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LETTER TO THE EDITOR

Self-avoiding walks on fractals studied by the Monte Carlo renormalization group

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Abstract. We have applied the Monte Carlo renormalization group (MCRG) method to study the problem of self-avoiding walks on the Sierpinski gasket family of fractals. Each member of the family is labelled by an integer b, $2 \leqslant b \leqslant \infty$, and when $b \to \infty$ both the fractal d_f and spectral d_s dimension approach their Euclidean value 2. We have calculated the critical exponent ν, associated with the mean square end-to-end distance, up to $b = 80$. Our MCRG results deviate at most 0.03% from the available exact results (for $2 \leqslant b \leqslant 9$). The obtained data show clearly that ν *monotonically decreases* with b and *crosses the Euclidean value* $\nu = \frac{3}{4}$ at $b \approx 27$, that is, before entering the fractal to Euclidean crossover region that occurs in the limit $b \to \infty$.

The statistics of self-avoiding walks (SAWs) on random fractals, and in particular on critical percolation clusters, has acquired the attribute of being a rather controversial problem in the past decade (see, for example, Lam (1990) and Kim (1990)). The main query concerns correct values of the critical exponent ν for the mean square end-to-end distance of SAWs on fractals, defined by $\langle R_N^2 \rangle \sim N^{2\nu}$, where N is the number of steps. In addition to various numerical approaches to the problem, several Flory-type formulae for ν have been proposed (see, for example, Roy and Blumen (1990) and references quoted therein). Almost all of these proposals have been tested against available results for ν of SAWs on deterministic fractals (Rammal *et al* 1984). For this reason, knowledge of exact values of ν on a class of non-trivial deterministic fractals provides a systematic test of the phenomenological proposals. However, so far only a limited sequence of results for the Sierpinski gasket class of fractals has been available (Elezović *et al* 1987).

The limited sequence of the Sierpinski gasket results, that served (Dekeyser *et al* 1987, Aharony and Harris 1989) as a testing ground for the phenomenological proposals, deserved to be extended in its own right. Indeed, the exact results of Elezović *et al* (1987), together with the related finite-size scaling arguments of Dhar (1988), engendered an interesting puzzle. Each member of the Sierpinski gasket class of fractals is labelled by an integer b ($2 \leqslant b \leqslant \infty$), and when b approaches very large values both the fractal dimension d_f and spectral dimension d_s approach their Euclidean value 2 (with the correction terms $\ln 2/\ln b$ and $\ln(\ln b)/\ln b$, respectively). Now, the exact values of ν, known for $2 \leqslant b \leqslant 9$ (Dhar 1978, Elezović *et al* 1987, Bubanja and Knežević 1991), are larger than the Euclidean value $\nu = \frac{3}{4}$ (Nienhuis 1982) and monotonically decrease with increasing b. On the other hand, using finite-size scaling arguments, Dhar (1988) predicted that ν should tend to $\frac{3}{4}$ from below when $b \to \infty$, that is, with a negative correction term proportional to $\ln(\ln b)/\ln b$. This implies that ν, as a function of b, should be a *non-monotonic function*, such that at some puzzling *finite* $b > 9$ crosses the Euclidean value $\frac{3}{4}$, which does not seem very plausible. To unravel this puzzle we apply the Monte Carlo renormalization group (MCRG) method, since the exact calculation of ν cannot be pushed much farther beyond $b = 9$.

For the sake of introducing the MCRG method it is useful to outline the exact renormalization group approach of calculating ν for the Sierpinski gasket class of fractals. First, it is necessary to recall that each member (characterized by b) of the class can be constructed in stages. At the initial stage ($n = 1$) of the construction there is an equilateral triangle (generator) that contains b^2 identical smaller triangles of unit side length, out of which only the upward oriented are assumed to be physically present (see, for example, figure 1 in the paper by Elezović *et al* (1987)). The subsequent fractal stages are constructed self-similarly. Fractals constructed in this way allows of formulating exact renormalization group (RG) suitable for calculating critical exponents for SAW. To calculate the critical exponent ν we need to study the one-parameter renormalization group transformation

$$B' = \sum_{N=b}^{b(b+1)/2} a_N B^N \tag{1}$$

where B is the weight (fugacity) of one SAW step that traverses the unit triangle, a_N is number of all possible SAW of N steps that traverse (see figure 1) the fractal generator, and B' is the corresponding renormalized fugacity. The specific value of ν, for a given b, follows from

$$\nu = \frac{\ln b}{\ln \lambda} \tag{2}$$

where λ is the relevant eigenvalue of the RG equation (1) at the non-trivial fixed point $0 < B^* < 1$ (Elezović *et al* 1987)

$$\lambda = \left.\frac{\mathrm{d}B'}{\mathrm{d}B}\right|_{B^*}. \tag{3}$$

Thus the central task in evaluation of ν, for a given b, consists of determining number a_N of all possible SAWs of N steps that traverse the fractal generator. Unfortunately, the exact enumeration of SAWs cannot be easily done for b larger than $b = 9$ (for

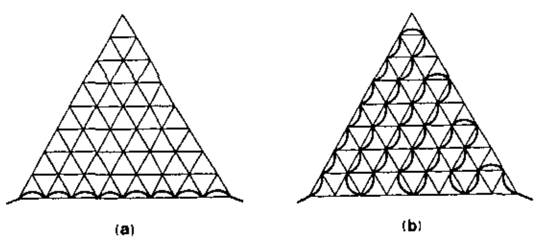

Figure 1. The SAW traversing the $b = 8$ fractal generator with the minimum (a) and maximum (b) number of steps. The SAW paths are represented by the wavy solid lines. One should note that the walker is not allowed to cross any downward oriented unit triangle, and if it crosses an upward oriented unit triangle it is never allowed to enter it again.

example, to calculate in this way ν for $b=10$ it would require about 85 days of continuous operating of the IBM 3090 mainframe).

For the reasons explained in the preceding paragraph, we apply the MCRG method to learn ν for SAW on the fractals with $b>9$. It can be expected that, due to both the inherent self-similarity and the finite ramification of the underlying fractals, this method works better here than in the case of regular lattices. The starting point of the method (Reynolds and Redner 1980) consists of treating B' as the grand canonical partition function that comprise all possible SAW that enter and exit the fractal generator at two fixed apexes. Accordingly, the relation (1) can be written in the following form

$$\frac{\mathrm{d}B'}{\mathrm{d}B}=\frac{B'}{B}\langle N(B)\rangle \tag{4}$$

where $\langle N(B)\rangle$ is given by

$$\langle N(B)\rangle=\frac{1}{B'}\sum_{N=b}^{b(b+1)/2} Na_N B^N \tag{5}$$

which seems to be the average number of steps made, at fugacity B, by all possible SAW that pass the generator. Comparing (3) and (4), we obtain the equality $\lambda=\langle N(B^*)\rangle$, and thereby we find

$$\nu=\frac{\ln b}{\ln\langle N(B^*)\rangle}. \tag{6}$$

This formula enables us to determine the critical exponent ν by calculating $\langle N(B^*)\rangle$ via the constant-fugacity MCRG method (Redner and Reynolds 1981).

For a given b, we begin with determining the critical fugacity $B^*=1/\mu$, where μ is the connectivity constant (Elezović *et al* 1987). To this end, we start the Monte Carlo (MC) simulation with an initial guess for the fugacity B_0 in the region $0<B_0<1$. Here B_0 can be interpreted as the probability of making the next step along an available direction from the vertex that the SAW walker has reached. Let us assume that S_0 is the total number of the MC simulations of SAW (at the chosen B_0), and let S_0^{t} of them be those that traverse the fractal generator. Hence the ratio S_0^{t}/S_0 can be accepted as the renormalized fugacity B_0' of the coarse-grained fractal structure. In this way we get the value of the sum (1) without specifying the set a_N. Then, the next values B_n $(n\geqslant 1)$, at which the MC simulation should be performed, can be found by using the 'homing' procedure (Redner and Reynolds 1981), which can be terminated at the stage when the difference B_n-B_{n-1} becomes less than the statistical uncertainty associated with B_{n-1}. Consequently, B^* can be identified with the last value B_n found in this way.

Having found B^* we can evaluate $\langle N(B^*)\rangle$ by performing the MC simulation at this particular value. During this simulation it is important to record the number S_N^{t} of SAW that traverse the fractal generator in N steps. These data allow us to write

$$\langle N(B^*)\rangle=\frac{1}{S_{\mathrm{c}}^{\mathrm{t}}}\sum_{N=b}^{b(b+1)/2} NS_N^{\mathrm{t}} \tag{7}$$

where $S_{\mathrm{c}}^{\mathrm{t}}$ is the number of all SAW that traverse the fractal generator at the critical fugacity B^*. Thereby we can learn the value of $\langle N(B^*)\rangle$ and, through formula (6), the critical exponent ν. Using the HP9000/S800 computer, we have in this way been able to calculation ν up to $b=80$. The time needed for this calculation increases exponentially with b (for example, 10^5 simulations, for $b=10$ and $b=80$, at the corresponding critical fugacities, required 10 minutes and 46 hours of the available CPU time, respectively).

Our results for the critical exponent ν for $b \geq 10$ are given in table 1, whereas results for $2 \leq b \leq 9$ we compare here with the available exact results. For $b=2$ Dhar (1978) found the exact value $\nu=0.798\,62$, while we have obtained $\nu=0.798\,46 \pm 0.000\,53$. For $3 \leq b \leq 8$, the set of exact values {0.793 64, 0.788 40, 0.784 01, 0.780 33, 0.777 17, 0.774 41}, calculated by Elezović *et al* (1987), should be compared with the set of our MCRG results {0.793 66 ± 0.000 39, 0.788 23 ± 0.000 33, 0.784 02 ± 0.000 29, 0.780 10 ± 0.000 27, 0.777 28 ± 0.000 25, 0.774 24 ± 0.000 24}. Finally, for $b=9$ we can compare the exact value $\nu=0.771\,96$, obtained recently by Bubanja and Knežević (1991), with our result $\nu=0.772\,18 \pm 0.000\,23$. All our results quoted here have been obtained by performing 2×10^5 simulations. We can see that each of our results deviates at most 0.03% from the relevant exact value, and thus we can conclude that the agreement between the exact and the MCRG results is strikingly good.

In figure 2 we have depicted our results for ν, together with the available exact results. From this figure, and from table 1, it follows that ν is a monotonic function of b (*in the entire region* $2 \leq b \leq 80$), and crosses the Euclidean value $\nu=\frac{3}{4}$ at $b \approx 27$. This finding, in conjunction with the prediction of Dhar (1988) about the limit $b \to \infty$, implies that ν should display a minimum at some $b_{\min} > 80$. In other words, if the prediction (Dhar 1988) that ν should approach the Euclidean value $\frac{3}{4}$ in the limit $b \to \infty$ from below (that is, with the negative correction term of the type $\ln(\ln b)/\ln b$) is valid, then ν for SAW should be a *non-monotonic function* of b, and this function should have a minimum at some value of b *larger than* $b=80$.

Table 1. The MCRG results for the critical exponent ν of SAW on the Sierpinski gasket type of fractals for $10 \leq b \leq 80$. The particular values of b have been chosen in such a way as to make the corresponding data as much as possible uniformly distributed on the $1/b$ scale. The given error bars are determined by statistics of the method applied (Redner and Reynolds 1981).

b	No of MC realizations	B^*	$\langle N(B^*) \rangle$	ν
10	10^6	0.395 86 ± 0.000 07	19.908 ± 0.008	0.769 80 ± 0.000 10
12	2×10^5	0.380 37 ± 0.000 13	25.64 ± 0.02	0.765 94 ± 0.000 20
15	2×10^5	0.363 96 ± 0.000 11	34.95 ± 0.03	0.761 99 ± 0.000 18
17	3×10^5	0.355 93 ± 0.000 08	41.79 ± 0.03	0.759 02 ± 0.000 14
20	5×10^5	0.346 81 ± 0.000 06	52.59 ± 0.03	0.756 03 ± 0.000 11
22	2×10^5	0.341 97 ± 0.000 08	60.31 ± 0.05	0.754 00 ± 0.000 16
26	2×10^5	0.336 02 ± 0.000 08	72.44 ± 0.06	0.751 58 ± 0.000 15
26	2×10^5	0.334 44 ± 0.000 07	76.61 ± 0.07	0.750 93 ± 0.000 15
27	3×10^5	0.332 85 ± 0.000 06	81.04 ± 0.06	0.749 91 ± 0.000 12
30	2×10^5	0.328 76 ± 0.000 07	94.33 ± 0.08	0.748 05 ± 0.000 14
35	1.2×10^5	0.323 50 ± 0.000 08	117.6 ± 0.1	0.745 74 ± 0.000 18
40	2×10^5	0.319 36 ± 0.000 06	142.9 ± 0.1	0.743 36 ± 0.000 15
50	10^5	0.313 96 ± 0.000 07	197.8 ± 0.1	0.739 91 ± 0.000 10
60	1.4×10^5	0.310 11 ± 0.000 06	256.7 ± 0.2	0.737 98 ± 0.000 12
70	10^5	0.307 45 ± 0.000 06	322.1 ± 0.6	0.735 70 ± 0.000 22
80	10^5	0.305 46 ± 0.000 06	391.6 ± 0.7	0.733 96 ± 0.000 21

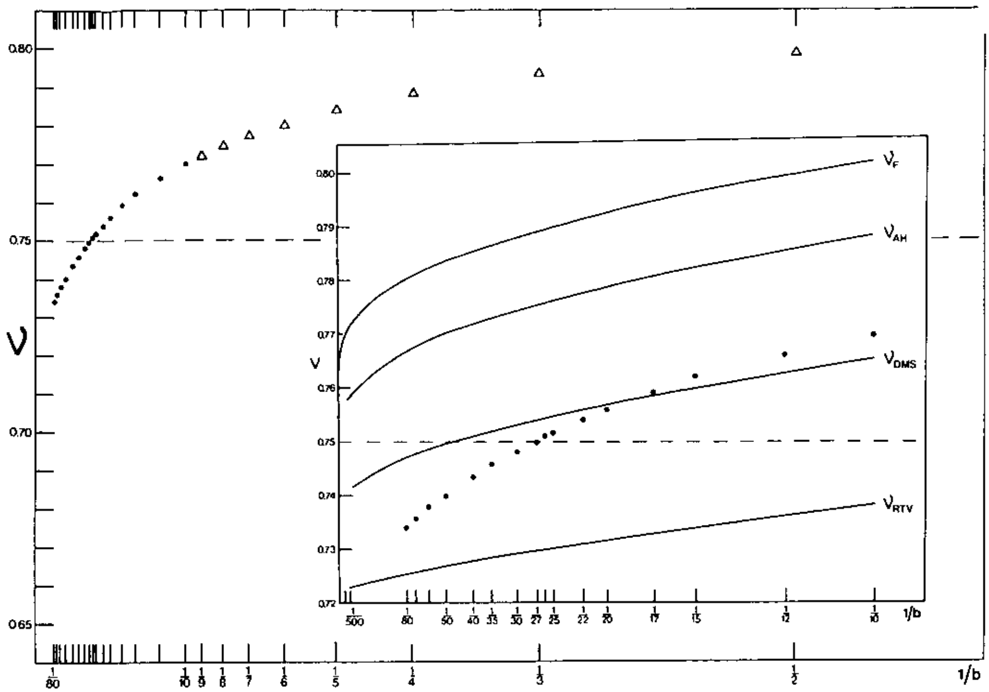

Figure 2. The MCRG (solid circles) and exact (small open triangles) results for the critical exponent ν as a function of $1/b$. The horizontal broken line represents the Euclidean value $\nu = \frac{3}{4}$ (Nienhuis 1982). In the inset the MCRG results are compared with the results that follow from the phenomenological formulae ν_F, ν_{RTV}, ν_{AH} and ν_{DMS} given by relations (8), (9), (10) and (11), respectively. The related curves ν_{RTV}, ν_{AH} and ν_{DMS} are plotted up to $b = 650$, which corresponds to the last calculated value of the requisite spectral dimension (Milošević *et al* 1988). The error bars related to the MCRG data are not depicted in the figure since they are at most of the size of the radii of the solid circles that represent the data.

The observed decrease of ν in the region $2 \leq b \leq 80$, and the expected decrease beyond $b = 80$, imply, according to the formula (6), that $\langle N(B^*) \rangle$ increases faster than b. This decrease of ν can be explained in the following way. For values of b close to $b = 2$, the dominant number of SAWs are those that quickly traverse the fractal generators (see figure 1(a)), whereas for larger b the walks that contain many rebounds from the generator edges (see figure 1(b)) begin to predominate, which makes the walk look like the Hamiltonian walk (see, for example, Bradley 1989). This argument can be corroborated numerically. Indeed, for the Hamiltonian walks $\nu = 1/d_f$, and, when $b \to \infty$, the asymptotic form $\nu = \frac{1}{2} + \ln 2/(4 \ln b)$ is valid. On the other hand, a straightforward numerical analysis of our data for $b > 20$ reveals that the best fit of ν can be obtained assuming the variable $1/\ln b$.

In the inset of figure 2 we present a comparison of the MCRG results, for $b \geq 10$, with the results that follow from various phenomenological formulae for ν. All these formulae stem from attempts to find a finite set of fractal properties which determine the SAW critical exponents. The simplest formula

$$\nu_F = 3/(2 + d_f) \qquad (8)$$

is a straightforward generalization (Kremer 1981, Sahimi 1984) of the Flory formula

$\nu = 3/(2+d)$, where d is the Euclidean dimension of a substratum. The next formula

$$\nu_{RTV} = 3d_s/d_f(2+d_s) \tag{9}$$

includes both the fractal d_f and spectral d_s dimension (Rammal *et al* 1984). Recently several groups of authors (Aharony and Harris 1989, Bouchaud and Georges 1989, Roy and Blumen 1990) proposed a new relation between ν and the fractal properties, which in the case of the Sierpinski gasket fractals has the form

$$\nu_{AH} = (4d_f - d_s)/[d_f(2d_f - d_s + 2)]. \tag{10}$$

Finally, we quote here the formula

$$\nu_{DMS} = (2d_f + d_s)/[d_f(2+d_f)] \tag{11}$$

which follows from the work of Dekeyser *et al* (1987). One should notice that the last three formulae predict, in agreement with the finite-size scaling argument (Dhar 1988), that ν should approach the Euclidean value $\frac{3}{4}$, when $b \to \infty$, with the negative correction term proportional to $\ln(\ln b)/\ln b$. However, one can also notice that none of the quoted formulae provide satisfactory fit to the existing values of ν for SAWs on the Sierpinski gasket type of fractals.

In conclusion, we would like to point out that the application of the MCRG method to the study of SAWs on the Sierpinski gasket family of fractals produced results that agree quite well with the previously known exact results. Besides, new results confirm that the critical exponent ν crosses the Euclidean value $\frac{3}{4}$ *before entering* the fractal to Euclidean crossover region that appears in the limit $b \to \infty$. This finding, together with the fact that all phenomenological proposals deviate significantly from the MCRG results, may serve as an instructive caveat in the future quests for a proper theory of SAWs on random fractals, such as the critical percolation clusters.

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References

Aharony A and Harris A B 1989 *J. Stat. Phys.* **54** 1091
Bubanja V and Kneževič M 1991 to be published
Bouchaud J P and Georges A 1989 *Phys. Rev.* B **39** 2846
Bradley R M 1989 *J. Phys. A: Math. Gen.* **22** L24
Dekeyser R, Maritan A and Stella A 1987 *Phys. Rev. Lett.* **58** 1758
Dhar D 1978 *J. Math. Phys.* **19** 5
—— 1988 *J. Physique* **49** 397
Elezović S, Knežević M and Milošević S 1987 *J. Phys. A: Math. Gen.* **20** 1215
Kim Y 1990 *Phys. Rev.* A **41** 4554
Kremer K 1981 *Z. Phys.* B **45** 149
Lam P M 1990 *J. Phys. A: Math. Gen.* **23** L831
Milošević S, Stassinopoulos D and Stanley H E 1988 *J. Phys. A: Math. Gen.* **21** 1477
Nienhuis B 1982 *Phys. Rev. Lett.* **49** 1062
Rammal R, Toulouse G and Vannimenus J 1984 *J. Physique* **45** 389
Redner S and Reynolds P J 1980 *J. Phys. A: Math. Gen.* **14** L55
—— 1981 *J. Phys. A: Math. Gen.* **14** 2679
Roy A K and Blumen A 1990 *J. Stat. Phys.* **59** 1581
Sahimi M 1984 *J. Phys. A: Math. Gen.* **17** L379