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LETTER TO THE EDITOR

'True' self-avoiding walk on fractals

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Abstract. We investigate the 'true' self-avoiding walk on fractal spaces. The number S_N of sites visited during an N-step walk and the root-mean-square displacement R_N are calculated via extensive Monte Carlo simulations on the 2D Sierpinski gasket. For all positive values of the repulsion parameter g, we found the same exponents: $s' = 0.815 \pm 0.001$ and $\nu' = 0.510 \pm 0.005$ respectively. Both R_N and S_N are shown to exhibit a simple scaling behaviour in N and g. We compare our results with a simple Flory-like prediction for the exponent ν'.

Recently there has been an increasing interest in the problem of random walks on fractal lattices and on percolation clusters. The infinite percolation cluster at percolation threshold is just a simple example of fractal structures in physics. The next step is naturally the study of the self-avoiding walks (SAWs) on fractals. Different types of walks are expected to probe in general different properties of a fractal space. For instance the simple random walks (RWs) have simple properties (Alexander and Orbach 1982, Rammal and Toulouse 1983, Angles d'Auriac *et al* 1983) and provide a powerful probe giving direct access to the spectral dimension $\tilde{d}$ which governs the density of states of low energy excitations. Similarly, it was argued recently (Rammal *et al* 1983) that SAWs will probe the fractal $\bar{d}_B$ and spectral $\tilde{d}_B$ dimensionalities of the backbone (i.e. doubly connected component) of the fractal structure. Following the same line of ideas, we investigate in this paper the 'true' self-avoiding walk (TSAW) on fractals. Only recently, Amit *et al* (1983) have shown that the problem of a walker who steps randomly, but tries to avoid places he has already visited, is actually different from the SAW problem. They called this problem the TSAW and show that the upper critical dimensionality d_c of such a walk is two while it is known to be four for SAWs (see Peliti 1983, Obukhov and Peliti 1983). The TSAW on a given lattice corresponds to a walker who can move to one of the nearest neighbours of the site he is at. The probability to move to a site j depends on the number of times n_j that the site has already been visited and is given by

$$P_{i\to j} = \exp(-gn_j) \Big/ \sum_j \exp(-gn_j). \qquad (1)$$

The normalising sum runs over all nearest neighbours j of i. The parameter g measures the intensity with which the path avoids itself ($g > 0$). The limit $g = 0$ corresponds to the RW problem but, except in the case of the linear chain, the TSAW is not equivalent to the standard SAW at $g = \infty$. The parameter g evidently becomes irrelevant at $d > d_c$ and the TSAW reduces to the RW problem.

We first consider a fractal structure of fractal and spectral dimensionalities $\bar{d}$ and $\tilde{d}$ respectively. The following heuristic argument (see Amit *et al* 1983) can be used for the estimation of the mean-square displacement R_N^2 for large N. For a RW ($g=0$), one would of course have $R_N^2 \simeq N^{2\nu_{\mathrm{RW}}}$, where $\nu_{\mathrm{RW}} = \tilde{d}/2\bar{d}$. The number of self-intersections of such a walk is of order $N^2/R_N^{\bar{d}} \sim N^{2-\tilde{d}/2}$. The self-repulsion has the net effect to increase R_N^2. We obtain, therefore, the following estimation:

$$R_N^2 \simeq N^{2\nu_{\mathrm{RW}}} + CN^{2-\tilde{d}/2} \simeq N^{2\nu_{\mathrm{RW}}}(1 + CN^{2-\tilde{d}/2-2\nu_{\mathrm{RW}}}) \tag{2}$$

where C denotes a numerical factor. The correction due to the fact that the walk is self-avoiding is asymptotically negligible for: $2-\tilde{d}/2-2\nu_{\mathrm{RW}}<0$, and may alter the asymptotic behaviour for

$$k \equiv 2-\tilde{d}/2-\tilde{d}/\bar{d} > 0. \tag{3}$$

Otherwise, if (3) is fulfilled the self-repulsion parameter g becomes relevant and deviations from RW statistics are expected to occur. The condition (3) is to be compared with the analogous result (Rammal and Toulouse 1983) for the SAW: $4-\tilde{d}>0$, which involves only the spectral dimension $\tilde{d}$ without any reference to the fractal dimension $\bar{d}$. As it should, (3) reduces to the known result: $2-d>0$ on Euclidean spaces ($\tilde{d}=\bar{d}=d$). In the latter case, important corrections due to g are mainly limited to $d=1$. In opposition, (3) is fulfilled for all d, in two important examples of fractal spaces: the family of Sierpinski gaskets and the infinite percolation clusters at threshold. In the first example, $\bar{d}=\ln(d+1)/\ln 2$, $\tilde{d}=2\ln(d+1)/\ln(d+3)$ and $k>0$ for all d. For percolation clusters, (3) reduces to $\bar{d}>1$, which holds for all d, if the value $\tilde{d}=\frac{4}{3}$ (Rammal and Toulouse 1983) is used as an estimation for $\tilde{d}$.

The above result shows that fractal structures provide a rich field for the investigation of the TSAW statistics. In the following, we consider results for TSAWs on the 2D Sierpinski gasket. Using the same methods we presented previously (Angles d'Auriac *et al* 1983, Rammal *et al* 1984) we simulated about 10^4 TSAWs of $N\sim 5000$ steps, for different values of the repulsion parameter $g \geqslant 0$. All the calculations were performed (in assembly language) on processor M 68000. The gaskets were generated iteratively, and chosen to contain some 10^4 sites (being of 8th order of iteration for $d=2$). For each realisation of the TSAW, both starting points and displacements (equation (1)) were randomly chosen according to standard Monte Carlo procedure. Two statistical properties were investigated: the root-mean-square displacement R_N and the average number S_N of distinct visited sites during N-step walks (range). The usual Euclidean metric has been used to measure the displacements of the walker.

In figure 1 are shown the Monte Carlo results for S_N at different values of the repulsion parameter $0<g<\infty$. After a short transient regime, different initial slopes converge towards a well defined value s' independent of $g>0$. For $g=0$, we recover with a very high accuracy the known value $s=\tilde{d}/2=0.682$, which corresponds to the RW limit. For all positive values of g, *including* $g=\infty$, we obtain a different value for the corresponding exponent: $S_N \sim N^{s'}$. From the best fit of data at large N, we have obtained the following estimation: $s'=0.815\pm 0.001$. This estimation of s' is also supported by a much more extended analysis at $g=0.5$, where averages over 3×10^4 runs were performed. As expected, the exponent s' is enhanced ($s'>s$) by the self-repulsion. The limiting case $g=\infty$ appears to be controlled by the same exponent, making a net difference with Euclidean spaces where $g=\infty$ plays a special role in the TSAW problem.

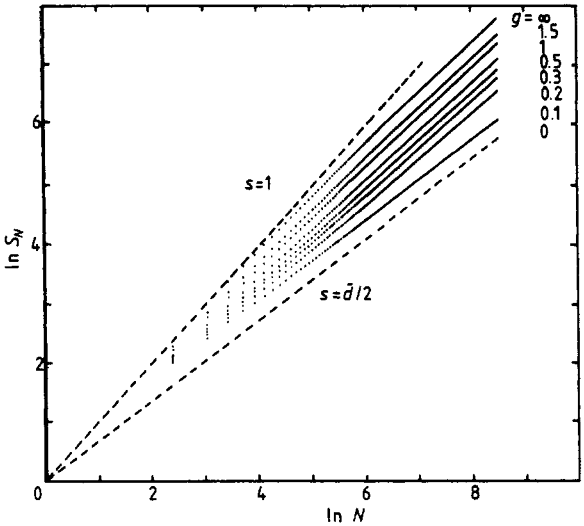

Figure 1. Average range S_N of the TSAW, on a 2D Sierpinski gasket, for different values of the repulsion parameter: $g=\infty$, 1.5, 1, 0.5, 0.3, 0.2, 0.1 and 0. For each value of g, average over 10^4 runs of up to $N=5000$ steps was performed. Broken lines, of slopes $s=1$ and $s=\bar{d}/2$ respectively, are shown for comparison ($\tilde{d}=1.365$, $\bar{d}=1.585$). Different initial slopes merge into the asymptotical slope $s'=0.815$ for large N, independent of the value of $g>0$.

Figure 2 gives the results for the root-mean-square displacement R_N. Again, different initial slopes merge into an asymptotical slope ν' at large N, for all values of $g>0$. As it should be, $\nu=\tilde{d}/2\bar{d}$ is recovered in the RW limit ($g=0$). However, the estimation of ν' is less accurate than that of s'. Indeed, using the best fit of our data

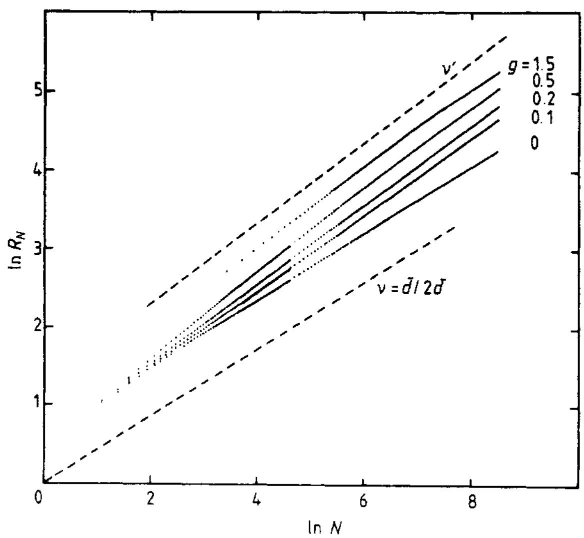

Figure 2. The same plot as figure 1, for the root-mean-square displacement R_N. Broken lines of slopes $\nu=\tilde{d}/2\bar{d}$ and $\nu'=0.51$ corresponding to $g=0$ and $g>0$ are shown for comparison.

at large N, we have found $\nu' = 0.510 \pm 0.005$. In trying to extract ν' (or ν) on fractal space, one encounters several difficulties, mainly related to spatial fluctuations of the structure. It should be noticed that such a complication is not present in the calculations of S_N, which provide very accurate results for s' (or s).

Within the accuracy of our estimations, we conclude that on a gasket, the exploration is *compact*, in the following sense: $S_N \sim R_N^{\bar{d}}$, i.e. $s' = \nu' \bar{d}$. This is the case for $g = 0$ and seems to occur also for all positive values of g. Already visited sites have a high probability of revisitation (in spite of the repulsion!), so that, given a compact volume which contains the walker, most points inside this volume are visited before a new site outside the volume is explored. An example of compact exploration is of course the one-dimensional RW or TSAW (Rammal *et al* 1984).

The value of the exponent ν' so obtained lies between (see table 1) the corresponding value for the RW and that recently calculated for the SAW (Rammal *et al* 1983). In particular, this shows that the TSAW statistics at $g = \infty$ is definitely distinct from that of the SAW on the same structure. In table 1, we have summarised the relevant results for different RW problems on the gaskets.

Table 1. Random walks exponents on the Sierpinski gaskets. RW: simple random walk, SAW: self-avoiding walk, TSAW: true self-avoiding walk. ν = exponent of the RMS displacement ($R_N \sim N^{\nu}$); s = exponent of the average range ($S_N \sim N^{s}$); d = Euclidean dimension; $\bar{d} = \ln(d+1)/\ln 2$: fractal dimension; $\tilde{d} = 2\ln(d+1)/\ln(d+3)$: spectral dimension.

			RW		SAW		TSAW	
d	$\bar{d}$	$\tilde{d}$	ν	s	ν	s	ν	s
1	1	1	1/2	1/2	1	1	2/3	2/3
2	1.5849	1.3652	0.4306	0.6826	0.798	1	0.510	0.815
3	2	1.5474	0.3868	0.7737	0.729	1		

In what follows we will show that the main asymptotical properties of the TSAW can be analysed with the help of a simple scaling argument. Following previous work on $d = 1$, it is natural to consider $z \equiv gN^k$ as a reduced parameter for the TSAW statistics. For instance, matching together the respective RW and TSAW power laws for S_N: $S_N \sim N^s$ and $S_N \sim N^{s'}$, one obtains the simple scaling function

$$S_N = N^s \phi(gN^k) \tag{4}$$

with the following limits

$$\begin{aligned} \phi(z) &\sim 1 && \text{at } z \ll 1, \\ &\sim z^{(s'-s)/k} && \text{at } z \gg 1. \end{aligned} \tag{5}$$

Stated otherwise, $gS_N^{k/s}$ is a universal function $\psi(z)$ of the scaling variable z, with

$$\begin{aligned} \psi(z) &\sim z && \text{at } z \ll 1, \\ &\sim z^{s'/s} && \text{at } z \gg 1. \end{aligned} \tag{6}$$

In figure 3, we have shown some of our data, according to the scaling suggested by equation (6). All points fall on the same universal curve, which shows in particular the expected RW-to-TSAW crossover at $z \sim 1$. In trying to extract k from this kind of

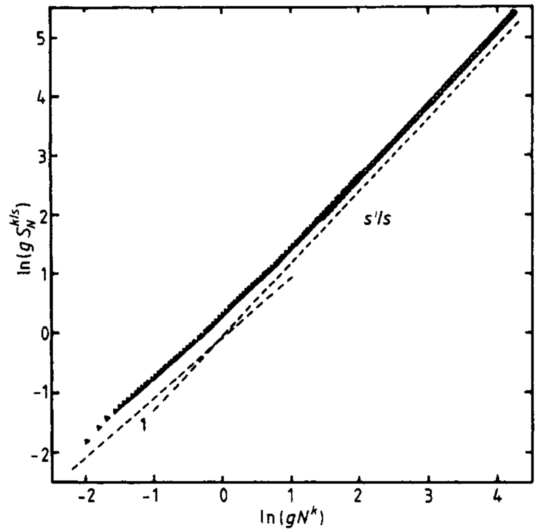

Figure 3. Universal plot of the average range S_N: $gS_N^{k/s}$ against gN^k, where $k = 2-\bar{d}/2-\tilde{d}/\bar{d}(=0.45604)$. For the sake of clarity, only data for $g=0.1$ and 1.5 were used in this plot. The expected crossover between two distinct regimes is clearly observed, at $gN^k \sim 1$.

plot, we have checked the validity of the heuristic argument leading to the proposed value (equation (3)) of the dimension of g. The universal plot of figure 3 strongly supports this argument as well as the scaling (equation (6)) in N and g.

We now discuss a simple Flory-like argument for the exponent ν'. Following a previous study of SAWs on fractals (Rammal *et al* 1983), a first important guess is that the combination $\nu'\bar{d}$ is an intrinsic property, independent of the space in which the fractal is embedded, whereas $\bar{d}$ and ν' both depend on this embedding. The simplest assumption is that $\nu'\bar{d}$ depends only on $\tilde{d}$. On the other hand, the Flory-like argument (Pietronero 1983, Bernasconi and Pietronero 1983) provides a satisfactory interpolation between the values of ν' for Euclidean lattices:

$$\nu' = 2/(d+2) \tag{7}$$

for $d \leqslant 2$. It is exact for $d=2$ and probably for $d \doteq 1$. This suggests a similar approximation for fractals, under the assumption that only $\tilde{d}$ plays a role

$$\nu' = (\tilde{d}/\bar{d})2/(\tilde{d}+2). \tag{8}$$

This is the simplest approximation that reduces to (7) for Euclidean spaces. However, (8) must be considered only as a working hypothesis. For the 2D Sierpinski gasket, (8) gives $\nu' = 0.5119$ which is surprisingly close to our numerical estimation for ν'. This 'agreement' is probably accidental, because ν' (as given by (8)) becomes lower than $\nu = \tilde{d}/2\bar{d}$ for $\tilde{d} > 2$.

In summary we have presented the first results for the TSAW statistics on fractal spaces. Our Monte Carlo simulation for the 2D Sierpinski gasket exhibits a compact exploration of space and a net deviation due to the self-repulsion parameter. A new type of critical behaviour with universal exponents ν' and s' (independent of the repulsive parameter g) was found. The proposed scaling analysis in N and g is found to be consistent with the Monte Carlo results, and can be used to understand the self-attracting regime ($g<0$). In view of the validity of the relation $\nu' = (\tilde{d}/\bar{d})2/(\tilde{d}+2)$, it is of great interest to check this working hypothesis on different fractal structures. A more detailed understanding of the universality classes for SAWS and TSAWS on fractals will be necessary to resolve that question.

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