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Finite-size scaling for random walks on fractals

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Abstract. Random walks are simulated on finite stages of construction of regular fractal lattices. It is proved that the mean-square displacement $\langle R_N^2 \rangle$ obeys a finite-size scaling hypothesis and the critical exponent v_w is estimated. The efficiency of the method is proved when applied to finitely ramified fractals in which the problem is exactly solvable. v_w is obtained with good accuracy ($\approx 1\%$) for a class of infinitely ramified fractals, the Sierpinski carpets. The results correct previous estimates based on simulations which did not use finite-size scaling. It is shown that v_w decreases when D_F decreases with very small corrections due to other geometrical properties such as lacunarity. The comparison with estimates of the ideal chain exponent v_c shows that the two problems are not equivalent on these fractals, and that in general $v_w > v_c$. Estimates of v_w with the same accuracy are obtained on two Sierpinski pastry shells ($2 < D_F < 3$), where anomalous diffusion is also observed.

1. Introduction

Random walks on fractals have been studied intensively in the last few years especially due to their relation to diffusion in disordered systems [1]. Their most important property is the anomalous diffusion: the mean-square displacement of the walker varies with the number of steps N as

$$\langle \mathcal{R}_N^2 \rangle \sim N^{2\nu_w} \tag{1}$$

with $v_w < \frac{1}{2}$ ($v_w = 1/D_w$, where D_w is the dimension of the random walk), while in Euclidean lattices $v_w = \frac{1}{2}$. The irregularities of the fractals are responsible for the delay of the diffusion [1].

In the random walk problem on a lattice, the walker at a certain site after N - 1 steps has equal probability to jump to any of its neighbouring sites in the Nth step. The statistical weight of the walk depends on the sites it visits if the coordination number of the lattice is not uniform [1, 2].

The ideal chain problem is closely related to the random walk. It is defined on the same ensemble of walks, but the statistical weight of the chain depends only on its length (x^N) , where x is the step fugacity). It is the equilibrium statistical problem of an ideal polymer (with no self-avoiding effects) in solution [3]. The mean square end-to-end distance of the ideal chain scales according to

$$\langle R_N^2 \rangle \sim N^{2\nu_c} \,. \tag{2}$$

In Euclidean lattices and also on fractals with uniform coordination number (e.g. the Sierpinski gasket), the random walk and the ideal chain have the same asymptotic behaviour, i.e. $v_w = v_c$ [1.4].

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However, the two problems have different behaviours in fractals with non-uniform coordination numbers, where the ideal chain is (statistically) attracted to the sites with highest coordination [5, 6]. When those sites form an infinite connected cluster, the ideal chain is more stretched than the random walk, so that $v_c > v_w$. But when those sites are isolated, they act as 'entropic traps', preventing the swelling of the chain and leading to localization effects: $v_c = 0$ and $\langle R_N^2 \rangle$ may grow, for instance, as $\log N$ [6]. All these properties have been observed in finitely ramified fractals where both problems can be solved exactly. The interesting features of random walks and ideal chains also made both problems useful tools for finding the effects of the fractal geometry on physical systems. More efforts to solve these problems in other regular fractals (constructed iteratively according to fixed rules) are also justified.



Figure 1. Iterative construction of a Sierpinski carpet whose fractal dimension is $D_F = \ln 8 / \ln 3$.

In most of the infinitely ramified fractals, however, there are no exact solutions to these problems. It is the case of Sierpinski carpets (figure 1) and Sierpinski pastry shells. Some exact relations for RW in the carpets have been obtained [7, 8], but not the exact value of v_w .

Exact enumeration techniques were used to estimate v_c in the carpets, and some scaling properties of the chains suggested that they are asymptotically different from random walks [9].

Estimates of v_w were also obtained from several techniques. Gefen *et al* [10] used a bond-moving renormalization scheme, which was improved by Kim *et al* [8], who derived rigorous lower and upper bounds for v_w (with an accuracy of around 10%).

Simulations on finite stages of construction of the carpets have also been performed and estimates of v_w were obtained. These simulations used large lattices which, however, do not represent the fractal exactly, and the walks that touched their borders were discarded when taking the means [8]. These approximations may lead to incorrect results because they neglect the full connectivity of the fractals; for example, overestimating the effect of the central lacuna in the finite lattice. This problem was already pointed out for directed self-avoiding walks on the carpets: when series expansions methods which consider the true fractal limit were applied, the results were very different from simulations estimates [11, 12].

The purpose of this work is to obtain reliable and accurate estimates of v_w for the Sierpinski carpets and for Sierpinski pastry shells ($D_F > 2$), improving all previous estimates. Monte Carlo simulations of random walks on finite (not necessarily large) stages of construction of these fractals are performed. These simulations do not discard walks that touch the borders of the lattices, so that the problem of random walks confined in finite lattices is studied. It is shown that the mean-square displacement obeys a finite-size scaling hypothesis and v_w is obtained from it. These techniques have proved to be extremely

powerful in the study of the critical behaviour of magnetic models, using the data from simulations on finite lattices or exact results on small lattices [13–16].

This paper is organized as follows. In section 2 we present the finite-size scaling hypothesis for random walks and a brief description of the simulations techniques. In section 3 we analyse the results of simulations on fractals where the random walk problem can be solved exactly. In section 4 we use the same method to calculate v_w for the Sierpinski carpets. The results are carefully discussed, giving special attention to the effects of D_F , the lacunarities and the ramification of the fractals on v_w and v_c . In section 5 we apply the method to fractals with dimensions D_F between 2 and 3, the Sierpinski pastry shells. Section 6 contains our final conclusions.

2. Finite-size scaling for random walks

Consider a magnetic system in a lattice of length L at temperature T. The finite-size scaling hypothesis for a thermodynamic function $F_L(T)$ is expressed as [14]

$$F_L(T) \approx L^{-\lambda/\nu} f(L/\xi) \tag{3}$$

where f is a generic function of its argument L/ξ , ξ is the correlation length of the infinite system and the exponent λ describes the critical behaviour of the function F(T) in the infinite lattice. Equation (3) separates finite size effects and the true critical behaviour in a convenient way.

Using the correspondence between magnetic and geometric quantities and equation (3), we propose a finite-size scaling hypothesis adapted for a walk confined inside a lattice with length L:

$$\langle R_N^2 \rangle^{1/2} \approx L f(L N^{-\nu_w}) \,. \tag{4}$$

It is expected that

$$f(x) \sim x^{-1} \qquad x \to \infty \tag{5}$$

so that (1) is recovered when $L \to \infty$. When $N \to \infty$ in a finite system, (4) leads to

$$\langle R_N^2 \rangle^{1/2} \sim L \,. \tag{6}$$

Similar scaling properties have already been observed in self-avoiding walks confined inside spheres [17]. However, they have not been applied to fractals before.

In order to estimate v_w in a fractal, we simulate random walks confined on finite stages of its construction. The initial site for each walk is randomly chosen over the lattice and N_{max} is its maximum number of steps. At each step the walker has probability $1/z_i$ to move to any neighbouring site, where z_i is the number of neighbours of the actual site *i* (it is called the 'myopic ant rule' to construct a RW [5]). Averaging over a certain number of initial sites (number of generated walks), we obtain $\langle R_N^2 \rangle$ for each N in a stage with characteristic length L. Then we plot $\langle R_N^2 \rangle^{1/2}/L$ versus $LN^{-\nu_w}$ using several values of ν_w . The best estimate of ν_w will be the one which provides the collapse of the data for different stages (different L) in the same curve. This procedure is equivalent to some applications of finite-size scaling to magnetic systems [14-16].

3. Applications for finitely ramified fractals

The finite-size scaling hypothesis (equation (4)) will be tested for the fractals in figures 2(a) and (b).

The first test is in the 3-simplex fractal (figure 2(*a*)). The asymptotic behaviours of random walks on this fractal and on the Sierpinski gasket are equivalent, with $v_w = \ln 2/\ln 5 \approx 0.4306$ [4]. We performed simulations on stages n = 3, 4, 5 and 6 of its construction. They correspond to L = 8, 16, 32 and 64, respectively, taking the number



Figure 2. (a) Iterative construction of the 3-simplex fractal, the fractal dimension of which is $D_F = \ln 3/\ln 2$. (b) Iterative construction of the Sierpinski gasket with scale factor b = 3, the fractal dimension of which is $D_F = \ln 6/\ln 3$.



Figure 3. Plots of $(R_N^2)^{1/2}/L$ versus $LN^{-\nu_w}$ for random walks on finite stages of the 3-simplex.

of sites in one border as the length of the system. The number of walks generated in the simulations varied from 20000 for L = 8 to 100000 for L = 64, and the values of N_{max} were 60 and 8000 for these lattices, respectively. The results from different simulations indicate that the errors in $\langle R_N^2 \rangle$ are always less than 1% (for small walks, around 0.1%).

In figures 3(a) and (b) we plot $\langle R_N^2 \rangle^{1/2}/L$ versus $x = LN^{-\nu_w}$ for $\nu_w = 0.431$ (equal to the exact ν_w up to three decimal places) and $\nu_w = 0.444$ (3% above the exact value). These plots used non-uniformly separated values of N, but when all values of N are plotted we obtain almost continuous curves for the greatest lattices, so that the collapse of the data can be analysed in greater detail. The collapse in figure 3(a) is extremely good, and the divergence of the data in figure 3(b) proves the accuracy of the method. When the uncertainties of the simulations are considered, the plots for some values of ν_w around 0.431 show intersections of different lattices' data. From them we obtain an estimate $\nu_w = 0.431 \pm 0.006$ for the 3-simplex.

In the plot of figure 3(a) we note that the data for L = 8 slightly diverge from the other lattices' data when $x \approx 1$. It means that other finite-size effects (corrections to (4)) take place, but they rapidly decrease as L increases, so that (4) is sufficient to describe the behaviour of random walks on finite lattices.

The limit of (6) can be tested with simulations for very large numbers of steps, when a saturation of $\langle R_N^2 \rangle$ is observed. For example, $\langle R_N^2 \rangle$ in stage 6 (L = 64) saturates at around $N = 15\,000$. Estimates of $\langle R_\infty^2 \rangle$ ($\langle R_N^2 \rangle$ for $N \to \infty$) are obtained from the maximum and minimum values of $\langle R_N^2 \rangle$ for several N after that saturation, with an accuracy of around 2%. In figure 4 we plot $\langle R_\infty^2 \rangle^{1/2}$ versus L for the lattices studied. The straight line has an inclination of exactly 1, confirming equation (6) (with a slight deviation for the smallest lattice).

The other test is for the Sierpinski gasket with scale factor b = 3 (figure 2(b)). In this fractal $v_w = \ln 3/\ln(90/7) \approx 0.4301$ [5]. It is an important test because this fractal has non-uniform coordination number, in contrast to the 3-simplex and the usual Sierpinski



Figure 4. Plot of $(R_{\infty}^2)^{1/2}$ as function of L in four stages of the 3-simplex. The straight line has inclination 1.



Figure 5. Plot of $(R_N^2)^{1/2}/L$ versus $LN^{-\nu_w}$ for random walks on finite stages of the Sierpinski gasket with b = 3.

gasket (with scale factor b = 2). We simulated random walks on stages n = 2, 3, 4 and 5, corresponding to L = 9, 27, 81 and 243. In figure 5 we plot $\langle R_N^2 \rangle^{1/2}/L$ versus $x = LN^{-\nu_w}$ for $\nu_w = 0.429$, the value which provides the best data collapse. We note that the data for the smallest lattice (L = 9) diverge from the others, but the collapse of the data for L = 27, 81 and 243 is excellent. Our final estimate of ν_w is 0.429 ± 0.004 . This result includes the exact value and the centre of the error bar differs from it by only 0.3%.

4. Random walks on Sierpinski carpets

The Sierpinski carpets are constructed by the recursive iteration of a generator as shown in figure 1. An initial square is divided into b^2 subsquares and m of them are eliminated according to a fixed rule, and this procedure is applied recursively to the remaining subsquares. The lattice whose sites are in the vertices of the non-eliminated subsquares after an infinite number of iterations has fractal dimension [18]

$$D_F = \frac{\ln(b^2 - m)}{\ln b} \,. \tag{7}$$

We studied random walks on the carpets, the generators of which are shown in figures 6(a)-(h), numbered as 1 to 8 (with decreasing D_F), respectively. The characteristic length of a finite stage of construction n is $L = b^n$, as before.

Table 1. Stages *n* of construction of the carpets on which random walks were simulated, the maximum number of steps N_{max} on each lattice, the corresponding fractal dimensions D_F , the estimates of v_w and the estimates of v_c obtained with series expansion methods [9].

Carpet	DF	n	N _{max}	ν _w	ν _c
1	1.9746	2, 3, 4	500, 14 000, 300 000	0.492 ± 0.005	0.490 ± 0.002
2	1.9343	2,3	1500, 45 000	0.483 ± 0.005	0.470 ± 0.005
3	1.9343	2, 3, 4	1500, 45 000, 2 000 000	0.483 ± 0.005	0.480 ± 0.005
4	1.8957	2,3 -	.3000, 120 000	0.477 ± 0.004	0.455 ± 0.005
5	1.8957	2,3	3000, 120 000	0.475 ± 0.004	0.475 ± 0.015
6	1.8928	2, 3, 4, 5	100, 1000, 8000, 80 000	0.476 ± 0.005	0.45 ± 0.01
7	1.8617	2, 3	6000, 300 000	0.472 ± 0.004	
8	1.8617	2,3	6000, 300 000	0.471 ± 0.004	



Figure 6. Generators of Sierpinski carpets 1-8: (a) b = 5, m = 1; (b) and (c) b = 6, m = 4; (d) and (e) b = 7, m = 9; (f) b = 3, m = 1; (g) and (h) b = 8, m = 16.

In table 1 we present the stages of construction of the carpets on which random walks were simulated and the maximum number of steps (N_{max}) for each lattice. The total number of walks used in the statistics was 500 000, divided into five independent simulations. The only exception was the fourth stage of carpet 3 (L = 1296): as we had to generate very long walks (up to 2×10^6 steps) and due to computer time limitations, only 120 000 walks were generated.

The accuracy of the results was estimated from the dispersion of $\langle R_N^2 \rangle$ for each N in different simulations. It is less than 0.5% for lattices with L < 50, generally the smallest stages used. For the other lattices with L < 250 the errors rarely exceed 1% and for the largest lattices they are near 2%, even for long walks. The slow growth of the statistical errors in $\langle R_N^2 \rangle$ is due to the confinement of the walk, which limits its displacement.

In figures 7(a) and (b) we plot $\langle R_N^2 \rangle^{1/2}/L$ versus $x = LN^{-\nu_w}$ for carpets 3 and 6, respectively, using the value of ν_w (with three decimal places) which provides the best data collapse for each fractal.

For carpet 6, which has the smallest scale factor (b = 3), four stages were studied (see table 1). The data for n = 3, 4 and 5 (L = 27, 81 and 243) collapse into a single curve even for $x \approx 1$, where the finite-size effects are very intense (see figure 7(b)). The data for n = 2 diverge from the others probably due to its small length (L = 9), as already observed in the fractals of section 2. For carpet 3 we also observe the collapse of three lattices' data (see figure 7(a)). These results bring more confidence to the other estimates, most of them based on data of only two stages but with sufficiently large values of L ($L \ge 25$ in all cases).

In table 1 we show the final estimates of v_w for each fractal, obtained with the same procedure described in section 3. All those values agree with the lower and upper bounds for v_w obtained with bond-moving renormalization [8], but are much more accurate (error bars $\sim 1\%$).

The effect of the lacunarity on v_w is very small. Carpets 2 and 3 have the same D_F



Figure 7. Plot of $(R_N^2)^{1/2}/L$ versus $LN^{-v_{w}}$ for random walks on finite stages of: (a) carpet 3; (b) carpet 6.

but different lacunarities [10, 19], and the same holds for the pairs of carpets 4, 5 and 7, 8. In each pair, the first fractal has lower lacunarity, which means a more homogeneus distribution of mass. The differences of v_w are less than 0.5% in each pair.

In other models previously studied in the carpets, such as ideal chains or self-avoiding walks, the influence of the lacunarity on the critical exponents is very important [9,20]. Thus it is surprising that it is not so important to the asymptotic behaviour of random walks.

In figure 8 we plot $v_w \times D_F$ for the carpets 1 to 8. We observe that the general trend is that v_w decreases (D_w increases) when D_F decreases. Interpolating those data one can predict the values of v_w for other carpets with $D_F \ge 1.85$ with uncertainties close to the ones in table 1.

Phenomenological formulae for v_{SAW} as function of v_w and D_F have been proposed and analysed in many fractals [21-24], and other universal properties of physical systems on fractals are still being discussed [25, 26]. Our estimates and the possibility of interpolating them for other carpets may guide future investigations in which v_w is considered a relevant parameter.

In table 1 we also present some previous estimates for the ideal chain exponent v_c [9]. For lattices 2, 4 and 6 we obtain $v_w > v_c$, while for lattices 1, 3 and 5 $v_w \approx v_c$.

In finitely ramified fractals a statistical attraction of the chain to the highest coordination sites, which are isolated or connected along a single path, is observed. In the carpets, however, these sites (z = 4) are generally connected to similar sites in all directions, while the low coordination sites (z = 3) are in the borders of the lacunas. Then the highest coordination sites form an infinite connected cluster, with narrow corridors only between some lacunas of high lacunarity lattices (like carpets 3, 5 and 8).



Figure 8. Plot of the exponent v_w versus the fractal dimension D_F for carpets 1–8. The data for carpets with the same dimension are shown using near error bars.

The result $v_c < v_w < \frac{1}{2}$ in some carpets indicates that the compression of the ideal chain is greater than the compression of the random walk (relative to both systems in two dimensions). It seems that the compression of the ideal chain is due not only to the lacunas but also to their borders (sites with z = 3), while for random walks only the repulsion of the lacunas exists. This speculation is based on the (statistical) attraction of the chain to the highest coordination sites discussed above [5, 6]. In fractals where $v_w \approx v_c$, either this effect is reduced (carpet 1) or it is compensated for by the stretching of the chain in some corridors between lacunas (carpets 3 and 5).

The results of previous simulations which did not use finite-size scaling techniques for carpets 1, 3, 5 and 8 are different than ours [8]. Probably it was due to an overestimation of the compression of the central lacunas, although the lattices used were large. It would have been convenient to test that method in fractals where exact solutions are known to analyse its efficiency.



Figure 9. Generators of Sierpinski pastry shells: (a) b = 3, m = 1; (b) b = 5, m = 27. Internal bonds of the generator are shown only in (a).



Figure 10. Plots of $(R_N^2)^{1/2}/L$ versus $LN^{-\nu_{w}}$ for random walks on finite stages of pastry shell 1.

5. Random walks on fractals with $2 < D_F < 3$

We studied random walks on two Sierpinski pastry shells [18], the generators of which are shown in figures 9(a) and (b), numbered 1 and 2, respectively. They are constructed iteratively like the carpets, with small cubes substituted by the generator at each stage. After an infinite number of iterations, the fractal lattice whose sites are in the vertices of the non-eliminated cubes has dimension

$$D_F = \frac{\ln(b^3 - m)}{\ln b} \tag{8}$$

where b is the scale factor and m is the number of eliminated cubes in the generator.

Table 2. Estima	ttes of v_w for	pastry shells	1 and 2 and thei	r fractal dimensions	D _F .
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Pastry shell	D_F	Vw
1	2.9656	0.492 ± 0.006
2	2.8488	0.478 ± 0.004

In table 2 we present the dimensions of the two fractals studied and the estimates of v_w . The great number of lattice sites to be allocated in the computer for the simulations was the stronger reason to study only these lattices: they have small scale factors and at least two stages with length not very small.

In figure 10 we plot $\langle R_N^2 \rangle^{1/2}/L$ versus $x = LN^{-\nu_w}$ for pastry shell 1, using the value of ν_w which provides the best data collapse. We note that the data for stage n = 2 (L = 9) diverge from the following stages' data (n = 3 and 4), the same phenomena observed in other fractals.

The estimates of v_w prove that there is anomalous diffusion in these fractals, as expected. According to them we may also propose that v_w decreases when the decrease of D_F is large, as observed in the carpets.

Simulations in other Sierpinski pastry shells with equal dimensions and different lacunarities would be interesting to find the extension of the properties of random walks on the carpets. However, one would have to deal with lattices with many sites and special techniques of simulation may have to be developed.

6. Conclusion

Finite-size scaling techniques were used to calculate the anomalous diffusion exponent v_w in various regular fractals, using data from simulations on their finite stages of construction. Applications to fractals where the problem is exactly solvable proved that reliable and accurate estimates can be obtained.

For the Sierpinski carpets new results were presented. For example, the relation $v_w > v_c$ was found in many lattices, in contrast to the result $v_w < v_c$ in some finitely ramified fractals. It was also shown that the dependence of v_w on D_F is much stronger than its dependence on other geometrical properties such as lacunarity, in contrast to some related systems (e.g. ideal chains or self-avoiding walks).

For Sierpinski pastry shells $(2 \leq D_F \leq 3)$ estimates of $v_w < \frac{1}{2}$ were also obtained.

The comparison with other techniques to study critical phenomena on fractal lattices shows the advantage of finite-size scaling. Simulations on large lattices but not analysed with this technique give biased estimates of critical exponents and renormalization techniques for infinitely ramified fractals make approximations of the lattices. Series expansions methods, although considering the true fractal limit, generally do not provide such accurate results due to the small orders of the series. Also note the possibility of studying fractals with $D_F \approx 3$, which would be much more difficult with the other methods.

Other problems can be studied using this technique, such as self-avoiding walks on fractals. Then many classes of fractals can be studied and some open questions, the solutions of which depend on accurate estimates of critical parameters, may be answered. Work along these lines is in progress.

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