directed SAWs, crossing configurations as the one of Figure 14 are impossible.

In addition, for squares of size greater than $K^2 \times K^2$, there are more walks crossing square from one side to the opposite one (or turning into a square) than for K-Fractal-SAW (see Figure 15), and there are 19 such walks which go from one side of a 3×3 square to the opposite side, 18 which turn into a 3×3 square and 22 which cross into a 3×3 square. For 3-QuasiFractal SAWs, we get the following formula: $S = s^3 + 6st^4 + 4st^4c^2 + 2st^6 + 2s^3t^4c^2 + 4st^6c$

¹It is not possible to remove Condition 2. The main tool that we used for counting Fractal SAWs (or their variants) was that a $K^p \times K^p$ square inside a $K^{p+1} \times K^{p+1}$ square is like a vertex inside a $K \times K$ square. Using this tool implies that the squares are all independent (what "happens" inside a square does not depend on what happens in another one). Removing Condition 2 would add dependency between squares of different sizes: for instance, if a walk enter a square at a corner, it enters squares of all the smaller sizes by this corner.



Figure 12: A 3-QuasiFractal SAW



Figure 13: The three types of walks to be considered for counting K-QuasiFractal SAW

$$\begin{split} T &= s^2t + t^3 + 3t^5c^3 + s^2t^3c + 3s^2t^5 + 2s^2t^3 + t^7 + 2s^2t^5c^2 + 2s^2t^5c + 2t^5c \\ C &= s^4c + 2s^2t^4 + 8t^4c^5 + 4s^2t^4c + 6t^6c^2 + t^6 \end{split}$$

where $c(z) = \sum_{n \in N} C_k(n) z^n$, $C(z) = \sum_{n \in N} C_{k+1}(n) z^n$ and $C_k(n)$ is the number of walks which cross into a $3^k \times 3^k$ square. Using the finite lattice method, it is possible to compute similar formula for 5-QuasiFractal SAWs and 7-QuasiFractal SAWs, from which we can get the values of the connective constant μ in Figure 16.

K	μ		
3	1.862		
5	2.155		
7	2.312		

Figure 16: The Connective Constant μ for QuasiFractal SAWs



Figure 14: An impossible walk for K-QuasiFractal SAW



Figure 15: Examples of paths to be considered for 3-QuasiFractal-SAWs but not for 3-Fractal-SAWs. Only the cases in the top line occur in 3×3 squares. The other cases occur only in greater squares. A node in a $3^{p+1} \times 3^{p+1}$ square like the central one in the middle drawing of the second line corresponds (up to symmetries and rotations) to a path in a $3^p \times 3^p$ square like the ones in the two upper lines.

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