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Connective constant of SAWs on the Sierpinski gasket family

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Abstract. Using a graph counting technique suitable for regular fractals, an exact evaluation of the total number of embeddings of self-avoiding walks on the generalized Sierpinski gasket is obtained. Numerical estimates for the connective constants μ_b are quoted for the first time, where b is the generation parameter of the gaskets. It is shown that the number of distinct n-step SAWs per site c_n converges to the triangular lattice values when $b \to \infty$ ($D_f \to 2$). Our analysis indicates that μ_b converges to the Euclidean value in the same limit and an asymptotic expression is given.

1. Introduction

The statistics of self-avoiding walks (SAWs) on fractals has been extensively investigated using exact renormalization techniques [1–3], by finite-size scaling arguments [4], Monte Carlo techniques [5] and, more recently, with series expansions [6]. This problem is relevant to the study of polymers in a dilute solution confined to a highly disordered media.

These studies show that the critical properties of SAWs on fractals depend on several geometrical parameters besides the Hausdorff dimension D_f. A question that naturally arises is the convergence of critical exponents to Euclidean lattices values when D_f approaches an integer dimension. This work adresses this problem, which has been intensively investigated in the last few years [5, 7–9].

We study SAWs on a family of finitely ramified regular fractals embedded in the two-dimensional Euclidean space, the generalized Sierpinski gasket. Each member of this family is constructed from a generator characterized by a parameter b, where b is an integer which runs from two to infinity. Each generator is an equilateral triangle (see figure 1) containing b^2 smaller triangles from which the downward-oriented ones are discarded and the $b(b+1)/2$ upward-oriented triangles are left. The corresponding regular fractal is formed by reproducing iteratively the generator in each upward-oriented triangle. The lattice at an s-stage of construction (after s iterations) is then obtained from the generator with all upward-oriented smaller triangles filled with the reproductions of the previous $(s-1)$-stage. The lattice at the first stage is the generator.

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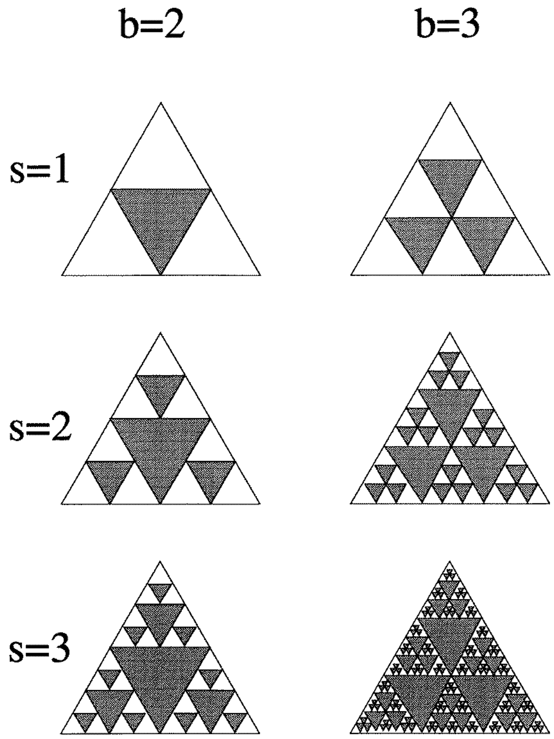

Figure 1. First steps of construction of b-triangles (for $b = 2, 3$).

In the limit $s \to \infty$, a fractal lattice is obtained (we call it a b-triangle) with dimension:

$$D_f = \ln[b(b+1)/2]/\ln b. \qquad (1)$$

From (1), when $b \to \infty$, $D_f \to 2$. It was argued that [3] as the limiting generator, when $b \to \infty$, is only the wedge of the primitive triangle, the members of the generalized Sierpinski gasket family should converge to a wedge of the triangular lattice. This, however, does not insure the convergence of the critical parameters of SAWs on these lattices towards the correspondent Euclidean values. The critical properties of SAWs on any lattice are obtained when the number of steps n tend to infinity. This means that in order to obtain the critical properties of SAWs on the limiting Euclidean lattice from the fractal family, one should take the limit $b \to \infty$ first and then analyse the statistics of SAWs as $n \to \infty$. On the other hand, when one analyses the convergence of critical parameters of SAW on a fractal family as $b \to \infty$, it means that the limit $n \to \infty$ was taken before the limit $b \to \infty$.

The statistics of SAWs on the Sierpinski gasket ($b = 2$) was obtained exactly from a renormalization-group approach [2]. SAWs were also studied on a fractal family called truncated 3-simplices [1] which is in the same universality class as the generalized Sierpinski gasket family. For these lattices there are exact results when $2 \leqslant b \leqslant 8$, obtained via a renormalization group approach [3] and also numerical results for $b \leqslant 80$ obtained via the Monte Carlo renormalization group method [5].

It has been shown that the critical exponent ν crosses the two-dimensional value when $b \approx 26$ and decreases monotonically with b in the range studied. On the other hand, the exponent γ is greater than the two-dimensional value and increases monotonically with b

[7]. This behaviour is consistent with the scaling arguments of Dhar [4].

In other families of fractals this crossing at $\nu = \frac{3}{4}$ for $b \approx 26$ has also been observed [8], but the estimates of ν do not approach $\frac{3}{4}$ when $b \to \infty$ and $D_f \to 2$ (fractals with b up to 121 were studied). However, in the Φ family and the Koch family, when $b \to \infty$, $D_f \to 1$ and the critical exponents tend to the (trivial) one-dimensional values [9].

In this work, the critical behaviour of SAWs on b-triangles is analysed using the series-expansion method. We use an exact enumeration technique to calculate the density of n-step SAWs $c_n(b)$ for the b-triangles (section 2). This method has already been used to study the critical behaviour of SAWs on infinitely ramified fractals[6].

We show analytically that $c_n(b)$ converges to the triangular lattice (Euclidean) value $c_n(T)$ as $b \to \infty$ (section 3).

The connective constants μ_b are calculated for several b-triangles. As μ_b are non-universal quantities, they could not be inferred from the previous studies [3–5] of SAWs that have been performed on other fractal families. The analysis of the chain-generating function properties for SAWs on the b-triangles and the numerical values of μ_b indicate that μ_b converge to the triangular value μ_T when $b \to \infty$ (section 4).

2. Series expansions

Consider the chain-generating function for SAWs on a particular b-triangle:

$$C_b(x) = \sum_{n=1}^{\infty} c_n(b) x^n \tag{2}$$

where $c_n(b)$ is the total number of distinct n-step SAWs per number of sites of the lattice and x is the weight factor for each step.

The connective constant μ_b for SAWs on each b-triangle can be obtained from† [10]:

$$\mu_b = \lim_{n\to\infty} [c_n(b)]^{1/n}. \tag{3}$$

The coefficients $c_n(b)$ are obtained in the fractal limit (infinite lattice) from:

$$c_n(b) = \lim_{s\to\infty} \frac{G_n^b(s)}{N^b(s)} \tag{4a}$$

where $G_n^b(s)$ is the total number of embeddings of n-step SAWs in stage s and $N^b(s)$ is the number of sites in this stage.

The density of a particular SAW is given by:

$$c_{\mathrm{SAW}}(b) = \lim_{s\to\infty} \frac{G_{\mathrm{SAW}}^b(s)}{N^b(s)} \tag{4b}$$

where $G_{\mathrm{SAW}}^b(s)$ is its number of embeddings in stage s.

Clearly,

$$c_n(b) = \sum_{\mathrm{SAW}/n} c_{\mathrm{SAW}}(b) \tag{5}$$

where $\sum_{\mathrm{SAW}/n}$ is the summation over all distinct n-step SAWs.

In order to calculate $c_n(b)$, we generalize the method developed in [11] that relates the number of embeddings of a connected graph in two consecutive stages of construction of a regular fractal.

† The asymptotic form expected for $c_n(b)$ is ${\mu_b}^n n^{\gamma_b - 1}$.

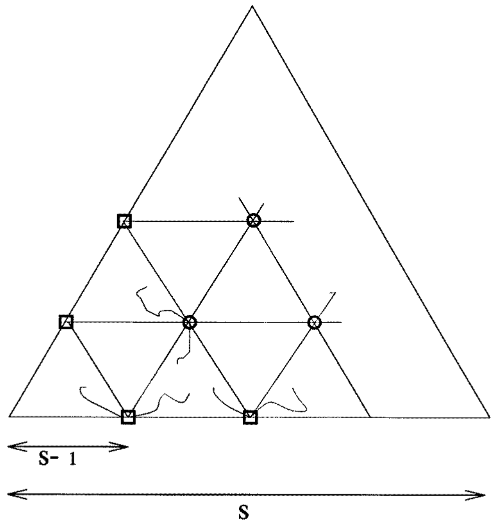

Figure 2. Examples of embedding which contribute to E_n^b and I_n^b terms. □ External connection sites; ○ internal connection sites.

For a particular n-step SAW and for a particular b-triangle there is a minimum lattice stage $s_0 + 1$ for which any embedding of the SAW cannot cross any reproductions of the s_0-stage in the (s_0+1)-stage. For $s > s_0$, the recursion relation between $G_n^b(s)$ and $G_n^b(s-1)$ is:

$$G_n^b(s) = A_1(b)G_n^b(s-1) + 3A_2(b)E_n^b + A_3(b)I_n^b. \tag{6}$$

$A_1(b)$ is the number of reproductions of stage $s-1$ in s, so the first term in equation (6) represents the total number of SAWs completely embedded in a single reproduction of stage $s-1$. $A_2(b)$ is the number of external sites connecting these reproductions at one side of the stage s, and E_n^b is the number of embeddings in stage s which crosses two reproductions of stage $s-1$ through external sites. Analogously, $A_3(b)$ and I_n^b refer to the embeddings passing through internal sites. Figure 2 shows two particular embeddings which contribute to E_n^b and one to I_n^b. Note that they do not depend on b nor s if these parameters are sufficiently large.

The coefficients $A_1(b)$, $A_2(b)$ and $A_3(b)$ are given by:

$$A_1(b) = b(b+1)/2 \tag{7a}$$

$$A_2(b) = (b-1) \tag{7b}$$

$$A_3(b) = (b-1)(b-2)/2. \tag{7c}$$

Analogously, we obtain the recursion formula for the number of lattice sites $N^b(s)$:

$$N^b(s) = A_1(b)N^b(s-1) - 3A_2(b) - 2A_3(b). \tag{8}$$

Iterating the recursion formula (6) up to $s_0 + 1$ we obtain:

$$G_n^b(s) = A_1^{s-s_0}G_n^b(s_0) + \frac{1-A_1^{s-s_0}}{1-A_1}[3A_2E_n^b + A_3I_n^b]. \tag{9}$$

E_n^b and I_n^b can be obtained considering the embeddings of n-step SAWs across two adjacent reproductions of stage s_0 [11]. In table 1 we present the values of s_0, $G_n^2(s_0)$, E_n^2 and I_n^2 for the 2-triangle for $1 \leqslant n \leqslant 5$.

Table 1. Numerical values of s_0, $G_n^2(s_0)$, E_n^2 and I_n^2 for $1 \leqslant n \leqslant 5$.

	s_0	$G_n^2(s_0)$	E_n^2	I_n^2
$n = 1$	1	9	0	0
$n = 2$	2	75	4	12
$n = 3$	2	171	24	72
$n = 4$	3	1389	100	300
$n = 5$	3	3264	344	1032

Table 2. Selected values of $c_n(b)$.

	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$	$n = 8$
$b = 2$	4	12	30.67	76	186.67	2691.11
$b = 3$	4.29	14.57	42.43	116.14	307.29	5740.33
$b = 4$	4.5	16.50	53.10	159.90	458.85	9759.63
$b = 5$	4.67	18	61.96	201.87	628.89	15 742.83
$b = 8$	5	21	80.44	297.33	1073.19	44 635.75
$b = 15$	5.37	24.32	101.47	412.18	1650.96	100 535.28
$b = \infty$	6	30	138	618	2730	224 130

Iterating equation (8) with $s_0 = 1$ one obtains:

$$N^b(s) = A_1^{s-1} N^b(1) + \frac{1 - A_1^{s-1}}{1 - A_1}[-3A_2 - 2A_3]. \tag{10}$$

$N^b(1)$, the number of sites of the generator of the b-triangle, is given by:

$$N^b(1) = \frac{(b+1)(b+2)}{2}. \tag{11}$$

Using (10) and (11), we can rewrite (4a) as:

$$c_n(b) = \lim_{s\to\infty} \frac{G_n^b(s)}{N^b(s)} = \frac{(A_1 - 1)G_n^b(s_0) + (3A_2 E_n^b + A_3 I_n^b)}{A_1^{s_0-1}[(A_1 - 1)N^b(1) - (3A_2 + 2A_3)]} \tag{12}$$

where A_1, A_2 and A_3 are given by (7).

In table 2 we present $c_n(b)$ up to $n = 8$ for some values of b between 2 and 15.

We have constructed series up to the order of $n = 14$ for b ranging from 3 to 20 and up to $n = 13$ for b ranging from 21 to 100.

3. Finite SAWs in the Euclidean limit

Consider a particular n-step SAW and let b be sufficiently large: in this case $s_0 = 1$. In figure 3 we show this SAW embedded in the generator. The total number of embeddings obeys the relation:

$$\tfrac{1}{2}(b - R + 1)(b - R + 2) \leqslant G_{\mathrm{SAW}}^b(1) \leqslant \tfrac{1}{2}(b+1)(b+2). \tag{13}$$

R is the greatest distance between two distinct sites belonging to the SAW, and the left-hand side of (13) is a lower bound of the number of embeddings of this SAW, that is, it is the number of embeddings of a (lattice) circle with diameter R, while the right-hand side is the number of sites of the generator.

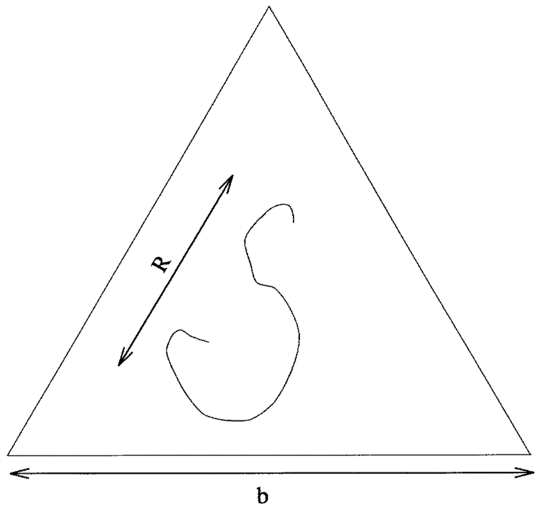

Figure 3. The number of starting sites is less than the total number of sites $\frac{1}{2}(b+1)(b+2)$ and bigger than this total number minus the excluded volume $\frac{1}{2}(b-R+1)(b-R+2)$.

We calculate the number of embeddings of this SAW, $c_{\mathrm{SAW}}(b)$ using the procedure shown in the last section. Using inequality (13) we obtain:

$$\frac{\left(\frac{b(b+1)}{2}-1\right)\left(\frac{1}{2}(b-R+1)(b-R+2)\right)+3(b-1)E_{\mathrm{SAW}}+\frac{(b-1)(b-2)}{2}I_{\mathrm{SAW}}}{\left(\frac{b(b+1)}{2}-1\right)\frac{(b+1)(b+2)}{2}-3(b-1)-(b-1)(b-2)} \leqslant c_{\mathrm{SAW}}(b)$$
$$\leqslant \frac{\left(\frac{b(b+1)}{2}-1\right)\left(\frac{1}{2}(b+1)(b+2)\right)+3(b-1)E_{\mathrm{SAW}}+\frac{(b-1)(b-2)}{2}I_{\mathrm{SAW}}}{\left(\frac{b(b+1)}{2}-1\right)\frac{(b+1)(b+2)}{2}-3(b-1)-(b-1)(b-2)} \tag{14}$$

where E_{SAW} and I_{SAW} have analogous definitions as I_n^b and E_n^b respectively.

In the limit $b \to \infty$ both sides of this inequality go to 1. So,

$$\lim_{b\to\infty} c_{\mathrm{SAW}}(b) = 1. \tag{15}$$

Using (5) it follows that:

$$\lim_{b\to\infty} c_n(b) = \sum_{\mathrm{SAW}/n} \lim_{b\to\infty} c_{\mathrm{SAW}}(b) = c_n(T). \tag{16}$$

This result means that the nth terms of the series expansions for SAWs on the b-triangles converge to the nth term of the series for the triangular lattice when $b \to \infty$.

4. Numerical results in the Euclidean limit

Considering b as a continuous parameter, the sequence of functions $\{[c_n(b)]^{1/n}\}$ is such that each term goes to $\{[c_n(T)]^{1/n}\}$ when $b \to \infty$, as shown in section 3. The inversion of the limits $n \to \infty$ and $b \to \infty$ is possible if the convergence of that sequence is uniform. Note in figure 4 the decreasing distance between the curves for subsequent n values, which is a necessary condition for a uniform convergence. With this assumption, we get:

$$\lim_{b\to\infty} \mu_b = \lim_{b\to\infty}\lim_{n\to\infty}[c_n(b)]^{1/n} = \lim_{n\to\infty}\lim_{b\to\infty}[c_n(b)]^{1/n} = \lim_{n\to\infty}[c_n(T)]^{1/n} = \mu_T. \tag{17}$$

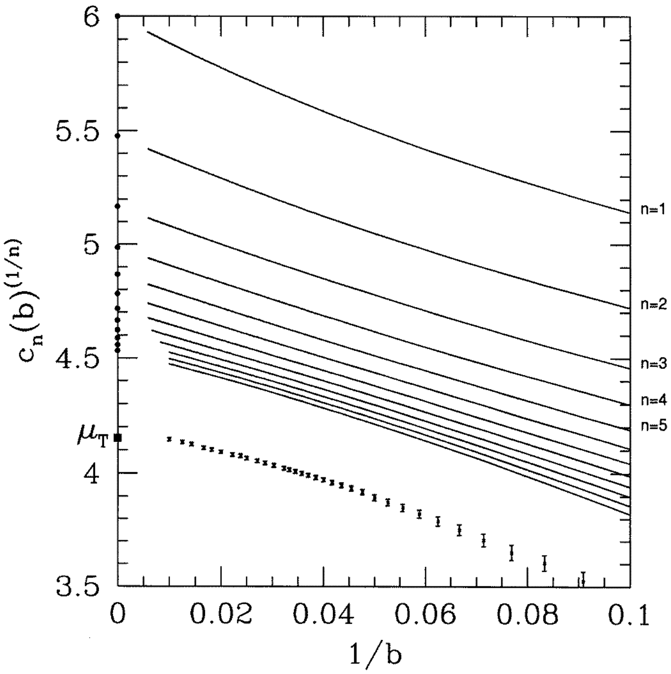

Figure 4. Plot of $[c_n(b)]^{1/n}$ versus $1/b$ for $1 \leqslant n \leqslant 12$ and $b \leqslant 170$. The dots are the limiting triangular values. The plot displays the characteristic behaviour of a uniform convergent series. The crosses are our estimates of μ_b (see text).

Equation (12) guarantees a rational expression for $c_n(b)$. Its finite value in the limit $b \to \infty$ implies that both polynomials are of the same degree k. Then,

$$c_n(b) = \frac{\alpha_0 b^k + \alpha_1 b^{k-1} + \cdots}{\beta_0 b^k + \beta_1 b^{k-1} + \cdots} \tag{18}$$

where α_i, β_i and k depend on n. From (16) and (18) and for b large:

$$\sqrt[n]{c_n(b)} \simeq \sqrt[n]{c_n(T)} \left(1 + \frac{\delta_n}{b}\right)^{1/n} \tag{19}$$

with

$$\delta_n = \frac{\alpha_1}{\alpha_0} - \frac{\beta_1}{\beta_0}. \tag{20}$$

In figure 5 we plot δ_n versus n calculated from (19). We obtain:

$$\delta_n \sim n^{0.8}. \tag{21}$$

Taking the limit $n \to \infty$ in equation (19) and using (3) and (21), we get that $\mu_b \to \mu_T$, with a null first-order correction in $1/b$.

Our numerical estimates of μ_b confirm this result. We calculate the linear extrapolated values for different sets of points in the plot $c_n(b)^{1/n}$ against $\frac{(\ln n)/n}{c_n(b)^{1/n} - c_1(b)}$. The estimates of μ_b are obtained averaging these values. The error bar is their standard deviation. This method parallels the construction of Neville tables [10]. Our results for the known cases $b = 2$ and for the triangular lattice are $\mu_2 = 2.2815 \pm 0.0067$ and $\mu_T \approx 4.154$, using series

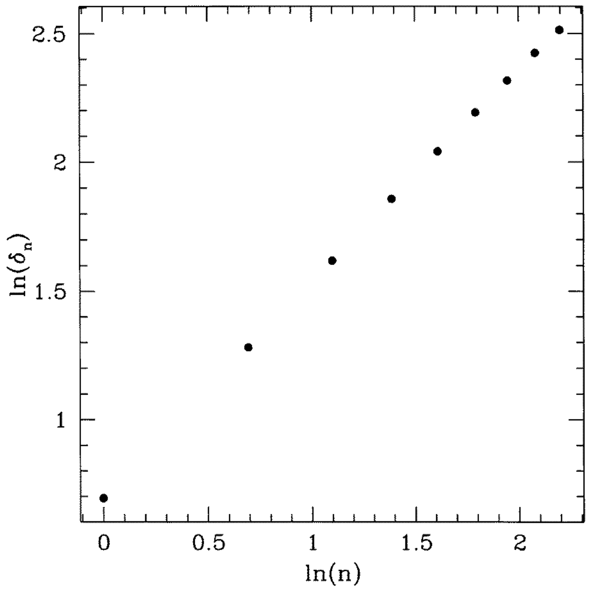

Figure 5. Log–log plot of δ_n versus n.

Table 3. Numerical estimates of μ_b.

b	μ_b	b	μ_b
2	2.282 ± 0.007	26	3.982 ± 0.009
3	2.49 ± 0.02	27	3.991 ± 0.009
4	2.686 ± 0.004	28	4.000 ± 0.008
5	2.82 ± 0.01	29	4.008 ± 0.008
6	2.92 ± 0.02	30	4.015 ± 0.008
7	2.99 ± 0.05	31	4.022 ± 0.008
8	3.13 ± 0.07	33	4.034 ± 0.008
9	3.27 ± 0.07	35	4.044 ± 0.008
10	3.39 ± 0.06	37	4.053 ± 0.007
11	3.52 ± 0.04	40	4.065 ± 0.007
12	3.60 ± 0.03	42	4.071 ± 0.007
13	3.65 ± 0.03	45	4.080 ± 0.007
14	3.71 ± 0.03	50	4.092 ± 0.007
15	3.75 ± 0.02	55	4.102 ± 0.007
16	3.79 ± 0.02	60	4.110 ± 0.007
17	3.82 ± 0.02	65	4.119 ± 0.007
18	3.85 ± 0.02	70	4.125 ± 0.007
19	3.87 ± 0.01	75	4.130 ± 0.007
20	3.89 ± 0.01	80	4.134 ± 0.008
21	3.92 ± 0.01	85	4.138 ± 0.008
22	3.93 ± 0.01	90	4.141 ± 0.008
23	3.95 ± 0.01	95	4.144 ± 0.008
24	3.96 ± 0.01	100	4.146 ± 0.008
25	3.972 ± 0.009		

up to the order of $n = 19$ and 14, respectively. They are in good agreement with the known results $\mu_2 = 2.288$ [2] and $\mu_T = 4.150\,75 \pm 0.0003$ [12].

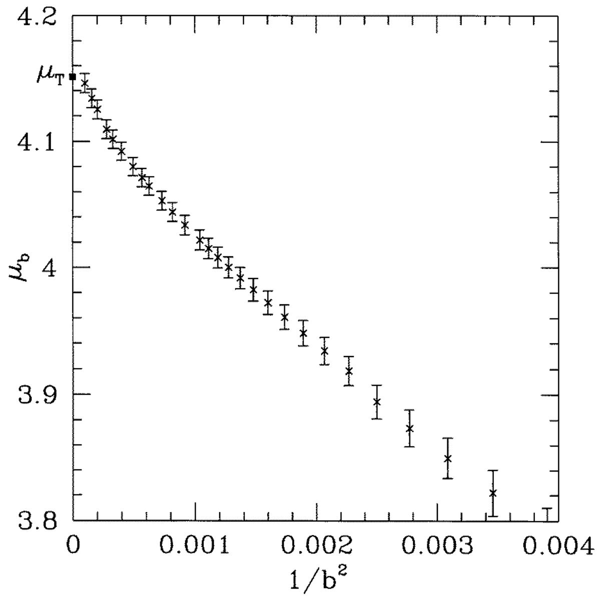

Figure 6. Plot of μ_b versus $1/b^2$. Convergence towards the Euclidean value μ_T is observed.

In table 3 we show the estimates of μ_b obtained using the procedure above for several b up to $b = 100$.

In figure 6 we plot μ_b versus $(1/b^2)$. From the numerical analysis of the data in table 3 we get asymptotically:

$$\mu_b = (4.148 \pm 0.003)\left(1 - \frac{(29.0 \pm 0.9)}{b^2} + \mathrm{o}\left(\frac{1}{b^3}\right)\right). \tag{22}$$

It confirms the convergence of μ_b to μ_T when $b \to \infty$. The limiting value of μ_b when $b \to \infty$ includes the triangular lattice value, and the first correction term is estimated.

The connective constants μ_b may also be obtained using an alternative method based on exact renormalization relations [1, 2]. For the Sierpinski gasket family, the non-trivial fixed point does not determine μ_b: one should study numerically the flow in the parameter space, as shown in [2] for the particular case of $b = 2$.

In [4], it is also suggested an asymptotic behaviour for the non-trivial fixed points of these renormalization equations, as $b \to \infty$. Nevertheless, as mentioned above, μ_b are not trivially related with the fixed points in the case of the Sierpinski gasket family, and so, it is not possible to draw any comparison with the asymptotic behaviour found in (22).

5. Conclusion

The main aim of this work is the study of the convergence of μ_b towards the Euclidean value μ_T when $b \to \infty$. As explained in the text, this convergence is not obvious due to an inversion of the limits $b \to \infty$ and $n \to \infty$ when one calculates $\lim_{b\to\infty} \mu_b$ or μ_T.

The direct computation of μ_b for large b according to (3) demands the evaluation of $c_n(b)$ for n and b sufficiently large. On the other hand, the exponential growth of $G_n^b(s_0)$ with n sets of upper values of n for which $c_n(b)$ can be evaluated for each b-triangle by (12).

In this treatment, the sequence of coefficients $c_n(b)$ are considered for each value of b independently. We then proceed with a new analysis and consider $c_n(b)$ as a sequence of functions (with index n) of the continuous parameter b. The asymptotic behaviour of $c_n(b)$ when $b \to \infty$ for each value of n is obtained and it is shown analytically that $\lim_{b\to\infty} c_n(b) = c_n(T)$, that is, each coefficient converges asymptotically to the triangular value.

Our analysis of the coefficients $c_n(b)$ indicate that $\lim_{b\to\infty} \mu_b = \mu_T$ with the first-order correction term of the order $\frac{1}{b^2}$.

The numerical estimates of μ_b confirm the above result. This is the first numerical evidence of the convergence of a critical parameter of SAWs to the corresponding Euclidean value when $b \to \infty$ in the family of generalized Sierpinski gaskets.

Using an exact enumeration technique to calculate $c_n(b)$ we obtain series expansions that are exact order by order. The results presented here for μ_b have good accuracy and can be systematically improved by enlarging the order of the series.

The investigation of the statistic of SAWsz on fractals based on the series-expansion method would also be helpful to settle some open question and conjectures regarding the limiting behaviour of the associated critical exponents as $b \to \infty$. Work along these lines is in progress.

Acknowledgments

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