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An investigation into the determination of critical dimension of self-avoiding random walk on a d-dimensional simplex fractal

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Abstract. By setting up the relevant recursion relations and by doing exact and approximate calculations, we show that there is no critical dimension in a self-avoiding random walk on a simplex fractal.

PACS. 05.40.+j Fluctuation phenomena, random processes, and Brownian motion – 36.20.Ey Conformation (statistics and dynamics)

1 Introduction

A branch of random walk that contains no self-intersection is called self-avoiding random walk (SAW). The properties of SAW have been investigated in the past twenty years [1–3]. Polymer collapse and polymer growth, as examples of phenomena occuring in nature, can be described as various types of random walk, such as indefinitely growing self-avoiding random walk and Hamiltonian walk [4–7]. A self-avoiding random walk is one of the most important geometric models that show critical behaviour. This critical behaviour can be characterized by a set of critical exponents. One of the critical exponents is ν, a universal exponent that characterizes the scaling behaviour R – the mean square distance between the end points in SAW. In other words

$$\langle R_N^2 \rangle \sim N^{2\nu}, \tag{1.1}$$

where N is the number of steps in the walk.

We shall consider indefinitely growing self-avoiding walk (IGSAW) [4,5], *i.e.* the SAW that neither stops nor gets trapped. Polymer growth, for instance, can be modeled as an IGSAW [5–10]. In IGSAW we shall consider the smart moves that start from a point A_1 and end at another point A_{d+1}, on the lattice. The average number of steps is proportional to some power ν of the distance between A_1 and A_{d+1} as $R \to \infty$, that is

$$\langle N \rangle \sim R^{\frac{1}{\nu}}, \tag{1.2}$$

with ν defined as in [4]. Note that the ν defined in equation (1.2) produces the result as if it were defined by equation (1.1). We have already studied SAW in up to four dimensions and have calculated ν and ν_H – the critical dimension of Hamiltonian walk [6–10].

Ordinary self-avoiding random walk on regular lattices shows a critical dimension at $d = 4$ [11], beyond which it is similar to ordinary walk (model for reflexible chain; here polymers behave as ideal chains). As for the fractals with decimation number b, some effective volume effect is present due to the media, and we have shown that up to $d = 4$ no critical dimension for $b = 2$ exists. This in turn implies that one should search for the answer at $d > 4$ (for $b = 2$).

Our aim here is to calculate the critical exponent ν of SAW on fractals in different dimensions, to see whether there exists any critical dimension. We have succeeded to calculate ν exactly in five dimensions and with a good approximation in higher dimensions, using real space renormalization group method. With a degree of certainty of order 10^{-3} we show that the critical exponent ν becomes less than a half for $d > 6$. Consequently, one should expect no critical dimension (we had to do approximate calculations, as otherwise one whole year of computing could not have sufficed!).

Although we consider a simplex in d dimensions, we note that it is embeddable in two dimensions; hence it is a 2-dimensional fractal lattice with a high fractal dimension (Fig. 1). In other words, there is a one-to-one mapping between this and $(d + 1)$-simplex lattice in d dimensions. This implies that it is a physical lattice with the distinction that the connections overlap. In studying polymer growth, with random walk as its mathematical model, the links among the monomers overlap, so no physical contradiction arises. We also note that by increasing d, we let the importance of the excluded volume effect decrease.

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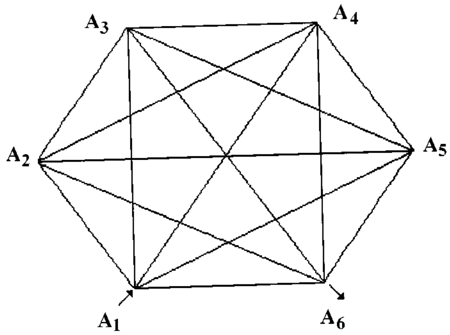

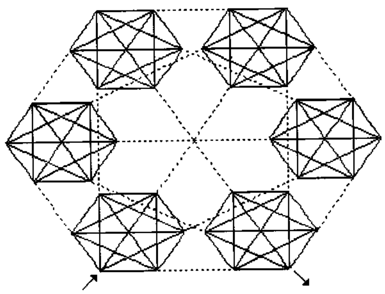

Fig. 1. Embeddability of a $d = 5$ dimensional simplex in two dimensions.

The paper is organized as follows: The $(d+1)$-simplex fractal is introduced in Section 2. In Section 3, we define the walks, generating functions and the recursion relations. We also calculate exactly some of the walks for arbitrary d. In Section 4 we exactly calculate ν for $d = 5$ and show that $d = 5$ cannot be the expected critical dimension. In Section 5, considering only these coefficients which can be calculated analytically, we obtain an approximate renormalization group equation. Using approximate recursion relation, we calculate ν with an accuracy of the order of 10^{-3}. Finally, with regard to the fact that the material quoted in the previous section can be useful in investigating Hamiltonian walk, we devote Section 6 to deal with this walk.

2 (d+1)-simplex fractals

A $(d+1)$-simplex fractal is a generalization of a two dimensional Sierpinski gasket to d dimensions such that its subfractals are $(d+1)$-simplices or d-dimensional polyhedra with $S_{(d+1)}$-symmetry. In order to obtain a fractal with decimation number b, we choose a $(d+1)$-simplex and divide all the links (that is the lines connecting sites) into b parts and then draw all possible d-dimensional hyperplanes through the links parallel to the transverse d-simplices. Next, having omitted every other inner polyhedra, we repeat this process for the remaining simplices or for the subfractals of the next higher generation. This way through $(d+1)$-simplex fractals are constructed. In order to calculate the fractal dimension, it is convenient to

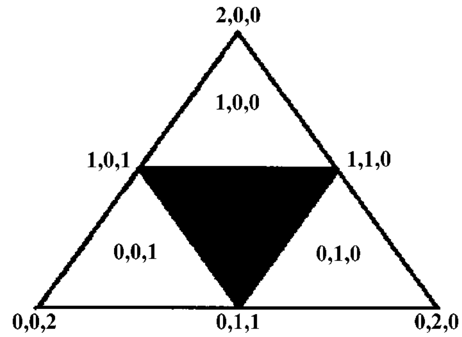

Fig. 2. Sierpinski gasket with $b = 2$.

label subfractals of generation $(n+1)$ in terms of partition of $(b-1)$ into $(d+1)$ positive integers $\lambda_1, \lambda_2, ..., \lambda_{d+1}$. Each partition represents a subfractal of generation n, and λ shows the distance of the corresponding subfractal from d-dimensional hyper-planes which construct the $(d+1)$ simplex. On the other hand, each vertex is denoted by partition of b into $(d+1)$ non-negative integers $\eta_1, \eta_2, \cdots, \eta_{d+1}$, and obviously the ith vertex of subfractal $(\lambda_1, \lambda_2, \cdots, \lambda_{d+1})$ is denoted by $\eta_j = \lambda_j + \delta_{i,j}$, where $j = 1, 2, \cdots, d+1$. As an illustrating example we show in Figure 2 the method of labelling a Sierpinski gasket with decimation number $b = 3$. Obviously the number of all possible partitions is equal to the distribution of $(b-1)$ objects amongst $(d+1)$ boxes, which is the same as the Bose-Einstein distribution of $(b-1)$ identical bosons in $(d+1)$ quantum states. This is equal to

$$C = [(b+d-1)!]/[(b-1)!d!]. \tag{2.1}$$

As is well-known, the fractal dimension D_f of a self-similar object is defined according to [12,13]

$$NL^{D_f} = 1,$$

where N is the number of similar objects, up to translation and rotation, here being equal to the number of subfractals of generation n, and l is the scale of subfractal of generation n. Hence

$$N = C^r, L = b^{-r}.$$

Therefore,

$$D_f = \ln c / \ln b,$$

or

$$D_f = \ln((b+d-1)!/(b-1)!)/\ln b. \tag{2.2}$$

3 The walks, generating functions and recursion relations for SAW

Generally, in order to study the SAW in $(d+1)$-simplex fractal with decimation number b, we shall need to calculate the mean number of steps in a subfractal of order l, that is $\langle N_l \rangle$, in order to calculate $\langle N \rangle$ in the limit

$l \to \infty$. Therefore, we need to define the walks $P_{r,l}^{(d)}(N)$ as the number of SAWs with N steps in which the walker enters the subfractal of generation l at A_1 (input subfractal) and having re-entered r times ($r = 0, 1, \cdots, [\frac{d+1}{2}]$; where [ ] indicates the greatest integer part) it exits at A_{d+1} (the output subfractal), without violating the self-avoiding condition. The generating functions of step l are defined in the following way

$$X_{r,l}^{(d)}(z) = \sum_{N=0}^{\infty} P_{r,l}^{(d)}(N) z^N, \qquad \left(r = 0, 1, \cdots, \left[\frac{d+1}{2}\right]\right). \tag{3.1}$$

The recursion relation for the generating functions is

$$X_{r,l+1}^{(d)}(z) = F_{r,l+1}^{(d)}[(X_{q,l}^{(d)}(z)], \tag{3.2}$$

where $F_{r,l}^{(d)}$ are some polynomial functions which are to be determined. One can write $\langle N_{r,l}^{(d)} \rangle$ in terms of the generating functions

$$\langle N_{r,l}^{(d)} \rangle = \lim_{l \to \infty} \frac{\sum_{N=0}^{\infty} N P_{r,l}^{(d)}(N)}{\sum_{N=0}^{\infty} P_{r,l}^{(d)}(N)} = \lim_{l \to \infty z \to 1} \frac{1}{X_{r,l}^{(d)}} \frac{dX_{r,l}^{(d)}}{dz}. \tag{3.3}$$

To find ν, we use the real space renormalization group technique. This means that in order to calculate $\langle N \rangle$, we must linearize the recursion relation (3.2) around the fixed point. Therefore

$$N_{r,l}^{\prime(d)} X_{r,l}^{(d)} = \sum_q \frac{\partial F_{r,l}^{(d)}}{\partial X_{q,l}^{(d)}} X_{q,l}^{(d)} N_{q,l}^{(d)}, \quad \left(r, q = 0, 1, 2, \cdots, \left[\frac{d+1}{2}\right]\right), \tag{3.4}$$

or in matrix form

$$N_{r,l}^{\prime(d)} = \sum_q a_{r,q}^{(d)}(l) N_{q,l}^{(d)}, \qquad \left(r, q = 0, 1, 2, \cdots, \left[\frac{d+1}{2}\right]\right), \tag{3.5}$$

where

$$a_{r,q}^{(d)}(l) = \frac{1}{X_{r,l}^{(d)}} \sum_q \frac{\partial F_{r,l}^{(d)}}{\partial X_{q,l}^{(d)}} X_{q,l}^{(d)}, \quad \left(r, q = 0, 1, 2, \cdots, \left[\frac{d+1}{2}\right]\right). \tag{3.6}$$

We know that ν is given by

$$\frac{1}{\nu} = \frac{\log \lambda_{max}}{\log b}, \tag{3.7}$$

in which λ_{max} is the largest eigenvalue of the matrix defined in (3.5). We see that investigation of SAW on a $(d+1)$-simplex practically reduces to establishing of recursion relations (3.2). It is obvious that $F_{r,l}^{(d)}[(X_{q,l}^{(d)}(z)]$ are polynomials in z such that

$$X'_r = F_r(X_q), \qquad r = 0, 1, \cdots, \left[\frac{d+1}{2}\right] \tag{3.8}$$

$$X'_r = \sum_{n_0=0}^{d+1} \sum_{n_1=0}^{d+1} \cdots \sum_{n_{[\frac{d+1}{2}]}=0}^{d+1} G_r^{(d)}(n_0, n_1, \cdots, n_{[\frac{d+1}{2}]}) \times X_{0,l}^{(d)}(z) X_{1,l}^{(d)}(z) \cdots X_{[\frac{d+1}{2}],l}^{(d)}(z)$$

with the following constraint

$$n_0 + n_1 + \cdots + n_{[\frac{d+1}{2}]} < d + 1, \tag{3.9}$$

where n_i is the number of subfractals visited by the walker, with $i = 0, 1, \cdots, n_{[\frac{d+1}{2}]}$ as the number of re-entrances. In this article we restrict ourselves only to decimation number $b = 2$.

Let us first derive $G_0^{(d)}(n_1, 0, 0, \cdots, 0)$. With a view to the following two facts that (a) for this type of walk there exists neither re-entrance nor re-exit, thus the walker does not visit any of the subfractals more than once, and (b) the number of subfractals is equal to $(d+1)$, and it is a must for the walker to visit the input/output subfractals, thereby leaving the remaining $(d+1) - 2 = (d-1)$ subfractals to be visited in d ways; then the other $(d-2)$ subfractals in $(d - n_1 + 2)$ ways and so forth, we conclude that in total we shall have

$$G_0^{(d)}(n_1, 0, \cdots, 0) = (d-1)(d-2) \cdots (d - n_1 + 2), \quad \text{with } n_1 < d + 1. \tag{3.10}$$

In order to find the coefficient of $G_0^{(d)}(n_0, 1, 0, \cdots)$ we note again that as for a given generator, there is just one possibility of re-entrance for every subfractal, therefore this re-entrance can occur either in the fixed input/output subfractals or in one of the inner subfractals:

(a) Occurence of re-entrance in input/output subfractals:
According to the sample path shown below (the re-entered subfractals are shown in bold-face letters)

$$\mathbf{A_1} A_2 A_3 \cdots A_j \mathbf{A_1} A_{j+1} \cdots A_{n_0} A_{d+1}, \tag{3.11}$$

the re-entrances occur at the input subfractal after visiting $j - 1$ inner subfractals. Obviously j can take values between 2 and n_0, therefore, there are $(n_0 - 2)G_0^{(d)}(n_0 + 1, 0, 0, \cdots)$ different paths in which the re-entrance can occur in the fixed input subfractal. Similarly, one can show that there are $(n_0 - 2)G_0^{(d)}(n_0 + 1, 0, 0, \cdots)$ different paths in which the re-entrance can occur in the fixed output subfractals. Therefore, in total, we have $2(n_0 - 2)G_0^{(d)}(n_0 + 1, 0, 0, \cdots)$ paths.

(b) Occurrence of re-entrance in one of the inner subfractals:
According to the following path:

$$A_1 A_2 A_3 \cdots \mathbf{A_j} A_{j+1} \cdots A_k \cdots \mathbf{A_j} A_{n_0} A_{d+1} \tag{3.12}$$

re-entrance occurs at the inner subfractal $\mathbf{A_j}$ after visiting the other $(k-j)$ inner subfractals. For a given j, k takes the values between $(j+2), \cdots, n_0$. Therefore, the number of paths in which the re-entrance can occur in the jth subfractal is equal to $n_0 - j - 2$. On the other hand, j itself varies between 2 and $n_0 - 2$. Thus the total number of paths is

$$\sum_{j=2}^{n_0-2} (n_0-j-2) = \frac{(n_0-2)(n_0-3)}{2} G_0^{(d)}(n_0+1, 0, 0, \cdots). \tag{3.13}$$

Summing up the paths in (a) and (b) we obtain

$$G_0^{(d)}(n_0, 1, 0, \cdots) = \frac{(n_0-2)(n_0+1)}{2} G_0^{(d)}(n_0+1, 0, 0, \cdots). \tag{3.14}$$

To calculate $G_0^{(d)}(n_0, 2, 0 \cdots)$ we need to sum up the following three types of paths:

(a) The re-entered subfractals are the fixed input/output subfractals. In this case, according to the following sample path:

$$\mathbf{A_1} A_2 A_3 \cdots A_j \mathbf{A_1} A_{j+1} \cdots A_k \mathbf{A_{d+1}} A_{k+1} \cdots A_{n_0+1} \mathbf{A_{d+1}} \tag{3.15}$$

the sum of this kind of paths is

$$(n_0^2 - n_0 + 1) G_0^{(d)}(n_0 + 2, 0, \cdots). \tag{3.16}$$

(b) The re-entered subfractals are one of the fixed subfractals (*i.e.*, either input or output) and another of the inner ones. A typical path is shown below

$$\mathbf{A_1} A_2 A_3 \cdots A_{j-1} \mathbf{A_j} A_{j+1} \cdots A_k \mathbf{A_1} A_{k+1} \times \cdots A_l \mathbf{A_j} A_{l+1} \cdots A_{n_0+1} A_{d+1}. \tag{3.17}$$

The number of paths as such is

$$n_0(n_0 - 1)(n_0 - 2) G_0^{(d)}(n_0 + 2, 0, \cdots). \tag{3.18}$$

(c) Both of the re-entered subfractals belong to the inner ones; an example of which is

$$A_1 A_2 \cdots A_{j-1} \mathbf{A_j} A_{j+1} \cdots \mathbf{A_k} A_{k+1}. \cdots A_l \mathbf{A_j} A_{l+1} \times \cdots A_m \mathbf{A_k} A_{m+1} \cdots A_{n_0+1} A_{d+1}. \tag{3.19}$$

The sum of this kind of paths is

$$\frac{n_0(n_0-1)(n_0-2)(n_0-3)}{8} G_0^{(d)}(n_0 + 2, 0, \cdots). \tag{3.20}$$

The total number of paths in (a), (b) and (c) is

$$G_0^{(d)}(n_0, 2, \cdots) = \frac{(n_0+1)(n_0^3 + n_0^2 - 6n_0 + 8)}{8} \times G_0^{(d)}(n_0 + 2, 0, \cdots). \tag{3.21}$$

In calculating $G_0^{(d)}(n_0, 3, 0 \cdots)$ we need to consider the following three types of paths:

(a) The re-entered subfractals are the fixed input/output and one of the inner subfractals. In this case, according to the following sample path:

$$\mathbf{A_1} A_2 \cdots A_i \mathbf{A_1} A_{i+1} \cdots A_j \cdots \mathbf{A_{d+1}} A_{j+1} \times \cdots A_{k-1} \mathbf{A_k} A_{k+1} \cdots A_m \mathbf{A_k} A_{m+1} \cdots A_{n_0+2} \mathbf{A_{d+1}} \tag{3.22}$$

the sum of the paths is

$$\frac{(n_0+1)(3n_0^3 + 7n_0^2 - 7n_0 - 6)}{6} G_0^{(d)}(n_0 + 3, 0, \cdots). \tag{3.23}$$

(b) The re-entered subfractals consist of one of the fixed (*i.e.* either input or output) subfractals and the other two are a pair of the inner ones. A typical path is shown below

$$\mathbf{A_1} A_2 \cdots \mathbf{A_j} A_{j+1} \cdots A_k \mathbf{A_1} A_{k+1} \cdots A_l \mathbf{A_j} A_{l+1} \times \cdots \mathbf{A_m} A_{m+1} \cdots \mathbf{A_m} A_{p+1} \cdots A_{n_0+2} A_{d+1}. \tag{3.24}$$

The sum of these paths is

$$\frac{(n_0+2)(n_0+1)n_0(n_0-1)(n_0-2)}{4} G_0^{(d)}(n_0 + 3, 0, \cdots). \tag{3.25}$$

(c) Three of the re-entered subfractals belong to the inner ones; an example of which is

$$A_1 \cdots \mathbf{A_j} A_{j+1} \cdots \mathbf{A_k} A_{k+1} \cdots A_l \mathbf{A_j} A_{l+1} \cdots A_m \mathbf{A_k} A_{m+1} \times \cdots \mathbf{A_p} A_{p+1} \cdots A_q \mathbf{A_p} A_{q+1} \cdots A_{n_0+2} A_{d+1}. \tag{3.26}$$

The sum of paths as such is

$$\frac{(n_0+2)(n_0+1)n_0(n_0-1)(n_0-2)(n_0-3)}{48} \times G_0^{(d)}(n_0 + 3, 0, \cdots). \tag{3.27}$$

The total sum of the paths in (a), (b) and (c) is

$$G_0^{(d)}(n_0, 2, \cdots) = \frac{(n_0+1)(n_0^5 + 8n_0^4 + 11n_0^3 + 24n_0^2 - 20n_0 - 48)}{48} \times G_0^{(d)}(n_0 + 3, 0, \cdots). \tag{3.28}$$

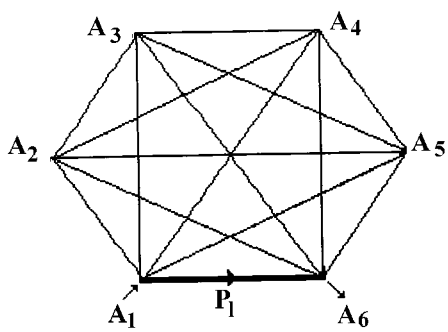

Fig. 3. The walk P_l of a six simplex fractal.

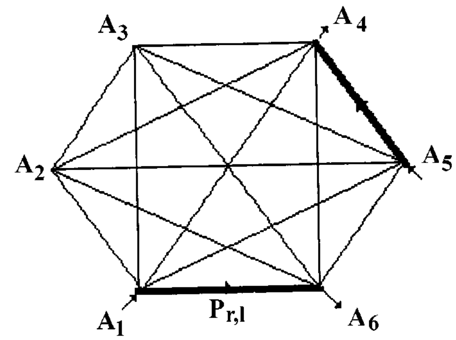

Fig. 4. The walk $P_{r,l}$ of a six simplex fractal.

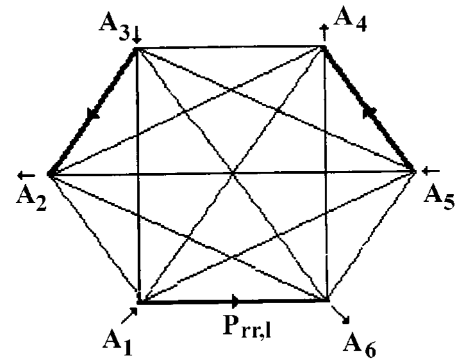

Fig. 5. The walk $P_{rr,l}$ of a six simplex fractal.

Similarly, one can calculate $G_1^{(d)}(n_0,0,0,\cdots)$ and $G_1^{(d)}(n_0,1,0,\cdots)$. The end results are:

$$G_1^{(d)}(n_0,0,0,\cdots)=(n_0-3)(d-3)(d-4)\cdots(d-n_0+2), \tag{3.29}$$

and

$$G_1^{(d)}(n_0,1,0,\cdots) = \frac{4(n_0^2-5n_0+7)}{n_0-2}G_1^{(d)}(n_0+1,0,\cdots) + \frac{(n_0^2-7n_0+14)(d-n_0+1)}{2}G_1^{(d)}(n_0,0,\cdots). \tag{3.30}$$

With the above prescription and some tedious work, one can calculate the other coefficients. We shall, however, see below that to determine the critical exponent ν the coefficients $G_0^{(d)}(n_0,0,\cdots), G_0^{(d)}(n_0,1,0,\cdots), G_1^{(d)}(n_0,0,0,\cdots)$ and $G_1^{(d)}(n_0,1,0,\cdots)$ are sufficient. The omission of the other coefficients will lead to errors of order 10^{-3}, which are not so important in the investigation of the critical dimension.

In order to compare the results of the approximate calculations with those of the exact one, and also to have an insight into the exact calculation, we exactly find the critical exponent ν of 6-simplex fractal with decimation number $b=2$, in the next section.

4 Exact solution of self-avoiding random walks on 6-simplex fractal

In this section we exactly calculate the critical exponent ν of SAW in six simplex fractals. To calculate $< N_l >$, according to the general prescription of Section 3, we need to define the following walks:

P_l: the number of SAWs in which the walker enters the subfractal of generation l at A_1 and exits at A_6 (Fig. 3).

$P_{r,l}$: the number of SAWs in which the walker enters the subfractal of generation l at A_1 and exits at A_6, then re-enters at A_5 and re-exits at A_4 (Fig. 4).

$P_{rr,l}$: the number of SAWs in which the walker enters the subfractal of generation l at A_1 and exits at A_6, then having re-entered at A_3 and re-exited at A_2, it enters at A_5 and exits at A_4 (Fig. 5).

We define the generating functions of generation l in the following way:

$$x_l(t) = \sum_{N=0} P_l(N)t^N, \tag{4.1a}$$

$$y_l(t) = \sum_{N=0} P_{r,l}(N)t^N, \tag{4.1b}$$

$$z_l(t) = \sum_{N=0} P_{rr,l}(N)t^N, \tag{4.1c}$$

where $t \le 1$. We find that $x(t)$, $y(t)$ and $z(t)$ satisfy the following recursion relations:

$$\begin{aligned} x' = {} & 25008y^4z^2 + 528y^5 + 20544y^5z + 6576y^6 \\ & + 11328xy^3z^2 + 528xy^4 + 15264xy^4z \\ & + 8688xy^5 + x^2 + 36x^2y^2 + 384x^2y^3 \\ & + 4992x^2y^3z + 5544x^2y^4 + 4x^3 + 24x^3y \\ & + 312x^3y^2 + 1728x^3y^2z + 2592x^3y^3 \\ & + 12x^4 + 120x^4z^2 + 120x^4y + 480x^4yz \\ & + 960x^4y^2 + 24x^5 + 48x^5z + 216x^5y + 24x^6, \end{aligned} \tag{4.2a}$$

$$\begin{aligned} y' &= 86000y^2z^4 + 76800y^3z^3 + 22y^4 + 48160y^4z^2 \\ &+ 372y^5 + 23520y^5z + 5440y^6 + 16672xy^3z^2 \\ &+ 440xy^4 + 17120xy^4z + 6576xy^5 + 2832x^2y^2z^2 \\ &+ 176x^2y^3 + 5088x^2y^3z + 3620x^2y^4 + 4x^3y \\ &+ 64x^3y^2 + 832x^3y^2z + 1232x^3y^3 + x^4 \\ &+ 26x^4y + 144x^4yz + 324x^4y^2 + 4x^5 + 16x^5z \\ &+ 64x^5y + 6x^6, \qquad (4.2b) \\ z' &= 844z^5 + 436704z^6 + 668yz^4 + 14176yz^5 \\ &+ 14928y^2z^4 + 93408y^3z^3 + 43440y^4z^2 \\ &+ 14448y^5z + 2940y^6 + 176xy^2z^3 + 6252xy^4z \\ &+ 2568xy^5 + 1416x^2y^3z + 954x^2y^4 + 208x^3y^3 \\ &+ 54x^4y^2 + 6x^5z + 12x^5y + x^6, \qquad (4.2c) \end{aligned}$$

with the phase space defined as

$$\begin{aligned} x' &= x_{l+1}(t), \qquad & x &= x_l(t), \\ y' &= y_{l+1}(t), \qquad & y &= y_l(t), \\ z' &= z_{l+1}(t), \qquad & z &= z_l(t), \end{aligned} \qquad (4.3)$$

or, simply as

$$X' = F(X), \qquad (4.4)$$

with

$$X' = (x', y', z'), \qquad (4.5)$$

and

$$X = (x, y, z). \qquad (4.6)$$

Iteration of equations (4.2) leads to construction of flow in the phase space.

To calculate ν, we use the real space renormalization technique. We benefit from Newton's algorithm [14] for solving the system of nonlinear equations in order to obtain the fixed points of the recursion relations (4.2). The only relevant fixed point of the recursion relations is

$$x = 0.262399, \quad y = 0.017568 \quad \text{and} \quad z = 0.000051. \qquad (4.7)$$

To calculate $\langle N \rangle$ we define

$$\begin{aligned} \langle N \rangle &= \frac{\sum_{N=0}^{\infty} NP(N)}{\sum_{N=0}^{\infty} P(N)} \\ &= \frac{1}{x(1)} \lim_{t\to 1} \frac{dx(t)}{dt} = DF(X_f). \end{aligned} \qquad (4.8)$$

D is the matrix which is shown explicitly in the following equation, and X_f is the fixed point, that is the partial derivative of the matrix at the fixed point.

We linearize equations (4.2) around the fixed point (4.7) and get for $\langle N \rangle$:

$$\begin{bmatrix} N_1' \\ N_2' \\ N_3' \end{bmatrix} = \begin{bmatrix} 3.347233 & 1.796974 & 0.111662 \\ 0.299496 & 0.411092 & 0.038912 \\ 0.013958 & 0.029184 & 0.008173 \end{bmatrix} \begin{bmatrix} cN_1 \\ N_2 \\ N_3 \end{bmatrix}. \qquad (4.9)$$

There are three eigenvalues for the 3×3 matrix of equation (4.9). They can be obtained by diagonalizing the matrix. The result is

$$\lambda_1 = 3.520932, \quad \lambda_2 = 0.240417, \quad \text{and} \quad \lambda_3 = 0.005148. \qquad (4.10)$$

Each row in the following matrix indicates eigen-vectors corresponding to λ_1, λ_2 and λ_3 respectively:

$$\begin{bmatrix} 0.995378 & 0.501251 & 0.029828 \\ 0.095920 & -0.861764 & -0.117158 \\ 0.004752 & -0.078164 & 0.992665 \end{bmatrix}. \qquad (4.11)$$

We see from equation (4.10) that λ_1 is bigger than 1, and the other two λ are less than it. This means that the flow is of nonlinear hyperbolic type by nature, and the fixed point is a saddle point. Therefore, it is quite natural to have a two-dimensional stable submanifold. With a good approximation, this unstable manifold in the neighbourhood of the fixed point is a plane which includes eigenvectors corresponding to the eigenvalues less than one, the equation of which is

$$0.995378\, x + 0.501251\, y + 0.029828\, z = 0.269993. \qquad (4.12)$$

One can also easily verify that the unstable manifold is normal to this plane and is the eigen-direction corresponding to the eigenvalue greater than one. Mathematically, stable (SM) and unstable manifolds (UM) are defined respectively as [15]:

$$\begin{aligned} SM &= \{x \in \text{phase space}, \ \ f^{(m)}(x) = \lim_{x\to+\infty} x^f\} \\ UM &= \{x \in \text{phase space}, \ \ f^{(m)}(x) = \lim_{x\to-\infty} x^f\}. \end{aligned} \qquad (4.13)$$

Now, we can readily calculate the exponent ν:

$$\nu = \frac{\ln 2}{\ln \lambda_1} = 0.550674. \qquad (4.14)$$

With regard to the above-mentioned renormalization group equation, we can calculate another characteristic parameter of random walk called μ which is defined as [11]

$$\begin{aligned} \ln \mu &= \frac{1}{N} \ln(\text{number of all possible walks with } N \text{ steps}) \\ &= \text{entropy of walks per step}, \end{aligned} \qquad (4.15)$$

which has already been shown to be equal to [16]

$$\mu = \frac{1}{z^c}\,. \tag{4.16}$$

As we have shown [7], the critical point z^c in equation (4.15) is the point of intersection of the direction of attraction, corresponding to eigenvalues less than 1, and the initial curve that by iteration leads to the fixed point (4.7). Therefore, we have $z^c = 0.271247$, which results in

$$\mu = 3.686673. \tag{4.17}$$

5 In quest of critical dimension

Using the results we have obtained thus far for ν in different dimensions up to $d = 4$ [6–10] and the one given in equation (4.14) for $d = 5$, the best fit we can get is

$$\nu = 1.058d^{-0.407}. \tag{5.1}$$

Now, considering only the coefficients $G_0^{(d)}(n_0, 0, \cdots)$, $G_0^{(d)}(n_0, 1, 0, \cdots)$, $G_0^{(d)}(n_0, 2, 0, \cdots)$, $G_0^{(d)}(n_0, 3, 0, \cdots)$, $G_1^{(d)}(n_0, 0, 0, \cdots)$ and $G_1^{(d)}(n_0, 1, 0, \cdots)$, the recursion relations given in equation (3.8) reduce to the following approximate recursion relations:

$$\begin{aligned} X_0' = X_0^2 &+ \sum_{n_0=3}^{d+1}(d-1)(d-2)\cdots(d-n_0+2)X_0^{n_0} \\ &+ \sum_{n_0=2}^{d}\frac{(n_0-2)(n_0+1)}{2} \\ &\times (d-1)(d-2)\cdots(d-n_0+1)X_0^{n_0}X_1 \\ &+ \sum_{n_0=2}^{d-1}\frac{(n_0^3+n_0^2-6n_0+8)(n_0+1)}{8} \\ &\times (d-1)(d-2)\cdots(d-n_0)X_0^{n_0}X_1^2 \\ &+ \sum_{n_0=2}^{d-2}\frac{(n_0^5+8n_0^4+11n_0^3+24n_0^2-20n_0-48)(n_0+1)}{2} \\ &\times (d-1)(d-2)\cdots(d-n_0-1)X_0^{n_0}X_1^3 \end{aligned}$$

and

$$\begin{aligned} X_1' = X_0^4 &+ \sum_{n_0=5}^{d+1}(n_0-3)(d-3)(d-4)\cdots(d-n_0+2)X_0^{n_0} \\ &+ \sum_{n_0=3}^{d}4(n_0^2-5n_0+7)(d-3)(d-4)\cdots(d-n_0+1)X_0^{n_0}X_1 \\ &+ \sum_{n_0=3}^{d}\frac{n_0^2-7n_0+14}{2}(d-n_0+1)(n_0-3) \\ &\times (d-3)(d-4)\cdots(d-n_0+2)X_0^{n_0}X_1. \end{aligned}$$

Table 1. Comparison of exactly and approximately calculated critical exponents ν_e and ν_a. Note that ν_e for $d = 6$ and 7 have been evaluated using equation (5.1).

d	ν_e	ν_a
2	0.798625	0.798625
3	0.674160	0.673761
4	0.600865	0.602129
5	0.550674	0.552765
6	0.520129	0.515875
7	0.491699	0.489155

Using the above recursion relations together with the algorithm given in Section 4, we can determine the approximate values of the critical exponent ν for different values of d. The results thus obtained, together with those calculated exactly, are given in Table 1.

Thus, according to equation (5.1), ν is a decreasing function of d (see Fig. 6). It, therefore, seems that there should be no critical dimension in the sense that self-avoidness does not play any role beyond it, as is the case in non-fractal lattices. Moreover, it appears that ν crosses the $\frac{1}{2}$ limit. This suggests that fractal lattices must be completely different from ordinary ones. To ascertain ourselves, we have carried out the calculations, although approximately, for $d = 6$ and $d = 7$. As the Table 1 indicates, the results are reliable up to within three decimals. Thus, we see that the curve $\nu(d)$ crosses the line $\nu = \frac{1}{2}$ at $6 < d < 7$. To put it differently, it seems, therefore, that the structure of simplex fractals induces an effective monomer-monomer interaction leading to further bending of polymers, modelized as self-avoiding random walks in fractal lattices.

6 Configurational entropy per monomer of a Hamiltonian walk

Hamiltonian walks are self-avoiding walks that visit every site in a lattice, and are often used as a model of collapsed polymer chains in the zero temperature limit [2,17]. With no exact knowledge of recursion relations for the generating functions of the Hamiltonian walk, the authors have presented an analytical proof that the exponent ν for simplex fractals in d dimension, with an arbitrary decimation number b, is given by [18]

$$\frac{1}{\nu} = \frac{\log[b(b+1)\cdots(b+d-1)]}{\log b}\,. \tag{6.1}$$

As in [17], the configurational connectivity constant μ_H is defined according to

$$\ln\mu_H = \lim_{N\to 0}\frac{1}{N}\ln[\text{number of possible walks}], \tag{6.2}$$

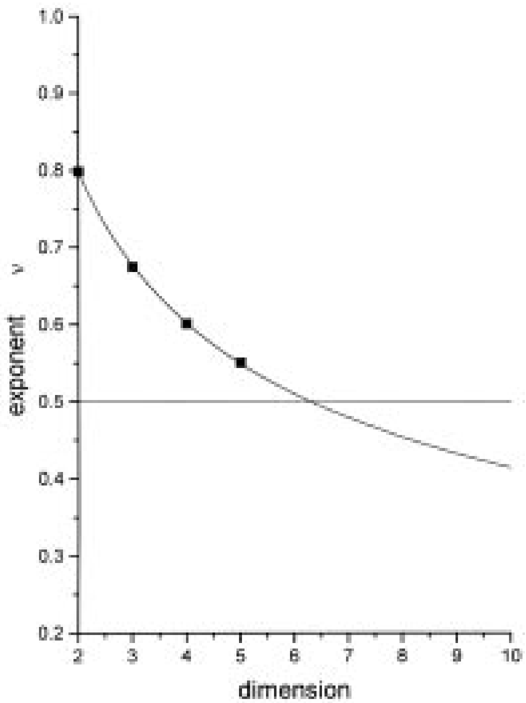

Fig. 6. Critical exponent ν as a function of dimension. The solid line corresponds to the fit (5.1).

where N is the number of points in a lattice. We show below the value of μ_H for lattices in different dimensions:

Table 2. Connectivity constant for Hamiltonian walks.

d	μ_H
2	1.200938
3	1.399710
4	1.748372

Now we calculate μ_H for $d = 5$, using the explicit recursion relations of generating functions for the Hamiltonian walk. As has already been indicated [19], the recursion relations for this type of the walk must be homogeneous polynomials of degree equal to the number of subfractals, which is six in this case. Therefore, we must consider the following equations

$$\begin{aligned} x' = {} & 25008y^4z^2 + 20544y^5z + 6576y^6 + 11328xy^3z^2 \\ & + 15264xy^4z + 8688xy^5 + 4992x^2y^3z + 5544x^2y^4 \\ & + 1728x^3y^2z + 2592x^3y^3 + 120x^4z^2 + 480x^4yz \\ & + 960x^4y^2 + 48x^5z + 216x^5y + 24x^6, \end{aligned} \tag{6.3a}$$

$$\begin{aligned} y' = {} & 86000y^2z^4 + 76800y^3z^3 + 48160y^4z^2 + 23520y^5z \\ & + 5440y^6 + 16672xy^3z^2 + 17120xy^4z + 6576xy^5 \\ & + 2832x^2y^2z^2 + 5088x^2y^3z + 3620x^2y^4 + 832x^3y^2z \\ & + 1232x^3y^3 + 144x^4yz + 324x^4y^2 + 16x^5z \\ & + 64x^5y + 6x^6, \end{aligned} \tag{6.3b}$$

$$\begin{aligned} z' = {} & 436704z^6 + 14176yz^5 + 14928y^2z^4 + 93408y^3z^3 \\ & + 43440y^4z^2 + 14448y^5z + 2940y^6 + 176xy^2z^3 \\ & + 6252xy^4z + 2568xy^5 + 1416x^2y^3z + 954x^2y^4 \\ & + 208x^3y^3 + 54x^4y^2 + 6x^5z + 12x^5y + x^6, \end{aligned} \tag{6.3c}$$

where as before

$$x' = x_{l+1}, \quad y' = y_{l+1}, \quad \text{and} \quad z' = z_{l+1}. \tag{6.4}$$

We use equations (6.3) to obtain

$$X' = \frac{F(X,Y)}{H(X,Y)}, \tag{6.5}$$

and

$$Y' = \frac{G(X,Y)}{H(X,Y)} \cdot \tag{6.6}$$

The functions $F(X,Y)$, $G(X,Y)$ and $H(X,Y)$ are defined as

$$\begin{aligned} F(X,Y) = {} & 25008Y^4 + 20544Y^5 + 6576Y^6 \\ & + 11328XY^3 + 15264XY^4 + 8688XY^5 \\ & + 4992X^2Y^3 + 5544X^2Y^4 + 1728X^3Y^2 \\ & + 2592X^3Y^3 + 120X^4 + 480X^4Y \\ & + 960X^4Y^2 + 48X^5 + 216X^5Y + 24X^6 \end{aligned} \tag{6.7a}$$

$$\begin{aligned} G(X,Y) = {} & 86000Y^2 + 76800Y^3 + 48160Y^4 \\ & + 23520Y^5 + 5440Y^6 + 16672XY^3 \\ & + 17120XY^4 + 6576XY^5 + 2832X^2Y^2 \\ & + 5088X^2Y^3 + 3620X^2Y^4 + 832X^3Y^2 \\ & + 1232X^3Y^3 + 144X^4Y + 324X^4Y^2 \\ & + 16X^5 + 64X^5Y + 6X^6 \end{aligned} \tag{6.8b}$$

$$\begin{aligned} H(X,Y) = {} & 436704 + 14176Y + 14928Y^2 \\ & + 93408Y^3 + 43440Y^4 + 14448Y^5 \\ & + 2940Y^6 + 176XY^2 + 6252XY^4 \\ & + 2568XY^5 + 1416X^2Y^3 + 954X^2Y^4 \\ & + 208X^3Y^3 + 54X^4Y^2 + 6X^5 \\ & + 12X^5Y + X^6 \end{aligned} \tag{6.8c}$$

where

$$X = \frac{x_l}{z_l} = X_l, \qquad Y = \frac{y_l}{z_l} = Y_l,$$
$$X' = \frac{x_{l+1}}{z_{l+1}} = X_{l+1}, \qquad Y' = \frac{y_{l+1}}{z_{l+1}} = Y_{l+1}.$$

By iterating equations (6.5, 6.6) they quite rapidly tend to zero. This indicates that z dominates x and y.

Now, to calculate μ_H, *i.e.* the connectivity constant for Hamiltonian walk, we divide both sides of equations (6.3, 6.4) by 6^{l+1} and get the following recursion relation

$$\frac{\ln(z_{l+1})}{6^{l+1}} = \frac{\ln(z_l)}{6^l} + \frac{\ln(H_{l+1})}{6^{l+1}}\,. \tag{6.9}$$

In practice, we start with the initial values $x = 1$, $y = z = 0$ in equations (6.3), then calculate the values X and Y according to equations (6.8). We then insert them in the homogeneous iteration relations (6.7) and get

$$\lim_{l\to\infty} \frac{\ln(z_{l+1})}{6^{l+1}} = 0.720278. \tag{6.10}$$

This determines the value of the connectivity constant:

$$\mu_H = \exp(0.720278) = 2.055004. \tag{6.11}$$

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