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Hamiltonian walks on Sierpinski and *n*-simplex fractals

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Abstract

We study Hamiltonian walks (HWs) on Sierpinski and n-simplex fractals. Via numerical analysis of exact recursion relations for the number of HWs we calculate the connectivity constant ω and find the asymptotic behaviour of the number of HWs. Depending on whether or not the polymer collapse transition is possible on a studied lattice, different scaling relations for the number of HWs are obtained. These relations are, in general, different from the well-known form characteristic of homogeneous lattices which has thus far been assumed to also hold for fractal lattices.

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1. Introduction

Enumeration of Hamiltonian walks (HWs), i.e., self-avoiding walks (SAWs) that visit every site of a given lattice, is a classic problem in graph theory, but it also has an important role in the study of the configurational statistics of polymers. HWs are used to model collapsed polymers [1], polymer melting [2, 3], as well as protein folding [4, 5]. The number of all possible HWs on a lattice is related to the configurational entropy of a collapsed polymer system, and also to the optimal solutions to the travelling salesman problem [6, 7]. Enumeration of HWs, closed or open, is a difficult combinatorial problem, which has been exactly solved only for few lattices, namely, the two-dimensional Manhattan oriented square lattice [8, 9], the two-dimensional ice lattice [10], the two-dimensional hexagonal lattice [11, 12], the Sierpinski gasket fractal [6] and the 4-simplex fractal [13]. The number of HWs has also been calculated numerically for various lattices by means of direct enumeration [14, 15], transfer matrix methods [16–18] and Monte Carlo estimates [19, 20]. The field theory representation for this problem was introduced in [21], and further developed in [22, 23].

The purpose of this paper is to understand the topological properties of Hamiltonian walks on several families of fractal lattices. In order to do this, we study the asymptotic behaviour of the number of closed HWs C_N for a large number of vertices N. This analysis yields the values of the so-called connectivity constant ω which has the physical meaning of the average number of steps available to the walker having already completed a large number of steps. It also provides insight into the spatial distribution of walks present at large N; this can be related to detailed studies of knot delocalization in [24].

The number C_N is for homogeneous lattices with $N \gg 1$ expected to take the form

$$C_N \sim \omega^N {\mu_S}^{N^\sigma} N^a. \tag{1.1}$$

Here ω is the connectivity constant and the term with μ_S represents a surface correction ($\mu_S < 1$), with $\sigma = (d-1)/d$ (d being the dimensionality of the lattice). This differs from the ordinary SAW case, where no surface term ${\mu_S}^{N^\sigma}$ is expected, i.e., the number of SAWs of length N behaves as $\mu^N N^a$ for large N. Furthermore, the exponent a is universal in the SAW case, i.e., it depends only on the dimensionality of the lattice, whereas for HWs it may depend on other, not yet identified, characteristics of the lattice. To the lowest approximation in equation (1.1) $C_N \sim \omega^N$, and the connectivity constant can be defined as

$$\ln \omega = \lim_{N\to\infty} \frac{\ln C_N}{N}. \tag{1.2}$$

For a better understanding of these problems it is helpful to study HWs on fractal lattices. As was first recognized by Bradley [13], the self-similarity of fractal lattices is a useful tool for the exact and computationally fast iterative generation and enumeration of all HWs on an unlimitedly large corresponding fractal structure. In this paper, we extend Bradley's algorithm to two- and three-dimensional Sierpinski fractal families, as well as n-simplex fractals with $n > 4$. We consider several families of fractals in order to compare the obtained results and be able to draw more general conclusions about the character of the Hamiltonian walks on different classes of lattices. In the case of the two-dimensional Sierpinski fractal family an exact closed form result for the connectivity constant is obtained due to the simple form of the recursion relations for the numbers of HWs. For the three-dimensional Sierpinski fractals which can model physically more frequently encountered systems a numerical approach is necessary. The study of asymptotics of the number of HWs shows that the surface term in equation (1.1) only appears for fractals on which the collapse transition from the polymer coil to the globule phase is possible. This is the same class of lattices for which delocalized HWs dominate over localized ones for large N.

The paper is organized as follows. In section 2 we describe the two-dimensional Sierpinski fractal family and obtain exact recursion relations for the number of HWs, as well as the closed exact formula for ω. Recursion relations for HWs on three-dimensional Sierpinski fractals are given and analysed in section 3. A similar method for analysing HWs on 5- and 6-simplex lattices is presented in section 4. Finally, in section 5 we discuss all our findings and related results obtained by other authors.

2. Hamiltonian walks on two-dimensional Sierpinski fractals

We begin by defining the two-dimensional (2D) Sierpinski fractal family. Each member of the 2D SF family (labelled by b) can be constructed recursively, starting with an equilateral triangle that contains b^2 smaller equilateral triangles (generator $G_1^2(b)$). The subsequent fractal stages are constructed self-similarly, by replacing each of the $b(b+1)/2$ upward-oriented small triangles of the initial generator by a new generator. To obtain the lth-stage fractal lattice $G_l^2(b)$, which we shall call the lth-order generator, this process of construction has to be

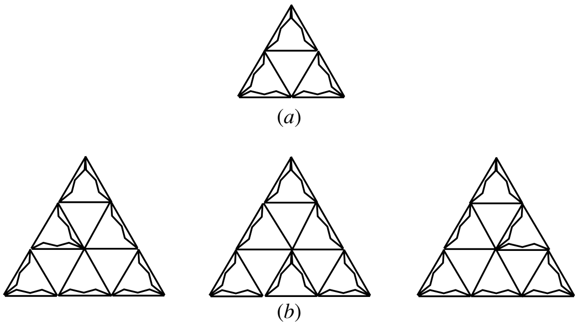

Figure 1. The $(l+1)$th-order generators $G_{l+1}(2)$ (a) and $G_{l+1}(3)$ (b) for $b = 2$ and $b = 3$ two-dimensional Sierpinski fractals, with the possible closed Hamiltonian walks configurations depicted. The small up-oriented triangles are the respective lth-order generators, and the lines that traverse them represent the open Hamiltonian walks.

repeated $l-1$ times, and the complete fractal is obtained in the limit $l \to \infty$. It is easy to see that, for any 2D SF, each closed HW on the $(l+1)$th generator comprises HWs which enter and exit lth-order generators. Let C_l be the number of closed HWs on the lth-order generator, whereas h_l and g_l are the numbers of HWs which enter the lth-order generator at one vertex, and leave it at the other, with or without visiting its third vertex, respectively. Then, it can be shown that a simple relation

$$C_{l+1} = Bh_l^{\alpha} g_l^{\beta} \tag{2.1}$$

is valid for $l \geqslant 1$ (see appendix A). Here B is a constant that depends only on SF parameter b, whereas exponents α and β are equal to

$$\alpha = b+1, \qquad \beta = \frac{(b+1)(b-2)}{2}. \tag{2.2}$$

For instance, the explicit form of the relation (2.1) for $b = 2$ is $C_{l+1} = h_l^3$ and for $b = 3$, $C_{l+1} = 3h_l^4 g_l^2$, which is illustrated in figure 1. One can also show (appendix A) that numbers h_l and g_l of open HWs obey the following closed set of recursion relations

$$h_{l+1} = Ah_l^x g_l^y, \qquad g_{l+1} = Ah_l^{x-1} g_l^{y+1}, \tag{2.3}$$

for all $l \geqslant 1$, where A is again a constant, different for every b, and

$$x = b, \qquad y = \frac{b(b-1)}{2}. \tag{2.4}$$

For $b = 2$ these relations have the form $h_{l+1} = 2h_l^2 g_l$, $g_{l+1} = 2h_l g_l^2$ and for $b = 3$, $h_{l+1} = 8h_l^3 g_l^3$, $g_{l+1} = 8h_l^2 g_l^4$ (see figure 2). From relations (2.3) it follows straightforwardly that

$$\frac{g_l}{h_l} = \frac{g_1}{h_1} = K, \tag{2.5}$$

for any $l \geqslant 1$, so that from (2.1) and (2.2) one gets $C_{l+1} = BK^{\beta} h_l^{b(b+1)/2}$. Since the number N_l of sites on the lth-order generator satisfies the recursion relation

$$N_{l+1} = \frac{b(b+1)}{2} N_l - (b^2 - 1), \tag{2.6}$$

according to (1.2) it then follows that

$$\ln \omega = \lim_{l \to \infty} \frac{\ln C_{l+1}}{N_{l+1}} = \lim_{l \to \infty} \frac{\ln h_l}{N_l}.$$

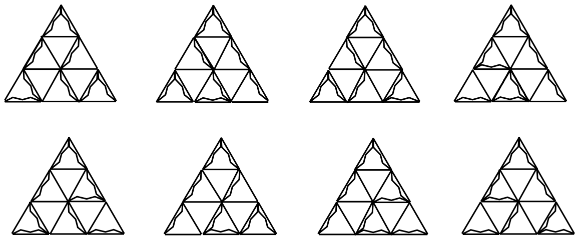

Figure 2. Schematic representation of the recursion relation for the number of open Hamiltonian walks (2.3) of h-type on $b = 3$ two-dimensional Sierpinski fractal structures.

Table 1. Values of the number A of Hamiltonian configurations relevant for the recursion relations (2.3), numbers h_1 and g_1 of open HWs on the generators of two-dimensional Sierpinski fractals, connectivity constant ω for HWs, and connectivity constant μ for SAWs (obtained via RG method—μ^{RG} and numerically estimated μ^{num} in [28]), for $2 \leqslant b \leqslant 8$.

b	A	h_1	g_1	ω	$\mu^{\mathrm{RG}}(\mu^{\mathrm{num}})$
2	2	2	3	1.317 98	2.288 (2.282 $\pm$ 0.007)
3	8	10	11	1.391 57	2.491 (2.49 $\pm$ 0.02)
4	40	92	112	1.461 86	2.656 (2.686 $\pm$ 0.004)
5	360	1852	2286	1.521 55	2.791 (2.82 $\pm$ 0.01)
6	3872	78 032	94 696	1.568 95	2.904 (2.92 $\pm$ 0.02)
7	62 848	6 846 876	8 320 626	1.610 11	3.005 (2.99 $\pm$ 0.05)
8	1287 840	1255 156 712	1527 633 172	1.645 28	(3.13 $\pm$ 0.07)

On the other hand, from (2.3)–(2.5) one has $h_{l+1} = AK^y h_l^{b(b+1)/2}$, i.e., $\ln h_l$ satisfies the difference equation $\ln h_{l+1} = \ln AK^y + \frac{b(b+1)}{2} \ln h_l$, whose solution is

$$\ln h_{l+1} = \frac{1 - [b(b+1)/2]^l}{1 - [b(b+1)/2]} \ln(AK^y) + \left(\frac{b(b+1)}{2}\right)^l \ln h_1. \tag{2.7}$$

From this equation, together with the explicit expression for the number of sites

$$N_{l+1} = \frac{b+4}{b+2}\left(\frac{b(b+1)}{2}\right)^{l+1} + 2\frac{b+1}{b+2}, \tag{2.8}$$

which follows directly from relation (2.6), one can derive the general form

$$\omega = A^{\frac{4}{b(b+4)(b^2-1)}} h_1^{\frac{4}{b(b+1)(b+4)}} g_1^{\frac{2}{(b+1)(b+4)}} \tag{2.9}$$

of the connectivity constant (1.2) for HWs on two-dimensional SFs. Consequently, in order to calculate ω for any particular 2D SF, one should find the numbers h_1 and g_1 of open HWs on the generator, and the number A of all Hamiltonian configurations which are relevant for recursion relations (2.3). In table 1 we present these numbers, together with the values of ω, for $2 \leqslant b \leqslant 8$. As one can see, for $b = 2$ and $b = 3$ the numbers g_1, h_1 and A are small and can be directly enumerated, whereas for larger values of b they quickly increase, so that enumeration should be computerized (calculation of the numbers A, g_1 and h_1 required 13 min for $b = 7$ case, and about 100 h for $b = 8$, both on a computer with a processor MIPS R10000, Rev 2.6 on 180 MHz). One should mention that the connectivity constant for the Sierpinski gasket ($b = 2$) has already been calculated in a different way by Bradley [6].

Combining equations (2.7)–(2.9) it is not difficult to see that $h_l = G\omega^{N_l}$, where G depends only on b, and correspondingly $C_l \sim \omega^{N_l}$. Comparing with (1.1) one can conclude that neither surface nor power correction terms are present in the scaling form for the number of closed HWs on two-dimensional Sierpinski fractals.

2.1. Comparison with the self-avoiding walk case

It is interesting to compare the value of the connectivity constant obtained for the case of Hamiltonian walks to that corresponding to all possible self-avoiding configurations on 2D SFs. Our algorithm for enumerating HWs is easily adjusted for that purpose. By means of an exact renormalization group (RG) approach [25, 26], these configurations can be used for calculating the connectivity constant μ for ordinary SAWs, which was done earlier only for the $b = 2$ case [26]. Here we extend an exact RG calculation of the connectivity constant μ for any b.

The connectivity constant μ for the SAW model is equal to $\mu = \lim_{N\to\infty}(c_{N+1}/c_N) = \lim_{N\to\infty}(p_{N+1}/p_N)$, where c_N (p_N) is the average number of distinct open (closed) n-step SAWs. In order to calculate μ within the exact RG approach, one should introduce two generating functions $B^{(l)}$ and $B_1^{(l)}$,

$$B^{(l)} = \sum_N \mathcal{B}_N^{(l)} x^N, \qquad B_1^{(l)} = \sum_N \mathcal{B}_{1,N}^{(l)} x^N,$$

where x is the statistical weight of each step of the SAW (fugacity), whereas $\mathcal{B}_N^{(l)}$ $(\mathcal{B}_{1,N}^{(l)})$ is the number of SAWs which enter the lth-order generator $G_l^2(b)$ at one vertex, and leave it at the second, without (with) visiting the third one. For every 2D SF lattice functions B and B_1 obey recursion relations of the following form,

$$B^{(l+1)} = \sum_{i,j} f_{i,j}(b)(B^{(l)})^i \left(B_1^{(l)}\right)^j, \qquad B_1^{(l+1)} = \sum_{i,j} g_{i,j}(b)(B^{(l)})^i \left(B_1^{(l)}\right)^j, \tag{2.10}$$

where $f_{i,j}(b)$ and $g_{i,j}(b)$ are coefficients that do not depend on l, but do depend on the fractal parameter b. The initial conditions are $B^{(0)} = x$, $B_1^{(0)} = x^2$ and the connectivity constant μ is equal to $1/x^*$, where x^* is the value of the fugacity for which one approaches the fixed point (B^*, B_1^*) of (2.10), after a large (infinite) number of iterations.

The explicit RG recursion relations for 2D SFs with $b = 2$ are

$$B' = B^2 + B^3 + 2BB_1 + \underline{2B^2B_1} + B_1^2, \qquad B_1' = B^2B_1 + \underline{2BB_1^2}$$

and for $b = 3$,

$$\begin{aligned} B' = {} & B^3 + 3B^4 + B^5 + 2B^6 + 3B^2B_1 + 12B^3B_1 + 4B^4B_1 + 8B^5B_1 + 3BB_1^2 + 16B^2B_1^2 \\ & + 5B^3B_1^2 + \underline{8B^4B_1^2} + B_1^3 + 8BB_1^3 + 2B^2B_1^3 + B_1^4 \end{aligned}$$

$$B_1' = B^4B_1 + 2B^5B_1 + 4B^3B_1^2 + 8B^4B_1^2 + 5B^2B_1^3 + \underline{8B^3B_1^3} + 2BB_1^4$$

whereas relations for $b = 4$ and 5 are given in appendix B. For $b = 6$ and 7 RG relations are too cumbersome to be quoted here, but they are available upon request. Underlined terms in quoted RG relations correspond to the Hamiltonian configurations, as one can check by direct comparison with relations (2.3); replacing g_l and h_l in (2.3) by B and B_1, respectively, one obtains underlined terms in the RG relations (values of coefficient A are given in table 1). It is obvious that for larger b values the number of SAW configurations is much larger than the number of Hamiltonian configurations, and for that reason we were not able to enumerate all SAW configurations on 2D SF beyond $b = 7$.

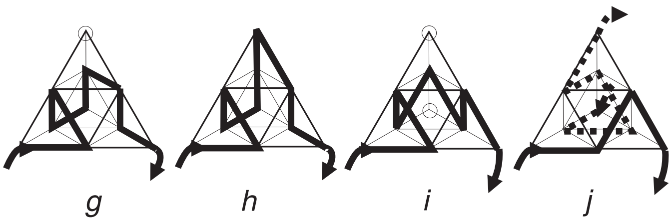

Figure 3. Examples of four possible types of open HWs on $G_1^3(2)$. Vertices not visited by the Hamiltonian walker are encircled.

For all b considered here recursive relations (2.10) have only one nontrivial fixed point $(B_b^*, 0)$, where B_b^* lies in the interval $0 < B_b^* < 1$. One can check that by setting $B_1 = 0$ in (2.10) RG equations used in [27] for calculating critical exponent ν (connected with the mean end-to-end distance) for SAWs on 2D SFs are recovered. Of course, the SAW model treated in [27] is slightly different (each unit triangle within the fractal can be traversed only along one side) from the usual one, treated here, but both of them belong to the same universality class, i.e., the critical exponent ν is equal for both considered SAW models. This is not the case with the connectivity constant, which is a nonuniversal quantity, so an extra RG parameter B_1 had to be introduced.

The final RG results μ^{RG} for the SAW connectivity constant are given in the last column of table 1, together with the corresponding values μ^{num} obtained in [28] using a graph counting technique. As one can expect, the connectivity constant μ for a SAW is larger than ω for HW model, for every considered SF, since the physical meaning of the connectivity constant is the average number of steps available to the walker after N steps completed, for large N. One can also see that the values of μ obtained by two different methods for $b = 4$ and 5 are not in good agreement. The RG method applied here is exact, implying that numerical estimations within the graph counting technique used in [28] were not accurate enough.

3. Hamiltonian walks on three-dimensional Sierpinski fractals

We proceed by analysing the properties of HWs on the three-dimensional (3D) SF family. A 3D SF can be constructed recursively as in the 2D case, the only difference being that the generator $G_1^3(b)$ of the fractal with the parameter b is no longer a triangle, but a tetrahedron that contains $b(b+1)(b+2)/6$ upward-oriented smaller tetrahedrons. Consequently, one should observe four types of open HWs that traverse the lth-order generator in order to obtain the overall number of closed HWs on 3D SF. The first three types are HWs which enter the generator at one vertex and leave it at another, meanwhile

- visiting the third, but not the fourth vertex (g-type),
- visiting both the third and the fourth vertex (h-type),
- visiting neither the third nor the fourth vertex (i-type).

HWs of the fourth possible type (j-type) consist of two self-avoiding branches, and correspond to the walks that enter the generator and leave it without visiting the remaining two vertices, then, after visiting other parts of the lattice, enter the same generator again at the third corner vertex and finally leave it at the fourth corner vertex. Examples of these types of walks are sketched in figure 3. In principle, it is possible to establish a closed set of recursion relations for the numbers g_l, h_l, i_l and j_l of the corresponding walks for any 3D SF in the following form,

$$
\begin{aligned}
g_{l+1} &= \sum_{n,m,k} \mathcal{G}(n,m,k) g_l^n h_l^m i_l^k j_l^{\frac{b(b+1)(b+2)}{6}-(n+m+k)}, \\
h_{l+1} &= \sum_{n,m,k} \mathcal{H}(n,m,k) g_l^n h_l^m i_l^k j_l^{\frac{b(b+1)(b+2)}{6}-(n+m+k)}, \\
i_{l+1} &= \sum_{n,m,k} \mathcal{I}(n,m,k) g_l^n h_l^m i_l^k j_l^{\frac{b(b+1)(b+2)}{6}-(n+m+k)}, \\
j_{l+1} &= \sum_{n,m,k} \mathcal{J}(n,m,k) g_l^n h_l^m i_l^k j_l^{\frac{b(b+1)(b+2)}{6}-(n+m+k)},
\end{aligned} \tag{3.1}
$$

where $\mathcal{G}(n,m,k)$, $\mathcal{H}(n,m,k)$, $\mathcal{I}(n,m,k)$ and $\mathcal{J}(n,m,k)$ are the numbers of open Hamiltonian configurations of the corresponding types, with n branches of g-type, m branches of h-type, k branches of i-type, and $[b(b+1)(b+2)/6 - (n+m+k)]$ branches of j-type. The number C_{l+1} of all closed HWs within the $(l+1)$th-order generator for any b is equal to

$$
C_{l+1} = \sum_{n,m,k} \mathcal{B}(n,m,k) g_l^n h_l^m i_l^k j_l^{\frac{b(b+1)(b+2)}{6}-(n+m+k)},
$$

where $\mathcal{B}(n,m,k)$ is the number of all closed Hamiltonian configurations with n branches of g-type, m branches of h-type, k branches of i-type, and $[b(b+1)(b+2)/6 - (n+m+k)]$ branches of j-type. As one can see, the recursion relations (3.1) for the number of open HWs on 3D Sierpinski fractals are much more complicated than the corresponding equations (2.3) for 2D SFs. Consequently, it is not possible to find an explicit expression, similar to (2.9), for the connectivity constant ω. Instead, one should perform a numerical analysis of the recursion relations (3.1) in order to find the value of ω. We shall demonstrate the method on the particular case of the $b = 2$ fractal.

By computer enumeration of the possible HW configurations within the $(l+1)$th-order generator $G_{l+1}^3(2)$ of the $b = 2$ 3D Sierpinski fractal, we found the following recursion relations,

$$
g' = 6g^2j^2 + 4g^3j + 2g^4 + 12ij^2h + 24igjh + 24ig^2h + 8i^2h^2, \tag{3.2}
$$

$$
h' = 24j^2hg + 16h^2ij + 16hg^3 + 32h^2gi + 24g^2hj, \tag{3.3}
$$

$$
i' = 12igj^2 + 12ig^2j + 8ig^3 + 8i^2jh + 16i^2gh, \tag{3.4}
$$

$$
j' = 8i^2h^2 + 48igjh + 22j^4 + 2g^4 + 8g^3j + 24ig^2h, \tag{3.5}
$$

where we have used the prime symbol as a superscript for the numbers of HWs on the $(l+1)$th-order generator $G_{l+1}^3(2)$ and no indices for the lth-order numbers. From the definition (1.2) of the connectivity constant and the formula for the number C_{l+1} of closed HWs within $G_{l+1}^3(2)$,

$$
C_{l+1} = 16g_l^2h_l^2, \tag{3.6}
$$

it then follows that

$$
\ln\omega = \lim_{l\to\infty} \frac{\ln C_{l+1}}{N_{l+1}} = \frac{1}{2}\lim_{l\to\infty}\frac{\ln g_l}{N_l} + \frac{1}{2}\lim_{l\to\infty}\frac{\ln h_l}{N_l}, \tag{3.7}
$$

where $N_l = 2(4^l + 1)$ is the number of sites in $G_l^3(2)$. On the other hand, from the recursion relation (3.2) for the numbers g_l one obtains

$$
\begin{aligned}
\lim_{l\to\infty}\frac{\ln g_{l+1}}{N_{l+1}} &= \frac{1}{2}\lim_{l\to\infty}\frac{\ln g_l}{N_l} + \frac{1}{2}\lim_{l\to\infty}\frac{\ln j_l}{N_l} \\
&\quad + \frac{1}{2}\lim_{l\to\infty}\frac{1}{4^{l+1}}\ln\left(6 + 4x_l + 2x_l^2 + 24y_lz_l + \frac{12y_lz_l}{x_l^2} + \frac{24y_lz_l}{x_l} + \frac{8y_l^2z_l^2}{x_l^2}\right)
\end{aligned} \tag{3.8}
$$

where $x_l = g_l/j_l$, $y_l = h_l/j_l$ and $z_l = i_l/j_l$. In a similar way, from (3.3) it follows that

$$\lim_{l\to\infty} \frac{\ln h_{l+1}}{N_{l+1}} = \frac{1}{4}\lim_{l\to\infty}\frac{\ln h_l}{N_l} + \frac{1}{4}\lim_{l\to\infty}\frac{\ln g_l}{N_l} + \frac{1}{2}\lim_{l\to\infty}\frac{\ln j_l}{N_l} + \frac{1}{2}\lim_{l\to\infty}\frac{1}{4^{l+1}}\ln 8\left(3 + 3x_l + 2x_l^2 + 4y_l z_l + \frac{2y_l z_l}{x_l}\right). \tag{3.9}$$

The new variables x_l, y_l and z_l fulfil recursion relations which are easy to deduce from their definitions and equations (3.2)–(3.5), and are not difficult to iterate (starting with initial values $x_1 = \frac{11}{14}$, $y_1 = 1$ and $z_1 = \frac{4}{7}$, following from the numbers $g_1 = 88$, $h_1 = 112$, $i_1 = 64$ and $j_1 = 112$, found by direct computer enumeration of the corresponding HWs within the generator $G_1^3(2)$). One quickly finds that x_l, y_l and z_l tend to zero, and $z_l \ll x_l \ll y_l$, $x_l^2 \sim y_l z_l$ for large l, meaning that the last terms on the right-hand side of equations (3.8) and (3.9) tend to zero. It is then straightforward to see that from (3.8) and (3.9) it follows that

$$\lim_{l\to\infty}\frac{\ln g_l}{N_l} = \lim_{l\to\infty}\frac{\ln h_l}{N_l} = \lim_{l\to\infty}\frac{\ln j_l}{N_l},$$

and, according to (3.7), one finds

$$\ln\omega = \lim_{l\to\infty}\frac{\ln j_l}{N_l}. \tag{3.10}$$

Instead of the number j_l, which rapidly grows with l, it is convenient to introduce yet another variable

$$u_l = \frac{\ln j_l}{4^l} - \frac{\ln 22}{3}\left(\frac{1}{4} - \frac{1}{4^l}\right), \tag{3.11}$$

which has the initial value $u_1 = \frac{\ln 112}{4}$. Numerically iterating its recursion relation, together with those for x_l, y_l and z_l, one can show that u_l tends to 1.250 778 8499… when $l \to \infty$. Finally, since $\ln\omega = \frac{1}{2}\lim_{l\to\infty} u_l + \frac{1}{24}\ln 22$, the connectivity constant for the $b = 2$ 3D Sierpinski fractal is equal to $\omega = 2.125\,87\ldots$.

In order to find the first correction to the leading-order behaviour of C_l one needs to know the asymptotic behaviour of the numbers x_l, y_l and j_l, according to the formula

$$\frac{\ln C_{l+1}}{N_{l+1}} = \frac{\ln 16}{N_{l+1}} + 2\frac{\ln x_l}{N_{l+1}} + 2\frac{\ln y_l}{N_{l+1}} + 4\frac{\ln j_l}{N_{l+1}}, \tag{3.12}$$

following from (3.6) and the definition of x_l and y_l. Keeping only the leading-order terms in the recursion relation for x_l one gets $x_{l+1} \approx \mathrm{const}\,x_l^2$, which means that x_l behaves as

$$x_l \sim \lambda^{2^l} \tag{3.13}$$

for large l. Numerically iterating the recursion relations for x_l, y_l and z_l one finds $\lambda = \lim_{l\to\infty}\frac{\ln x_l}{2^l} = 0.9055\ldots$. It then follows that $y_{l+1} \approx \frac{12}{11}x_l y_l$, $z_{l+1} \approx \frac{6}{11}x_l z_l$, implying that $\frac{y_l}{z_l} \sim 2^l$, which, together with the numerically established relation $x_l^2 \sim y_l z_l$, gives

$$z_l \sim 2^{-l/2}x_l \sim 2^{-l/2}\lambda^{2^l}, \qquad y_l \sim 2^{l/2}\lambda^{2^l}. \tag{3.14}$$

On the other hand, from the definition of u_l(3.11) and the corresponding recursion relation it follows that

$$\frac{\ln j_l}{4^l} = u_1 + \sum_{k=1}^{l-1}\frac{1}{4^{k+1}}\ln\left(1 + \frac{4}{11}x_k^3 + \frac{1}{11}x_k^4 + \frac{24}{11}x_k y_k z_k + \frac{12}{11}x_k^2 y_k z_k + \frac{4}{11}y_k^2 z_k^2\right) + \frac{\ln 22}{3}\left(\frac{1}{4} - \frac{1}{4^l}\right).$$

Then, using (3.10), one can write

$$\frac{\ln j_l}{4^l} = 2\ln\omega - \frac{1}{4^l}\frac{\ln 22}{3} - \sum_{k=l}^{\infty}\frac{1}{4^{k+1}}\ln\left(1+\frac{4}{11}x_k^3+\frac{1}{11}x_k^4+\frac{24}{11}x_k y_k z_k+\frac{12}{11}x_k^2 y_k z_k+\frac{4}{11}{y_k}^2 z_k^2\right),$$

and consequently, since

$$\sum_{k=l}^{\infty}\frac{1}{4^{k+1}}\ln\left(1+\frac{4}{11}x_k^3+\frac{1}{11}x_k^4+\frac{24}{11}x_k y_k z_k+\frac{12}{11}x_k^2 y_k z_k+\frac{4}{11}y_k^2 z_k^2\right) \leqslant \ln\frac{104}{11}\sum_{k=l}^{\infty}\frac{1}{4^{k+1}} = \frac{1}{3}\frac{1}{4^l}\ln\frac{104}{11},$$

which is not difficult to show, one obtains

$$\ln j_l = 2 * 4^l \ln\omega + O(1). \tag{3.15}$$

Finally, from (3.12)–(3.15) it follows that

$$\ln C_l = N_l \ln\omega + N_l^{1/2}\ln\lambda^{\sqrt{2}} + \tfrac{1}{2}\ln N_l + O(1),$$

which means that the behaviour (1.1) of the number of HWs, expected for homogeneous lattices, is also satisfied for this fractal lattice, with the following values of the exponents:

$$\sigma = \tfrac{1}{2}, \qquad a = \tfrac{1}{2}.$$

The number of all possible HW configurations within a generator of the 3D Sieprinski fractal grows rapidly with b. In appendix C we give the corresponding recursion relations for the numbers g_l, h_l, i_l and j_l found for the $b = 3$ 3D SF, together with their initial values, and the formula for the number C_{l+1} of closed HWs. The CPU time required for the enumeration and classification of HW configurations was so long for the $b = 3$ case that we could not go beyond it. However, the method used for $b = 2$ 3D SF in principle could be applied for any b with no qualitative difference. Analysing recursion relations given in appendix C in that manner, for the $b = 3$ 3D SF we found that the number C_l of closed HWs obeys a scaling form similar to that of the $b = 2$ 3D case with the following values for the connectivity constant ω and exponents σ and a:

$$\omega = 2.272\,2364\ldots, \qquad \sigma = \frac{\ln 3}{\ln 10}, \qquad a = 0.386\ldots.$$

4. Hamiltonian walks on *n*-simplex fractals

To complete our analysis of the nature of Hamiltonian walks on 2D and 3D Sierpinski fractal lattices, we now turn to n-simplexes, which are in some ways a generalization of SFs for $b = 2$ in $n - 1$ dimensions. To obtain an n-simplex lattice [25] one starts with a complete graph of n points and replaces each of these points by a new complete graph of n points. The subsequent stages are constructed self-similarly, by repeating this procedure. After l such iterations one obtains an *n-simplex of order l*, whereas the complete n-simplex lattice is obtained in the limit $l \to \infty$. It is trivial to see that the connectivity constant ω for HWs on 3-simplex lattice is equal to 1, whereas Bradley found that $\omega = 1.399710\ldots$ for the 4-simplex [13]. In principle, it is possible to establish an exact set of recursion relations for the numbers of suitably chosen prerequisite HWs on any n-simplex, as Bradley did for $n = 4$. Here we will demonstrate the method on $n = 5$ and $n = 6$ cases.

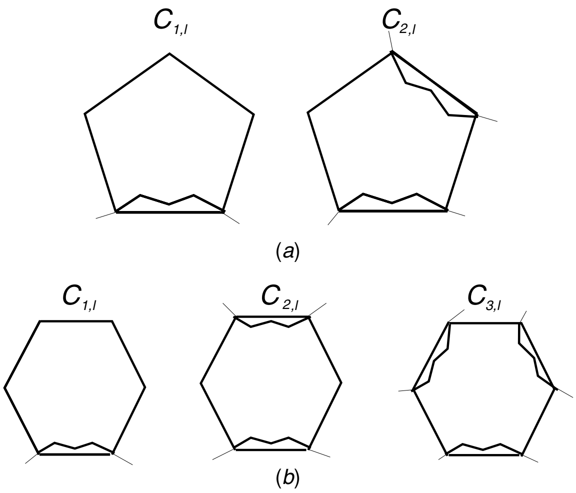

Figure 4. Schematic representation of types of open Hamiltonian walks through a (a) 5-simplex and (b) 6-simplex of order l.

4.1. 5-simplex

Any closed HW of order $(l+1)$ on this fractal can be decomposed into five open HWs through 5-simplices of order l. There are two possible types of these open HWs, as depicted in figure 4(a). The first corresponds to walks which enter the simplex at one corner, visit all vertices inside it, and leave it—we shall denote the number of these walks by $C_{1,l}$. A walk of the second type enters the simplex at one of its five corners, wanders around it visiting some of the vertices inside it, leaves it through the second corner, and afterwards enters it again at the third corner, visits all the remaining vertices, and finally leaves it—let the total number of these walks on the lth-order 5-simplex be $C_{2,l}$. The total number C_{l+1} of closed HWs is equal to

$$C_{l+1} = 12C_{1,l}^5 + 30C_{1,l}^4 C_{2,l} + 60C_{1,l}^3 C_{2,l}^2 + 132C_{2,l}^5 \tag{4.1}$$

which we found by computer enumeration, together with the recursion relations

$$\begin{aligned} C_{1,l+1} &= 6C_{1,l}^5 + 30C_{1,l}^4 C_{2,l} + 78C_{1,l}^3 C_{2,l}^2 + 96C_{1,l}^2 C_{2,l}^3 + 132C_{1,l} C_{2,l}^4 + 132C_{2,l}^5, \\ C_{2,l+1} &= 2C_{1,l}^5 + 13C_{1,l}^4 C_{2,l} + 32C_{1,l}^3 C_{2,l}^2 + 88C_{1,l}^2 C_{2,l}^3 + 220C_{1,l} C_{2,l}^4 + 186C_{2,l}^5. \end{aligned} \tag{4.2}$$

The initial values for these numbers are $C_{1,1} = 6$ and $C_{2,1} = 2$. From the recursion relation (4.1) it follows that

$$\frac{\ln C_{l+1}}{5^{l+1}} = \frac{\ln C_{2,l}}{5^l} + \frac{1}{5^{l+1}} \left(132 + 60x_l^3 + 30x_l^4 + 12x_l^5\right), \tag{4.3}$$

where the new variable $x_l = C_{1,l}/C_{2,l}$ satisfies the recursion relation

$$x_{l+1} = 6\frac{22 + 22x_l + 16x_l^2 + 13x_l^3 + 5x_l^4 + x_l^5}{186 + 220x_l + 88x_l^2 + 32x_l^3 + 13x_l^4 + 2x_l^5}, \tag{4.4}$$

obtained from (4.2). Numerically iterating this relation, starting with $x_1 = 3$, we find that $x_l \to 0.802\,318\,837\ldots$ when $l \to \infty$, and consequently, since $N_l = 5^l$, it follows that

$$\ln\omega = \lim_{l\to\infty} \frac{\ln C_{l+1}}{5^{l+1}} = \lim_{l\to\infty} \frac{\ln C_{2,l}}{5^l} + \lim_{l\to\infty} \frac{1}{5^{l+1}} \ln\left(1 + \frac{5}{11}x_l^3 + \frac{5}{22}x_l^4 + \frac{1}{11}x_l^5\right) = \lim_{l\to\infty} \frac{\ln C_{2,l}}{5^l}.$$

The last limiting value can be quickly calculated if we introduce the variable

$$y_l = \frac{\ln C_{2,l}}{5^l} - \frac{\ln 186}{4}\left(\frac{1}{5} - \frac{1}{5^l}\right) - \frac{\ln 2}{5},$$

which, according to (4.2), obeys the recursion relation

$$y_{l+1} = y_l + \frac{1}{5^{l+1}} \ln\left(1 + \frac{110}{93}x_l + \frac{44}{93}x_l^2 + \frac{16}{93}x_l^3 + \frac{13}{186}x_l^4 + \frac{1}{93}x_l^5\right), \tag{4.5}$$

and has the initial value $y_l = 0$. Then, iterating (4.5) simultaneously with (4.4) we find $y_l \to 0.141\,065\,489\,481\ldots$ for large l, and finally, since $\ln\omega = \lim_{l\to\infty} y_l + \ln 186/20 + \ln 2/5$, we obtain $\omega = 1.717\,769\ldots$.

To examine the leading-order correction to the number of Hamiltonian walks on the 5-simplex fractal, we note that for any k the quantity y_l can be written as $y_l = y_k + \sum_{m=k}^{l-1} (y_{m+1} - y_m)$. Taking the $l \to \infty$ limit and keeping k fixed in that equation, one obtains

$$\ln\omega = \frac{\ln C_{2,k}}{5^k} + \frac{\ln 186}{4\cdot 5^k} + \sum_{m=k}^{\infty} \frac{1}{5^{m+1}} \ln\left(1 + \frac{110}{93}x_m + \frac{44}{93}x_m^2 + \frac{16}{93}x_m^3 + \frac{13}{186}x_m^4 + \frac{1}{93}x_m^5\right).$$

Since $x_1 = 3$ and the array x_m is monotonically decreasing, the sum on the right-hand side of the above equation is bounded from above by

$$\ln(21.72)\sum_{m=k}^{\infty}\frac{1}{5^{m+1}} = \ln(21.72)\frac{1}{5^{k+1}}\left(1 + \frac{1}{5} + \cdots\right) = \frac{1}{4}\ln(21.72)\frac{1}{5^k}.$$

Therefore we can conclude that

$$\ln C_{2,k} = 5^k \ln\omega + O(1) \qquad \text{and} \qquad \ln C_{1,k} = \ln C_{2,k} + \ln x_k = 5^k \ln\omega + O(1). \tag{4.6}$$

Finally, for the number C_l of closed HWs, from (4.3), we obtain the same behaviour:

$$\ln C_l = 5^l \ln\omega + O(1). \tag{4.7}$$

Comparing with equation (1.1) we see that in the case of the 5-simplex fractal both the surface and the power correction to the number of HWs are absent.

4.2. 6-simplex

In addition to the $C_{1,l}$- and $C_{2,l}$-type walks, already defined for the 5-simplex, one should introduce another type of walks for complete enumeration of HWs on the 6-simplex lattice. These walks enter the 6-simplex three times, as depicted in figure 4(*b*). Let us denote their number on the 6-simplex of order l by $C_{3,l}$. The total number C_{l+1} of closed HWs within the 6-simplex of order $(l+1)$ is equal to

$$C_{l+1} = 60C_{1,l}^6 + 360C_{1,l}^5C_{2,l} + 1170C_{1,l}^4C_{2,l}^2 + 1920C_{1,l}^3C_{2,l}^3 + 3960C_{1,l}^2C_{2,l}^4 + 7920C_{1,l}C_{2,l}^5 + 5580C_{2,l}^6, \tag{4.8}$$

as we found by computer enumeration. Numbers $C_{1,l}$, $C_{2,l}$ and $C_{3,l}$ satisfy closed set of recursion relations, which can be numerically analysed in a way similar to, although more complicated than, that used in the case of the 5-simplex lattice (see appendix D). In contrast to the 5-simplex case, where numbers $C_{1,l}$, $C_{2,l}$ and C_l have the same asymptotic behaviour (4.6) and (4.7), here we obtained

$$\ln C_{1,l} = 6^l \ln\omega + 2^{l+1}\ln\lambda + O(1), \tag{4.9}$$

$$\ln C_{2,l} = 6^l \ln\omega + 2^l \ln\lambda + O(1), \tag{4.10}$$

$$\ln C_{3,l} = 6^l \ln \omega + O(1), \tag{4.11}$$

with $\omega = 2.0550\ldots$, $\lambda = 0.9864$ and

$$\ln C_l = N_l \ln \omega + N_l^\sigma \ln \mu_S + O(1), \tag{4.12}$$

with $N_l = 6^l$, $\sigma = \ln 2/\ln 6$ and $\mu_S = \lambda^3$. The surface correction to the number of HWs is present here, but still there is no term proportional to $\ln N_l$, which would imply the presence of the power correction. The same conclusion was obtained by Bradley [13] for the 4-simplex lattice, with $\sigma = 1/2$.

5. Discussion and conclusions

The values of the connectivity constant ω found by us, as well as some values previously found by other authors [13] are depicted in figure 5(a), as functions of the coordination number[3] z of the lattice, together with the Flory [29] and Orland [21] approximations, and ω for hexagonal [12], square [30], triangular [31] and cubic [15] lattices. One can clearly see that ω increases with z, which is in accord with Flory $\omega_F = (z-1)/e$ and Orland *et al* $\omega_O = z/e$ formulae, but it is obvious that ω depends on other lattice properties too. Furthermore, all values of ω lie between the values predicted by these two formulae, and it seems that these kinds of approximations give satisfying results for the fractal lattices studied here. Based on the information in this figure one may conclude that ω_O and ω_F are good upper and lower bounds for fractal HW connectivity constants.

In figure 5(b) the connectivity constant ω for 2D SFs is presented as a function of the reciprocal of the fractal scaling parameter b. It seems that for $b \to \infty$ the connectivity constant might approach its triangular lattice value. This is not surprising, since for $b = \infty$ the first step of the construction of the corresponding 2D SF is already the wedge of the triangular lattice. In the same limit, 3D SFs approach the corresponding three-dimensional Euclidean lattice, so it would be useful to obtain recursion relations for HWs on these fractals for larger b, since there are fewer results for more realistic three-dimensional lattices. This task requires faster computers, as well as establishing a better algorithm for enumerating the HW configurations within a generator of a fractal, which is something we are planning to do in the nearest future.

As for the correction to the leading-order asymptotic behaviour of the number of HWs, we have shown that the surface correction $\mu_s^{N^\sigma}$ appears for neither the two-dimensional Sierpinski fractals nor for the 5-simplex lattice. In contrast, for both three-dimensional Sierpinski fractals considered here, as well as for the 4-simplex [13] and the 6-simplex lattice, the surface correction is present, with the value of the exponent $\sigma = 1/d_f$, where d_f is the fractal dimension of the corresponding lattice[4]. This result is certainly not a simple generalization of the formula proposed for the homogeneous lattices: $\sigma = (d-1)/d$. This is actually not surprising: the correction term $\mu_S^{N^\sigma}$ in (1.1) was originally introduced in order to take into account possible surface tension effects, since at low temperatures a SAW forms a compact globule (see, for instance, [36]). The value $\sigma = (d-1)/d$ for homogeneous lattices then follows from the fact that the surface of such a globule is proportional to $N^{(d-1)/d}$. In the case of fractal lattices it is, however, questionable whether such surface effects exist at all. For instance, all sites of the $b = 2$ 3D SF lie on the surface, which is not the case for the $b = 3$ 3D SF, but for both lattices the number of HWs has the correction term $\mu_s^{N^\sigma}$. Or, in the case

[3] The coordination number z (the average number of nearest neighbours per site) for the n-simplex lattice is equal to n, whereas it can be shown that $z = 6(b+2)/(b+4)$ for 2D SF with the scaling parameter b, $z = 6$ for $b = 2$ 3D SF and $z = 6.75$ for $b = 3$ 3D SF.

[4] Fractal dimension for 3D SF is $d_f = \ln(b(b+1)(b+2)/6)/\ln b$, and for the n-simplex lattice $d_f = \ln n/\ln 2$.

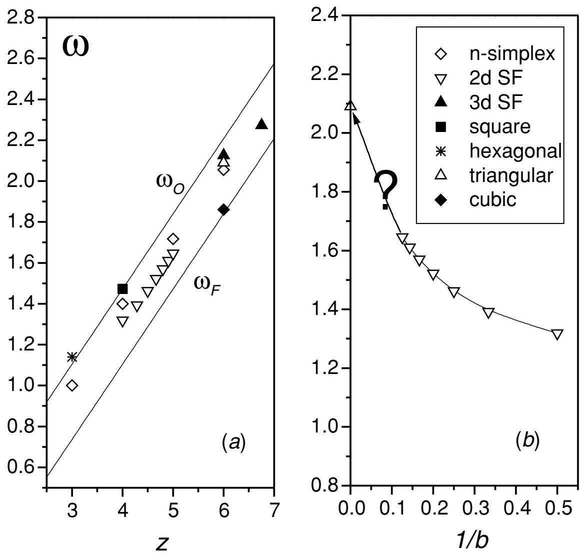

Figure 5. (*a*) Connectivity constant ω for Hamiltonian walks on Sierpinski fractals (∇ for 2D SF, and full triangles for 3D SF) and n-simplex lattices ($\diamond$) as functions of the coordination number z together with previously found results for 4-simplex [13], hexagonal [12] (star), square [29] ($\blacksquare$), triangular [30] ($\triangle$), and cubic [15] (full diamond) lattices, as well as Flory [28] and Orland [21] approximations, $\omega_F = (z-1)/e$ and $\omega_O = z/e$, respectively. (*b*) Connectivity constant for 2D SFs as a function of the reciprocal of the scaling parameter b, where line connecting triangles serves merely as the guide to the eye. Open up-oriented triangle on vertical axes depicts the value of ω for triangular lattice.

of an n-simplex lattice all sites have the same number n of neighbours, and one should not expect any surface correction, but still, for some of them the correction $\mu_s^{N^\sigma}$ was found. So, it seems that the term $\mu_S^{N^{1/d_f}}$, obtained for some of the studied fractals, does not originate from the surface effects, which is also supported by the fact that N^{1/d_f} is proportional to the mean radius of the globule formed by a HW, and not to its surface.

It is interesting to note here that the existence of the term $\mu_S^{N^{1/d_f}}$ in the scaling form for the number of HWs, coincides with the existence of the polymer coil to globule transition on the corresponding lattice. As was shown earlier, a polymer chain in a solvent, modelled by SAWs on the 2D Sierpinski fractals [27] and 5-simplex [32] can exist only in the swollen phase; on the 3D Sierpinski fractals [33–35], 4-simplex [25] and 6-simplex [32] lattices, when the temperature is lowered the polymer undergoes a collapse transition from an expanded state to a globule state (compact or semi-compact [34]). Analysing the asymptotic behaviour of different types of open HWs on fractals one can observe that the collapse transition exists on lattices whose topology allows for the statistical domination of HWs which are not localized. In particular, HWs on the 2D SG fractals cannot enter a generator of any order more than once, i.e., all the walks are localized. On the 5-simplex fractal this is possible (see figure 4(*a*)), but the number $C_{1,l}$ of localized HWs and the number $C_{2,l}$ of delocalized HWs (walks that enter every lth-order 5-simplex twice) are of the same order (see (4.6), i.e., the delocalized HWs do not dominate. On the other hand, the delocalized HWs on the 3D SG fractals (j-type, see figure 3) and on the 6-simplex ($C_{2,l}$- and $C_{3,l}$-type, see figure 4(*b*)), as well as on the 4-simplex [13], are possible, and furthermore, the number of these walks is much larger than the number of localized HWs (see sections 3 and 4.2). This observation strongly resembles the conclusion obtained in a series of recent papers [24] about the delocalization of knots in the low-temperature globular phase. Although the term 'delocalization' was not used in quite the same sense in these two contexts, it seems that the same effect is in question, and this problem deserves further investigation.

Finally, the power dependence of the overall number C_N of closed HWs on the number of sites N of the lattice was found only for the 3D SFs. A more detailed inspection of the calculation of the exponent a for these lattices reveals that

$$a = \text{const} \lim_{l\to\infty} \frac{\ln \frac{h_l}{i_l}}{l}.$$

The numbers h_l and i_l correspond to the localized open Hamiltonian configurations that visit the maximal (4) and the minimal (2) number of vertices, respectively, within the generator of order l (see figure 3). In the case of 2D SFs, numbers of open configurations visiting the maximal or the minimal number of vertices were h_l and g_l, respectively, and it was shown that the ratio h_l/g_l=const for every l. Consequently, $\lim_{l\to\infty} \ln(h_l/i_l)/l = 0$, which may be the formal explanation for the absence of the power correction to the number of HWs on a 2D SF. On the other hand, on the n-simplex lattices only one type of localized HW configurations is possible, so it appears that the power term in the scaling form for the number of HWs is obtained on lattices where a larger number of different types of localized configurations is possible.

In conclusion, we can say that the method of exact recursion relations turned out to be very powerful for the generation and the enumeration of extremely long Hamiltonian walks on the two- and three-dimensional Sierpinski and n-simplex fractals. Furthermore, it allows for a detailed numerical analysis of HWs of different topologies. This enabled us to find various scaling forms for the number of closed HWs on these lattices. In the case of two-dimensional Sierpinski fractals, a closed-form expression is obtained for the connectivity constant. Very interesting results were obtained for the three-dimensional Sierpinski fractals. This should be utilized for attaining deeper insight into the realistic physical problems which can be modelled by Hamiltonian walks.

Acknowledgments

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Appendix A. Recursion relations for HWs on 2D Sierpinski fractals

In this appendix, we present the derivation of relations (2.1) and (2.3) for open and closed HWs on 2D SFs, for general b.

It is obvious that the number of closed HWs on the $(l+1)$th-order generator is of the form $C_{l+1} = \sum_i B_i h_l^{\alpha_i} g_l^{\beta_i}$, where B_i is the number of all closed Hamiltonian configurations consisting of α_i steps of h-type and β_i steps of g-type ('step' is here a part of HW that traverses lth-order generator within the considered $(l+1)$th-order generator). By definition, a closed HW visits all sites of the $(l+1)$th generator, consequently it traverses all $b(b+1)/2l$th-order generators within it, so that

$$\alpha_i + \beta_i = \frac{b(b+1)}{2}. \tag{A.1}$$

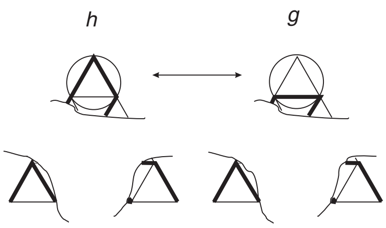

Figure A1. h- and g-type HWs on a G^2_{l+1} generator, which can be obtained from one another in a unique way. These two walks differ only in the parts surrounded by circles.

On the other hand, every h-type step occupies all three vertices of the lth generator it traverses, whereas a g-type step occupies only two vertices (the entering and the exiting one). This means that the numbers α_i and β_i also have to satisfy the following equation,

$$2\alpha_i + \beta_i = \frac{(b+1)(b+2)}{2}, \tag{A.2}$$

since the number of lth-order vertices inside the $(l+1)$th generator is $(b+1)(b+2)/2$. The system of equations (A.1) and (A.2) has a unique solution $\alpha_i = b+1$, $\beta_i = (b+1)(b-2)/2$ which completes the derivation of relation (2.1).

For open h-type HWs, in a similar way, we have $h_{l+1} = \sum_i A_i h_l^{x_i} g_l^{y_i}$, where exponents x_i and y_i satisfy the system $x_i + y_i = \frac{b(b+1)}{2}$, $2x_i + y_i = \frac{(b+1)(b+2)}{2} - 1$, whose only solution is $x_i = b$, $y_i = b(b-1)/2$. At the same time, every g-type HW on a generator G^2_{l+1} can be obtained from one and only one h-type HW (and vice versa), by substituting one h-step with a g-step, as depicted in figure A1. This means that all of these walks have exactly $(b-1)h$-steps and $[b(b-1)/2+1]$ g-steps, i.e. relations (2.3) are correct.

Appendix B. RG equations for the SAW model on a 2D SF

In this appendix, we give exact RG equations (2.10) for calculating the connectivity constant for the ordinary SAW model on the $b = 4$ and the $b = 5$ two-dimensional Sierpinski fractals. These equations were obtained via computer enumeration and classification of all SAW configurations within the corresponding fractal generator. RG relations (2.10) for $b = 6$ and 7 were also found, but they are too cumbersome to be quoted here and they are available upon request:

$b = 4:$

$$\begin{aligned}
B' = {} & B^4 + 6B^5 + 6B^6 + 9B^7 + 9B^8 + 9B^9 + 4B^{10} + 4B^3B_1 + 30B^4B_1 + 36B^5B_1 \\
& + 56B^6B_1 + 58B^7B_1 + 56B^8B_1 + 26B^9B_1 + 6B^2B_1^2 + 57B^3B_1^2 + 84B^4B_1^2 \\
& + 134B^5B_1^2 + 143B^6B_1^2 + 128B^7B_1^2 + 56B^8B_1^2 + 4BB_1^3 + 51B^2B_1^3 + 96B^3B_1^3 \\
& + 156B^4B_1^3 + 168B^5B_1^3 + 128B^6B_1^3 + \underline{40B^7B_1^3} + B_1^4 + 21BB_1^4 + 55B^2B_1^4 \\
& + 93B^3B_1^4 + 94B^4B_1^4 + 48B^5B_1^4 + 3B_1^5 + 14BB_1^5 + 28B^2B_1^5 \\
& + 20B^3B_1^5 + B_1^6 + 4BB_1^6
\end{aligned}$$

$$\begin{aligned}
B_1' = {} & B^6B_1 + 6B^7B_1 + 7B^8B_1 + 4B^9B_1 + 6B^5B_1^2 + 38B^6B_1^2 + 44B^7B_1^2 + 26B^8B_1^2 \\
& + 14B^4B_1^3 + 92B^5B_1^3 + 102B^6B_1^3 + 56B^7B_1^3 + 16B^3B_1^4 + 106B^4B_1^4 + 104B^5B_1^4 \\
& + \underline{40B^6B_1^4} + 9B^2B_1^5 + 58B^3B_1^5 + 40B^4B_1^5 + 2BB_1^6 + 12B^2B_1^6
\end{aligned}$$

$$
\begin{aligned}
b &= 5: \\
B' &= B^5 + 10B^6 + 20B^7 + 30B^8 + 54B^9 + 68B^{10} + 98B^{11} + 94B^{12} + 86B^{13} \\
&\quad + 38B^{14} + 16B^{15} + 5B^4B_1 + 60B^5B_1 + 140B^6B_1 + 228B^7B_1 + 443B^8B_1 \\
&\quad + 586B^9B_1 + 867B^{10}B_1 + 854B^{11}B_1 + 786B^{12}B_1 + 348B^{13}B_1 + 140B^{14}B_1 \\
&\quad + 10B^3B_1^2 + 146B^4B_1^2 + 402B^5B_1^2 + 718B^6B_1^2 + 1521B^7B_1^2 + 2137B^8B_1^2 \\
&\quad + 3203B^9B_1^2 + 3240B^{10}B_1^2 + 2918B^{11}B_1^2 + 1268B^{12}B_1^2 + 458B^{13}B_1^2 + 10B^2B_1^3 \\
&\quad + 184B^3B_1^3 + 610B^4B_1^3 + 1218B^5B_1^3 + 2846B^6B_1^3 + 4316B^7B_1^3 + 6433B^8B_1^3 \\
&\quad + 6648B^9B_1^3 + 5630B^{10}B_1^3 + 2306B^{11}B_1^3 + 664B^{12}B_1^3 + 5BB_1^4 + 126B^2B_1^4 \\
&\quad + 523B^3B_1^4 + 1209B^4B_1^4 + 3170B^5B_1^4 + 5307B^6B_1^4 + 7678B^7B_1^4 + 7960B^8B_1^4 \\
&\quad + 5960B^9B_1^4 + 2104B^{10}B_1^4 + \underline{360B^{11}B_1^4} + B_1^5 + 44BB_1^5 + 249B^2B_1^5 + 710B^3B_1^5 \\
&\quad + 2159B^4B_1^5 + 4118B^5B_1^5 + 5604B^6B_1^5 + 5554B^7B_1^5 + 3292B^8B_1^5 + 776B^9B_1^5 \\
&\quad + 6B_1^6 + 59BB_1^6 + 234B^2B_1^6 + 891B^3B_1^6 + 2031B^4B_1^6 + 2479B^5B_1^6 + 2086B^6B_1^6 \\
&\quad + 744B^7B_1^6 + 5B_1^7 + 36BB_1^7 + 214B^2B_1^7 + 630B^3B_1^7 + 626B^4B_1^7 + 324B^5B_1^7 \\
&\quad + B_1^8 + 28BB_1^8 + 117B^2B_1^8 + 72B^3B_1^8 + 2B_1^9 + 10BB_1^9 \\
B_1' &= B^8B_1 + 12B^9B_1 + 39B^{10}B_1 + 48B^{11}B_1 + 60B^{12}B_1 + 34B^{13}B_1 + 16B^{14}B_1 \\
&\quad + 8B^7B_1^2 + 102B^8B_1^2 + 344B^9B_1^2 + 432B^{10}B_1^2 + 556B^{11}B_1^2 + 314B^{12}B_1^2 \\
&\quad + 140B^{13}B_1^2 + 27B^6B_1^3 + 366B^7B_1^3 + 1278B^8B_1^3 + 1616B^9B_1^3 + 2098B^{10}B_1^3 \\
&\quad + 1156B^{11}B_1^3 + 458B^{12}B_1^3 + 50B^5B_1^4 + 722B^6B_1^4 + 2600B^7B_1^4 + 3254B^8B_1^4 \\
&\quad + 4128B^9B_1^4 + 2128B^{10}B_1^4 + 664B^{11}B_1^4 + 55B^4B_1^5 + 852B^5B_1^5 + 3148B^6B_1^5 \\
&\quad + 3808B^7B_1^5 + 4474B^8B_1^5 + 1968B^9B_1^5 + \underline{360B^{10}B_1^5} + 36B^3B_1^6 + 610B^4B_1^6 \\
&\quad + 2302B^5B_1^6 + 2590B^6B_1^6 + 2540B^7B_1^6 + 736B^8B_1^6 + 13B^2B_1^7 + 254B^3B_1^7 \\
&\quad + 981B^4B_1^7 + 948B^5B_1^7 + 592B^6B_1^7 + 2BB_1^8 + 54B^2B_1^8 + 220B^3B_1^8 \\
&\quad + 144B^4B_1^8 + 4BB_1^9 + 20B^2B_1^9.
\end{aligned}
\tag{B.1}
$$

Appendix C. Recursion relations for HWs within the $b = 3$ 3D SF

Here we give the recursion relations for the numbers g_l, h_l, i_l and j_l of open HW configurations within the $b = 3$ 3D SF, obtained via computer enumeration. With symbols g_{l+1}, h_{l+1}, i_{l+1}, j_{l+1}, g_l, h_l, j_l and i_l abbreviated to g', h', i', j', g, h, i and j, respectively, these relations have the following form:

$$
\begin{aligned}
g' &= 6120i^2g^3j^5 + 3312i^2g^4j^4 + 8176i^2g^5j^3 + 5068i^2g^6j^2 + 2964i^2g^7j + 776i^2g^8 \\
&\quad + 13\,296i^3gj^5h + 12\,688i^3g^2j^4h + 36\,832i^3g^3j^3h + 36\,504i^3g^4j^2h \\
&\quad + 27\,768i^3g^5jh + 9200i^3g^6h + 2080i^4j^4h^2 + 20\,224i^4gj^3h^2 + 40\,464i^4g^2j^2h^2 \\
&\quad + 46\,064i^4g^3jh^2 + 21\,856i^4g^4h^2 + 2848i^5j^2h^3 + 12\,192i^5gjh^3 \\
&\quad + 11\,328i^5g^2h^3 + 512i^6h^4
\end{aligned}
$$

$$
\begin{aligned}
h' &= 2928ig^4j^5 + 1288ig^5j^4 + 3296ig^6j^3 + 1760ig^7j^2 + 936ig^8j + 232ig^9 + 13\,296i^2g^2j^5h \\
&\quad + 10\,608i^2g^3j^4h + 28\,160i^2g^4j^3h + 23\,840i^2g^5j^2h + 16\,632i^2g^6jh \\
&\quad + 5168i^2g^7h + 12\,768i^3j^5h^2 + 14\,336i^3gj^4h^2 + 50\,176i^3g^2j^3h^2
\end{aligned}
$$

$$+63\,232i^3g^3j^2h^2+56\,624i^3g^4jh^2+21\,856i^3g^5h^2+13\,824i^4j^3h^3$$
$$+34\,432i^4gj^2h^3+48\,928i^4g^2jh^3+27\,968i^4g^3h^3+5824i^5jh^4+8192i^5gh^4$$

$$\begin{aligned}i' = {} & 12\,504i^3g^2j^5+7880i^3g^3j^4+19\,240i^3g^4j^3+13\,232i^3g^5j^2+8224i^3g^6j+2184i^3g^7\\ & +528i^4j^5h+4592i^4gj^4h+24\,224i^4g^2j^3h+36\,928i^4g^3j^2h+33\,728i^4g^4jh\\ & +13\,296i^4g^5h+1184i^5j^3h^2+8384i^5gj^2h^2+18\,880i^5g^2jh^2+13\,024i^5g^3h^2\\ & +640i^6jh^3+1600i^6gh^3\end{aligned}$$

$$\begin{aligned}j' = {} & 4308i^2j^8+5808i^2gj^7+17\,424i^2g^2j^6+11\,936i^2g^3j^5+19\,164i^2g^4j^4+14\,096i^2g^5j^3\\ & +9208i^2g^6j^2+3360i^2g^7j+544i^2g^8+11\,616i^3j^6h+21\,440i^3gj^5h\\ & +51\,024i^3g^2j^4h+66\,096i^3g^3j^3h+56\,056i^3g^4j^2h+28\,864i^3g^5jh\\ & +6400i^3g^6h+10\,312i^4j^4h^2+35\,296i^4gj^3h^2+53\,248i^4g^2j^2h^2\\ & +45\,440i^4g^3jh^2+14\,080i^4g^4h^2+5728i^5j^2h^3+12\,544i^5gjh^3\\ & +7168i^5g^2h^3+512i^6h^4.\end{aligned}$$

The initial values of these numbers are $g_1 = 497\,000$, $h_1 = 728\,480$, $i_1 = 340\,476$, $j_1 = 811\,468$ and the formula for the number C_{l+1} of closed HWs within $G^3_{l+1}(3)$ is

$$\begin{aligned}C_{l+1} = {} & 92g_l^8j_l^2+48g_l^9j_l+8g_l^{10}+1792i_lg_l^6h_lj_l^2+1248i_lg_l^7h_lj_l+384i_lg_l^8h_l\\ & +7568i_l^2g_l^4h_l^2j_l^2+7104i_l^2g_l^5h_l^2j_l+3008i_l^2g_l^6h_l^2+10560i_l^3g_l^2h_l^3j_l^2\\ & +13\,440i_l^3g_l^3h_l^3j_l+7680i_l^3g_l^4h_l^3+4480i_l^4h_l^4j_l^2+7680i_l^4g_lh_l^4j_l\\ & +6016i_l^4g_l^2h_l^4+512i_l^5h_l^5.\end{aligned}$$

Appendix D. Analysis of recursion relations for HWs on the 6-simplex lattice

Recursion relations for the numbers $C_{1,l}$, C_2 and $C_{3,l}$ of open HW configurations within the 6-simplex of order l have the following form,

$$\begin{aligned}C_1' = {} & 5544C_1^2C_2^4+1728C_1^3C_2^2C_3+2592C_1^3C_2^3+120C_1^4C_3^2+480C_1^4C_2C_3\\ & +960C_1^4C_2^2+48C_1^5C_3+216C_1^5C_2+24C_1^6+25\,008C_2^4C_3^2+20\,544C_2^5C_3\\ & +6576C_2^6+11\,328C_1C_2^3C_3^2+15\,264C_1C_2^4C_3+8688C_1C_2^5+4992C_1^2C_2^3C_3\end{aligned} \tag{D.1}$$

$$\begin{aligned}C_2' = {} & 94\,336C_2^2C_3^4+76\,800C_2^3C_3^3+48\,160C_2^4C_3^2+23\,520C_2^5C_3+6576C_1C_2^5+17\,120C_1C_2^4C_3\\ & +16\,672C_1C_2^3C_3^2+2832C_1^2C_2^2C_3^2+5088C_1^2C_2^3C_3+832C_1^3C_2^2C_3+3620C_1^2C_2^4\\ & +1232C_1^3C_2^3+144C_1^4C_2C_3+324C_1^4C_2^2+64C_1^5C_2+6C_1^6+16C_1^5C_3\end{aligned} \tag{D.2}$$

$$\begin{aligned}C_3' = {} & 541\,568C_3^6+94\,336C_2^3C_3^3+43\,200C_2^4C_3^2+14\,448C_2^5C_3+2940C_2^6+6252C_1C_2^4C_3\\ & +2568C_1C_2^5+1416C_1^2C_2^3C_3+954C_1^2C_2^4+208C_1^3C_2^3+54C_1^4C_2^2\\ & +6C_1^5C_3+12C_1^5C_2+C_1^6,\end{aligned} \tag{D.3}$$

where $C_i' = C_{i,l+1}$ and $C_i = C_{i,l}$, with the initial values $C_{1,1} = 24$, $C_{2,1} = 6$, $C_{3,1} = 1$. Introducing new variables

$$x_l = \frac{C_{1,l}}{C_{2,l}}, \qquad y_l = \frac{C_{2,l}}{C_{3,l}}, \qquad z_l = \frac{\ln C_{3,l}}{6^l} - \frac{\ln 541568}{5}\left(\frac{1}{6}-\frac{1}{6^l}\right),$$

one can obtain closed set of recursion relations which iterates towards $x_l, y_l \to 0, z_l \to 0.280\,204\ldots$ for $l \to \infty$. On the other hand, from (4.8) it follows that

$$\frac{\ln C_{l+1}}{6^{l+1}} = \frac{\ln y_l}{6^l} + \frac{\ln 5580}{6^{l+1}} + \frac{1}{6^{l+1}}\ln\left(1+\frac{44}{31}x_l+\frac{22}{31}x_l^2+\frac{32}{93}x_l^3+\frac{13}{62}x_l^4+\frac{2}{31}x_l^5+\frac{1}{93}x_l^6\right),$$

whereas from (D.2) one gets

$$\frac{\ln C_{2,l+1}}{6^{l+1}} = \frac{\ln C_{3,l}}{6^l} + 2\frac{\ln y_l}{6^{l+1}} + \frac{\ln 94\,336}{6^{l+1}} + \frac{1}{6^{l+1}}\ln\left(1 + \frac{600}{737}y_l + \frac{1505}{2948}y_l^2 + \frac{521}{2948}x_l y_l^2 + \frac{177}{5896}x_l^2 y_l^2 + \frac{735}{2948}y_l^3 + \frac{535}{2948}x_l y_l^3 + \frac{159}{2948}x_l^2 y_l^3 + \frac{1}{1474}x_l^5 y_l^4 + \frac{3}{47168}x_l^6 y_l^4\right),$$

and, consequently,

$$\ln\omega = \lim_{l\to\infty}\frac{\ln C_{3,l}}{6^l} + \frac{4}{3}\lim_{l\to\infty}\frac{\ln y_l}{6^l}.$$

Since the numerical analysis shows that $\ln y_l/6^l \to 0$, we finally obtain $\omega = 2.0550\ldots$

To find the leading-order asymptotic behaviour of the number of Hamiltonian walks on the 6-simplex fractal ($C_{1,l}, C_{2,l}, C_{3,l}$ and C_l), we conduct an analysis similar to that used in the case of the 5-simplex. However, we can tell right away that $C_{1,l}, C_{2,l}$ and $C_{3,l}$ will have mutually different asymptotics, since their ratios $x_l = \frac{C_{1,l}}{C_{2,l}}$ and $y_l = \frac{C_{2,l}}{C_{3,l}}$ were found to be approaching zero for large l. By iterating the recursion relations for x_l and y_l, one finds that the ratio of x_l and y_l quickly approaches a constant equal to $1.521\,868\ldots$. Keeping only the terms with the lowest sum of powers in x_l and y_l in the recursion relations, we find $x_{l+1} = 12\frac{1042y_l^2}{47\,168}$, $y_{l+1} = 2\frac{47\,168y_l^2}{541568}$, for $l \gg 1$ and the ratio x_{l+1}/y_{l+1} is indeed $1.521\,868\ldots$. From the above equation for y_{l+1}, one can see that

$$\ln y_l \approx 2^l\ln\lambda,\ \lambda = \text{const} = \lim_{l\to\infty}\frac{\ln y_l}{2^l} = 0.9864\ldots. \tag{D.4}$$

The asymptotic relation (4.11) can be obtained starting with $z_l = z_k + \sum_{m=k}^{l-1}(z_{m+1} - z_m)$ and following a procedure completely analogous to that used in the 5-simplex case. Relations (4.9) and (4.10) then follow from (4.11), (D.4) and the fact that x_l and y_l are proportional in the large l limit. From (4.9)–(4.11) it is apparent that in the limiting case $C_{1,l} \ll C_{2,l} \ll C_{3,l}$, since $\lambda < 1$. Therefore, it holds that $C_{l+1} \approx 5580C_{2,l}^6$, so finally $\ln C_l = 6^l\ln\omega + 3 * 2^l\ln\lambda$, which is equivalent to (4.12).

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