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# True self-avoiding walks on fractal lattices above the upper marginal dimension

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**Abstract.** We study by Monte Carlo simulations the critical behaviour and the cross-over scaling of the true self-avoiding walks (TSAW) on fractal lattices above the upper marginal dimension. We estimate the Flory exponent  $\nu$  which characterizes the RMS end-to-end distances of TSAW on a percolation cluster at percolation thresholds both in three and four dimensions and on a DLA cluster in three dimensions. Results were in good agreement with the predictions of the known Flory formulae. We also discuss the fractal-to-Euclidean and the RW-to-TSAW cross-over scaling. Monte Carlo data appear to collapse in the scaling regions for both cases; however, we found that the scaling function for the latter is different from that on the regular lattices.

## 1. Introduction

Since the development of the model, the true self-avoiding walks (TSAW) have attracted considerable interest mainly because they exhibit critical behaviour different from the ordinary self-avoiding walks (SAW) [1]. In contrast, the upper marginal dimension,  $d_c$  of SAW is 4 [2], while that of TSAW is known to be 2 [1]. On a  $d$ -dimensional lattice, the Flory formula for the exponent  $\nu$ , defined by the RMS end-to-end distances (or equivalently radii of gyration) of  $N$ -step walks via  $R_N \propto N^\nu$ , was obtained by a self-consistent approach [3] and Flory approximation [4] to be

$$\nu_{\text{TSAW}} = \frac{2}{d+2} \quad (1)$$

for any  $d \leq 2$ . Thus the only Euclidean dimension in which the TSAW attracts interest is in one dimension (1D), where  $\nu$  was found to be  $\frac{2}{3}$ , in agreement with equation (1) [5, 6].

The TSAW is the kinetic process, in which the probability  $P_{j \rightarrow i}$  of moving from site  $j$  to its nearest-neighbour site  $i$  depends on the number of previous visits  $n_i$  on the site  $i$  by

$$P_{j \rightarrow i} = e^{-gn_i} / \sum_k e^{-gn_k} \quad (2)$$

where the sum in the denominator runs over all sites neighbouring site  $j$  and the parameter  $g$  represents the strength of self-avoidance. The extreme limit  $g = 0$  corresponds to the ordinary random walks (RW). For any  $g < 0$ , the TSAW is self-attractive and the RMS end-to-end distances were found to yield an apparent saturation as the number of steps  $N$  increases [7]. For  $g > 0$ , the TSAW tends to avoid the previously visited sites, but it can intersect with itself with smaller probabilities. The excluded-volume effect of TSAW in this case is known to be different from that of SAW even in the extreme limit of  $g \rightarrow \infty$ .

Although the model of TSAW was designed originally from the theoretical motivation due to its unusual critical behaviour, it has later been shown that there exist relevant physical phenomena which can be described by this model. For example, the TSAW was found to describe the statistics of the typical polymers in a polydispersed solution with a broad distribution of chain sizes [4].

The TSAW on a regular lattice has attracted no further attention since the critical behaviour in physically interesting 2D and 3D is expected to be similar to that of non-interacting RW. However, with an increasing interest in fractals [8], the TSAW on fractals has also become an interesting topic in the field of critical phenomena. The first work of such problems is that of Angles d'Auriac and Rammal, who studied the TSAW on a Sierpinski gasket embedded in 2D [9]. They found that the exponent  $\nu$  of TSAW on a Sierpinski gasket was different from that on a regular lattice and, in addition, their estimate was very close to the prediction by Flory-type formula [10], given as

$$\nu_{\text{TSAW}}^R = \frac{d_s}{d_f} \frac{2}{d_s + 2} \quad (3)$$

where  $d_f$  and  $d_s$  are, respectively, the fractal and spectral dimensions of the underlying fractal lattice [11].

Recently, one of the present authors carried out extensive Monte Carlo simulations for TSAW on various fractal lattices, i.e. on Sierpinski gaskets in both 2D and 3D, on an infinite cluster and a backbone of 2D percolation [12, 13]. He obtained the Flory exponent  $\nu$  for such cases to be significantly different from that on a regular lattice. He also found that the estimates of  $\nu$  for all cases were in good agreement with the predictions from the Flory formulae suggested by Bouchaud and Georges [14] and by himself [13]. Bouchaud and Georges derived the Flory-type formula, based on statistical arguments concerning sums of long-range correlated random variables, given as

$$\nu_{\text{TSAW}}^{\text{BG}} = \frac{2\hat{d}}{d_f(2 + 2\hat{d} - d_s)} \quad (4)$$

where  $\hat{d}$  is the so-called spreading dimension of the underlying fractals [15]. On the other hand, Lee obtained, from the usual Flory approximation assuming the elastic free energy in the form  $F_{\text{el}} \propto (R/R_0)^x$  and choosing  $x = 2$  for short-range distributions of step sizes, the Flory formula for TSAW as

$$\nu_{\text{TSAW}}^L = \frac{d_f + d_s}{d_f(d_f + 2)} \quad (5)$$

Although the latter formula is simple in form without demanding knowledge of the spreading dimension of the underlying lattices, it has been found to describe the critical behaviour of TSAW just as well as the former.

All these works, however, were carried out on fractals of  $d_f < d_c$ , motivated by theoretical interest rather than understanding the corresponding physical phenomena. In this work, we study TSAW on random fractal lattices of  $d_f > d_c$ . One can readily think of such fractals as the infinite networks of percolation and DLA clusters embedded in the lattices of dimensions higher than 2. Since percolation clusters are known to describe the disordered media and TSAW corresponds to linear chain polymers in a polydispersed solution, at least one of these models may describe the relevant physics under certain circumstances.

On fractal lattices, Angles d'Auriac and Rammal [9] have redrawn the heuristic argument of Amit *et al* [1] and claimed that the self-avoidance of TSAW may increase the Flory exponent if

$$2 - d_s/2 - 2\nu_{\text{RW}} > 0 \quad (6)$$

holds. Since  $\nu_{\text{RW}} = d_s/2d_f$  [16] and  $d_s \simeq \frac{4}{3}$  [11] for percolation cluster, equation (6) reduces to  $d_f > 1$ , which is satisfied for all  $d > 1$ . Thus the TSAW on a percolation cluster is expected to show the critical behaviour different from that of RW for all  $d > 1$ . One can therefore raise the relevant question of what the value of  $\nu$  would be for TSAW on a percolation cluster in physical dimensions.

In order to address the answer to this question, we study by way of Monte Carlo simulations the TSAW on a 3D percolation cluster. To make our work more general, we also study TSAW on a 4D percolation cluster and on a 3D DLA cluster. We found that as the lattice dimension increases, the asymptotic behaviour of TSAW becomes unexpectedly slow, and accordingly, walks of a large number of steps should be generated to observe the correct asymptotic behaviour. We estimate the Flory exponent  $\nu$  from the Monte Carlo data for various values of  $g$ . Results are compared with the predictions by the known Flory formulae. We also study the fractal-to-Euclidean and the RW-to-TSAW cross-over scalings. The Monte Carlo data appear to collapse in the appropriate scaling regions for both cases; however, we found that the scaling function for the latter case is different from that on a regular lattice.

## 2. Monte Carlo methods

The Monte Carlo method of TSAW is well known. When the walk moves from site  $j$  to the neighbouring site  $i$ , the Boltzmann factor  $e^{-g^{\eta_i}}$  normalized by those of nearest-neighbour sites to  $j$  is taken as the probability  $P_{j \rightarrow i}$ . On a percolation cluster, the method is in principle similar to that on a regular lattice, except that the walk is restricted to a jump to the occupied neighbour sites. Thus, if the neighbouring site is empty, the probability of making a jump to it is assigned to be 0 and, otherwise, it is assigned according to equation (2).

Since the asymptotic behaviour of TSAW is slow on 3D and 4D percolation clusters as we mentioned earlier, we should construct clusters sufficiently large to avoid size effects. (We found that asymptotic behaviour can be observed for  $N$  over  $10^4$  steps.) If the underlying cluster is not sufficiently large, the walk would easily reach the boundaries and be reflected from them, causing finite-size effects which makes an accurate determination of the exponent  $\nu$  extremely difficult. However, obtaining such large clusters is not easy, particularly in high dimensions such as 3D and 4D. In order to reduce both the computing time and the size effects, we employ the periodic boundary condition. We generate a percolation cluster in a cell of  $L^d$  lattice sites. The largest cluster is then searched for and checked to see whether or not it spans along all coordinate directions and wraps around the lattice by a periodic boundary condition. If such a cluster is found, we assume it to be an infinite cluster, otherwise it is rejected and a new cluster is constructed.

Once we find an infinite cluster, we connect all isolated clusters near the edges which are members of the infinite cluster by periodic boundary conditions. We then select a starting point on an infinite cluster and generate a single  $N$ -step walk from the point. We repeat this procedure over many randomly selected starting points and the walk average is carried out over those walks on each cluster. The final disorder average is carried out over many different disorder configurations.

Our sampling technique defined here is different from that of the 'quenched average' defined for polymer chains on disordered media [17, 18]. The quenched average is often referred to as one-end fixed, i.e. the average should be carried out first over all walks from one starting point on each cluster and then over many different disorder configurations. However, we found that the difference is irrelevant for at least TSAW. We have carried out simulations on infinite clusters in 3D for selected values of  $g$ ,  $g = \infty, 0.5, 0.1, 0.05$

and 0.01, and for  $L = 64$ , using two different sampling methods. We found that the RMS end-to-end distances obtained were identical within statistical errors over all ranges of  $N$ . We believe this to be due to the correlations between two ends of chains being relatively weak and, after a large number of steps, the two ends are effectively uncorrelated, unlike the case of SAW.

When we generate the walks, we take full advantage of the wrapping condition employed for periodic boundaries. If the walk reaches one edge and exits the cell, we assume it to re-enter the cell through the opposite edge. This type of boundary condition requires additional attention in two respects. First, since the probability of each step depends on the history of the walk, one should keep the number of visits for each site. When the walk exits and re-enters the cell many times making loops, then keeping the number of visits would be very much more complex since it is difficult to work out whether the loops are true ones or artificial ones caused by the periodic boundary condition. Second, if the linear size of the walk is too large compared with the size of the cell,  $L$ , walks may pass through several replicated cells. In such a case, walks will eventually cross over to Euclidean lattices, thus, recovering the full lattice value of  $\nu$ .

Both of these problems, however, can be resolved if the size of the cell is sufficiently large so that the spanning distances of walks along each coordinate direction are always smaller than  $L$ . We have thus measured the spanning length of each walk along each coordinate direction and determined the number of steps  $N_{max}$  at which the spanning length exceeds  $L$  for the first time. Our data for  $N$  up to the smallest value of  $N_{max}$ 's are free of such problems as discussed. However, even for longer walks, since not all of them cause the problem, we did not discard the data beyond  $N_{max}$ . Our estimates of  $\nu$ , however, were obtained from the data up to  $N_{max}$  steps.

Another great advantage for the model of TSAW is that the walk averages seem to show relatively small fluctuations over different clusters, and thus, we have no need to generate a large number of different clusters. We found that the average over several clusters already yielded fairly consistent asymptotic behaviour. This behaviour is a characteristic of TSAW (and also of RW) and is different from that of SAW on a diluted lattice, where a large number of disordered configuration was essential to observe the correct asymptotic behaviour.

### 3. Results and discussions

We have carried out simulations for TSAW on an infinite cluster of percolation in both 3D and 4D and calculated the RMS end-to-end distances. The effective exponent  $\nu_N$  was calculated from the Monte Carlo data, and the Flory exponent  $\nu$  was obtained by extrapolating  $\nu_N$  in the limit of  $N \rightarrow \infty$ . The  $\nu_N$  can be defined in several different ways, similarly to the SAW on diluted lattices, among which the most effective and less fluctuative one is given as [19]

$$\nu_N = \frac{1}{2(N-M)} \left( N \ln R_N^2 - M \ln R_M^2 - \int_M^N \ln R_n^2 dn \right). \quad (7)$$

We have calculated the walk average over  $2.5 \times 10^4$  walks on a given disorder and the disorder average over 20 clusters. (We have added more clusters in the average for a selected value of  $g$ , but we found that 20 clusters are just enough to observe correct asymptotic behaviour for this particular problem.) We repeated calculations for various values of  $g$  to estimate the convergent exponent.

3.1. Flory exponent

Since an infinite cluster does not exist below  $p_c$ , the RMS distance of TSAW does not exceed the mean size of the cluster and thus saturates as

$$R_N \propto R_{\infty}(S) \quad \text{as } N \rightarrow \infty \tag{8}$$

where  $R_{\infty}(S)$  is the saturation value of  $R_N$  on a cluster of size  $S$  and diverges as  $R_{\infty} \sim (p_c - p)^{-\gamma \nu_{\text{perc}} / (d \nu_{\text{perc}} - \beta)}$  ( $\gamma$ ,  $\beta$  and  $\nu_{\text{perc}}$  being the exponents for mean cluster size, order parameter, and correlation length, respectively) as  $p \rightarrow p_c$ . The Flory exponent is thus trivial for  $p < p_c$  and therefore, we focus our study for  $p \geq p_c$ .

In 3D, we have generated percolation clusters on a simple cubic (SC) lattice of linear size  $L$ . We have chosen  $p = 0.312$  as  $p_c$ , where the best known value is  $p_c = 0.3117 \pm 0.0003$  [20] and carried out simulations for various values of  $g$ , ranging  $0 \leq g \leq \infty$ .

In order to see if there is any size effect, we have repeated simulations for various values of  $L$ ,  $L = 64, 80, 100, 120$ . The finite-size effect, if it exists, is expected to be more pronounced on the data for larger values of  $g$  since the walks for larger  $g$  probe wider regions of underlying fractal than the walks of smaller  $g$  can probe. The effective exponent  $\nu_N$  of TSAW for relatively large  $g$  is expected to be similar to that of SAW for small  $N$  and, as  $N$  increases, it should decrease towards the value of  $\nu$  for TSAW on a percolation cluster. However, since the finite-size effect yields TSAW to cross over to a Euclidean lattice behaviour, a sharp upturn in  $\nu_N$  is expected if the size effect exists. Such a behaviour was indeed observed in our data for  $L = 64$  and, as we increased the size of system, it became less appreciable, as expected. We found that  $L = 120$  is sufficient to eliminate any size effect on the data up to  $10^4$  steps. We thus present our data for  $L = 120$  in what follows.

Plotted in figure 1 is our Monte Carlo data, in comparison with those on a regular lattice. Two important consequences should be pointed out. First, data for  $g > 0$  yield the critical behaviour different from those of  $g = 0$ . This is clear from the figure, where the asymptotic slopes of the plots for  $g = 0.1$  and  $\infty$  are considerably larger than the

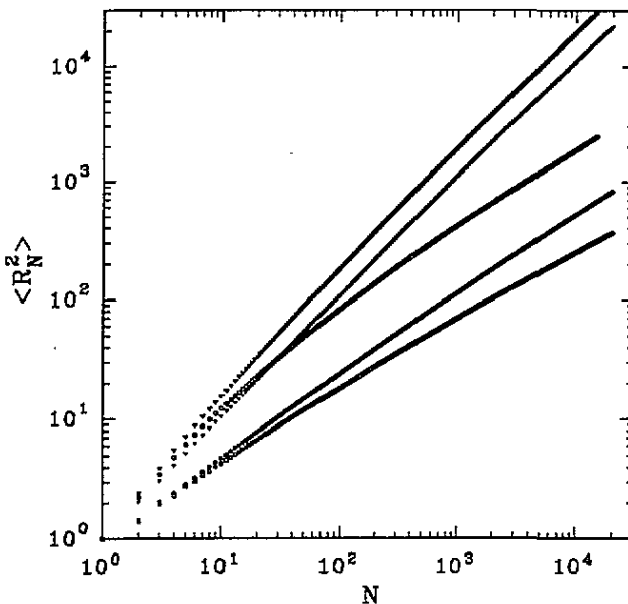


Figure 1. Double logarithmic plot of the mean square end-to-end distances of TSAW. Data are, from the top, for  $g = \infty, 0.1$  on a regular sc lattice and for  $g = \infty, 0.1$  and  $0$  on a percolation cluster at  $p_c$ .

corresponding data for  $g = 0$ , indicating that the self-avoidance enhances the RMS distances even on a percolation cluster. Second, the asymptotic slope for TSAW (for  $g > 0$ ) on a percolation cluster is smaller than that on a regular lattice. This implies that the Flory exponent  $\nu$  decreases considerably as the concentration of disordered sites becomes critical. Similar behaviour was also observed in the previous work in 2D [12] and is clearly different from that of SAW, where the Flory exponent was claimed to increase at  $p_c$  [21, 18].

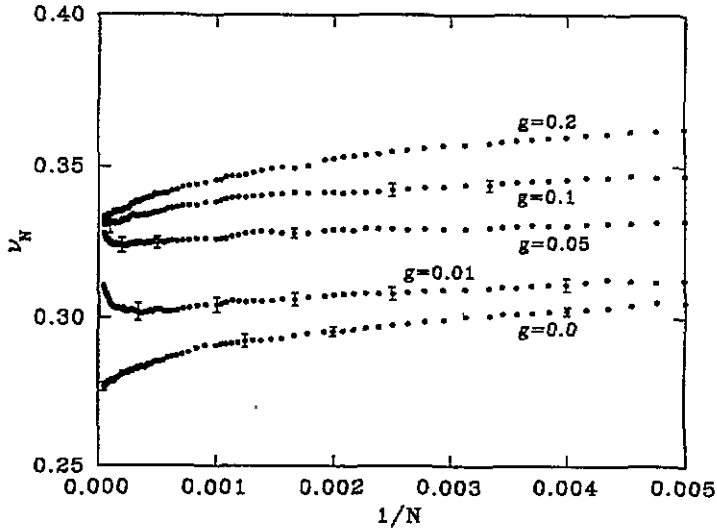


Figure 2. The effective exponent  $\nu_N$  as a function of  $N$  for TSAW on a 3D percolation cluster at  $p_c$ . The errors were estimated from the five batches of data, each of which was averaged over four disorder configurations.

The Flory exponent was estimated from the plot of  $\nu_N$  against  $N^{-1}$ . For TSAW on a regular lattice for various  $g$ 's,  $g = 0.005, 0.02, 0.1, 0.5$ , and  $\infty$ , data converge directly to the mean-field value of  $\frac{1}{2}$ , as expected from the usual critical phenomena above  $d_c$  (not shown). On a percolation cluster at  $p_c$ , data are plotted in figure 2. For  $g = 0$ , i.e. for RW (TSAW for  $g = 0$  corresponds to 'myopic ant' model [22] in the terminology of the 'ant in the labyrinth' [23])  $\nu_N$  is expected to converge onto the value  $\nu_{RW} = d_s/2d_f \approx 0.26$  ( $d_s \approx 1.33$  [24] and  $d_f \approx 2.52$  [25]) as  $N \rightarrow \infty$ ; however, as can be seen from the plot, our data appear to show slightly larger values up to 20 000 steps. This might be due to the fact that the RMS distance of RW on a critical percolation cluster exhibits unusually large correction terms, unlike the case in low dimensions. In order to confirm this, we assume the mean square end-to-end distance of the form

$$R_N^2 = AN^{2\nu}(1 + BN^{-\Delta} + CN^{-1} + \dots) \quad (9)$$

then, the effective exponent defined in equation (7) becomes

$$\nu_N = \nu + aN^{-\Delta} + bN^{-1} + \dots \quad (10)$$

From this, it is clear that if  $\Delta < 1$  a naive extrapolation versus  $N^{-1}$  gives wrong results. In order to estimate the exponent  $\nu$ , we have chosen  $\Delta$  as a parameter and plotted  $\nu_N$  versus  $N^{-\Delta}$ . The best linear fit was obtained for a  $\Delta$  of about 0.22, and, for this, the exponent  $\nu$  was estimated to be  $\nu \approx 0.26$ . Figure 3 shows the best fit of equation (10); the inset shows the linear fitting of  $\nu_N$  against  $N^{-\Delta}$ . (However, detailed knowledge for RW requires

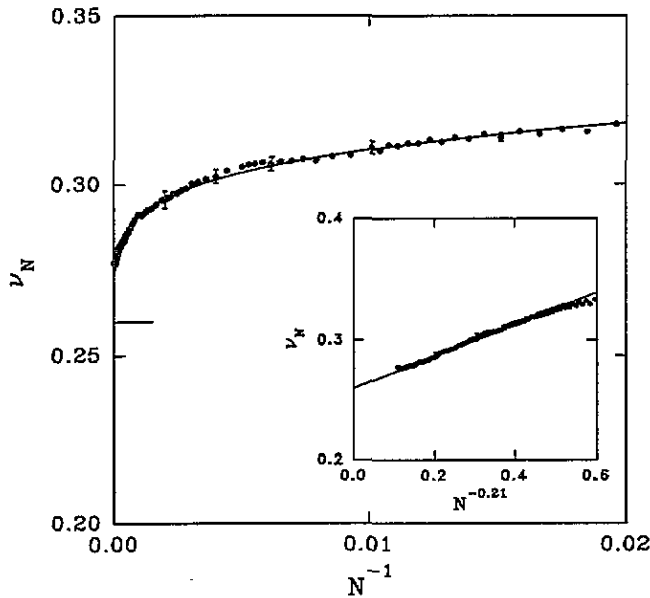


Figure 3. The correction-to-scaling fit of (10) for the effective exponent  $\nu_N$  of TSAW for  $g = 0$  (i.e. RW) against  $N^{-1}$ , using  $\Delta = 0.22$ ,  $a = 0.133$  and  $\nu = 0.26$ . The inset is the linear regression fitting of  $\nu_N$  versus  $N^{-\Delta}$ ;  $\Delta \approx 0.22$  shows the best result.

more careful analysis using both blind and myopic ant models, and we will leave this for a separate paper.)

For  $g > 0$ , all data for  $g = 0.05, 0.1$  and  $0.2$  appear to converge onto a single value on the ordinate and we obtain from the plot

$$\nu_{p_c}^{3D} = 0.330 \pm 0.005$$

which is within 4% of the predictions by the known Flory formulae. For  $g = 0.01$ , on the other hand, it is rather unclear that  $\nu_N$  would also converge to the same value on the ordinate. We, however, believe that it would do so according to the universality. Since for sufficiently small  $g$ , such as  $g \leq 0.01$ , TSAW behaves like RW for the first number of steps, the  $\nu_N$  is expected to be similar to that of RW for small  $N$ . (Note that we plotted data for  $N \geq 200$  in figure 2.) However, according to the universality, TSAW for all  $g > 0$  is expected to show the same asymptotic behaviour. The upturn in figure 2 appears to validate such a RW-to-TSAW cross-over, and the detailed cross-over behaviour shall be discussed in the subsequent subsection.

We have also carried out similar simulations in 4D. Although 4D is not a physical dimension, TSAW on an infinite percolation cluster at  $p_c$  is still an interesting problem.

Simulations were repeated for  $L = 30, 40$  and  $50$ , and we found that the data for  $L = 50$  are free of the size effect up to  $10^4$  steps. The asymptotic behaviour of TSAW on a 4D percolation cluster is basically similar to that in 3D. Shown in figure 4 are the effective exponents  $\nu_N$  for various values of  $g$  on a cluster generated at (or near)  $p_c$ . While the known value of  $p_c$  is about 0.197 [25], we have chosen  $p_c = 0.1988$  for all  $g$ 's except for  $g = 0.02$  where  $p_c = 0.1995$  was selected. Since an infinite cluster is known to exhibit a fractal nature in the region  $r < \xi$  ( $\sim |p - p_c|^{-\nu_{perc}}$ ), TSAW within this region is expected to show the same critical behaviour even though  $p$  is slightly away from  $p_c$ . This can be confirmed from our data in figure 4, where data for all  $g$ -values converge onto the same



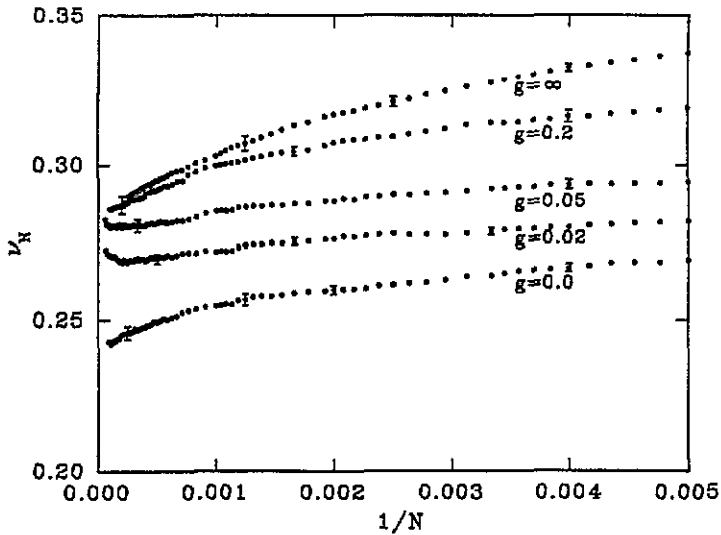


Figure 4. As of figure 2 for TSAW on a 4D percolation cluster at  $p_c$ .

value in the thermodynamic limit of  $N \rightarrow \infty$ .

For  $g = 0$ , the effective exponent again appears to show corrections, as in 3D. While the expected value of  $\nu_{RW}$  is about 0.22 from the scaling law  $\nu_{RW} = d_s/2d_f$  ( $d_s \simeq 1.33$  [24] and  $d_f \simeq 3.05$  [26]), our data up to 20 000 steps would yield about 0.24 if no corrections are assumed. However, the analysis of these data in a similar way to 3D yielded  $\Delta \simeq 0.19$  and  $\nu \simeq 0.22$ .

For  $g > 0$ , data for various  $g$ 's appear to converge onto the same value on the ordinate. Estimated from the plot is

$$\nu_{p_c}^{4D} = 0.283 \pm 0.005$$

which is considerably larger than the RW value, but smaller than the mean-field value on a regular lattice,  $\frac{1}{2}$ . Again, this is close to all the predictions by the Flory formulae but agrees better with equations (4) and (5).

So far we have discussed the TSAW on a percolation cluster in 3D and 4D. The estimates of  $\nu$  were found to be very close to the predictions of the known Flory formulae. With the work of TSAW on percolation clusters alone, however, it is not possible to work out whether such agreement is due to the excellency of the approximations made in deriving such formulae, or whether it is merely fortuitous and appropriate for TSAW only on a percolation cluster. In order to see if those formulae are good on other random fractals as well, we have studied TSAW on a 3D DLA cluster. The 3D DLA cluster has the fractal dimension close to that of 3D infinite percolation cluster but the geometrical structures are known to be very different. While percolation clusters possess many loops, DLA clusters instead have many branches. Since these branches grow as the clusters grow, it is rather difficult to generate TSAW on it if the clusters are not sufficiently large. In order to reduce the size effect we have chosen the diameters of DLA 150, 180 and 220 and generated TSAW from the seed sites. We found that if the number of steps is too large compared with the size of DLA, the effective exponent decreases sharply near the end of walks. This is due to the size effect being caused when TSAW reaches the growing boundary of DLA. We found, however, that if the number of steps are not very large, the  $\nu_N$  shows a convergent behaviour independent of the size of DLA and

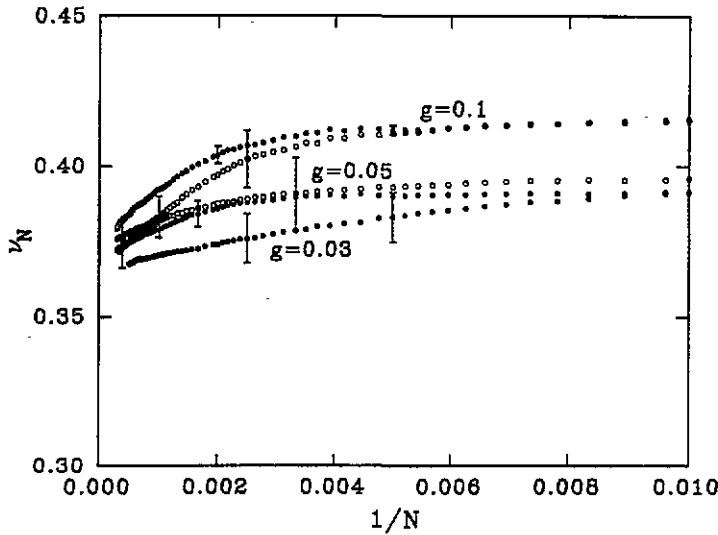


Figure 5. As of figure 2 for TSAW on a DLA cluster in 3D. The full symbols are for the RMS end-to-end distances and the open symbols for the radii of gyration.

Table 1. Summary of predictions from various Flory formulae for TSAW in comparison with the Monte Carlo estimates obtained in the present work.

	3D infinite cluster	4D infinite cluster	3D DLA cluster
$d_F$	2.51	3.05	2.50
$\hat{d}$	1.82 <sup>a</sup>	1.88 <sup>a</sup>	2.45 <sup>b</sup>
$d_s$	1.33	1.32	1.30 <sup>b</sup> ~ 1.35 <sup>c</sup>
Equation (3)	0.318	0.261	0.32
Equation (4)	0.336	0.278	0.35
Equation (5)	0.339	0.284	0.34
This work	$0.330 \pm 0.005$	$0.283 \pm 0.005$	$0.37 \pm 0.01$

<sup>a</sup> Reference [26].

<sup>b</sup> Reference [24] and references therein.

<sup>c</sup> Reference [27].

of the  $g$ -values for selected values of  $g$ , as shown in figure 5. Estimated from the figure is

$$\nu_{\text{TSAW}}^{\text{DLA}} = 0.37 \pm 0.01.$$

This value deviates slightly from the predictions of the Flory formulae,  $\nu_{\text{TSAW}}^{\text{BG}} \simeq 0.35$  and  $\nu_{\text{TSAW}}^L \simeq 0.34$  from equations (4) and (5), respectively, obtained using the known values of  $d_f$ ,  $d_s$  and  $\hat{d}$  [24], compared to the previous two cases, but is still close within the statistical errors. We thus conclude that the known Flory formulae appear to yield fairly good approximations on other random fractals, as well as on percolation clusters, for at least equations (4) and (5). We summarize our results in table 1, in comparison with the predictions by Flory formulae.

### 3.2. Crossover scaling of RMS distances

An infinite percolation cluster is known to exhibit a fractal nature in the region  $r < \xi$ , while for  $r > \xi$  it exhibits a Euclidean lattice structure. Thus one can expect that the asymptotic

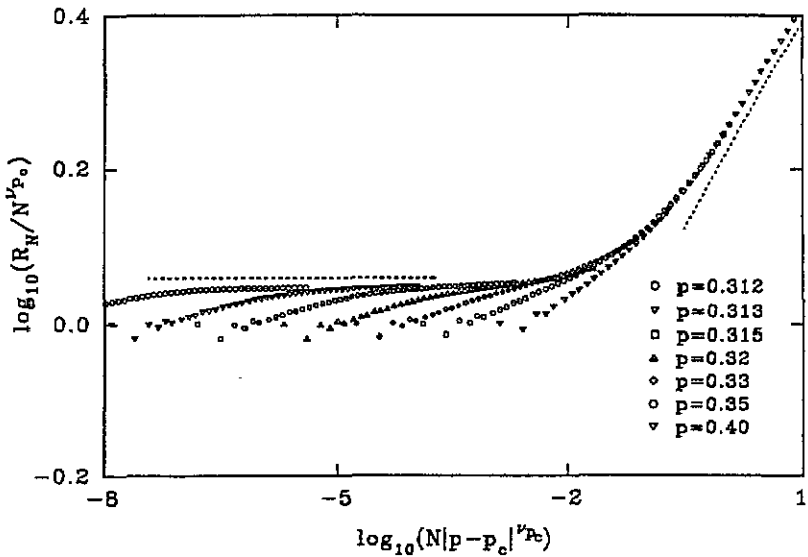


Figure 6. Fractal-to-Euclidean cross-over scaling function of RMS end-to-end distances for TSAW on a 3D percolation cluster. The dashed lines are for two asymptotic limits expected by theory.

behaviour of TSAW for  $R_N < \xi$  is different from that for  $R_N > \xi$ . Since the correlation length  $\xi$  diverges as  $p \rightarrow p_c$ , the TSAW must cross over from fractal behaviour to Euclidean behaviour as both  $N$  and  $p$  increase. This kind of cross-over is generally expected near  $p_c$  and has already been discussed for SAW on diluted lattices [28, 29].

From the usual scaling assumption, the cross-over scaling function can be written as

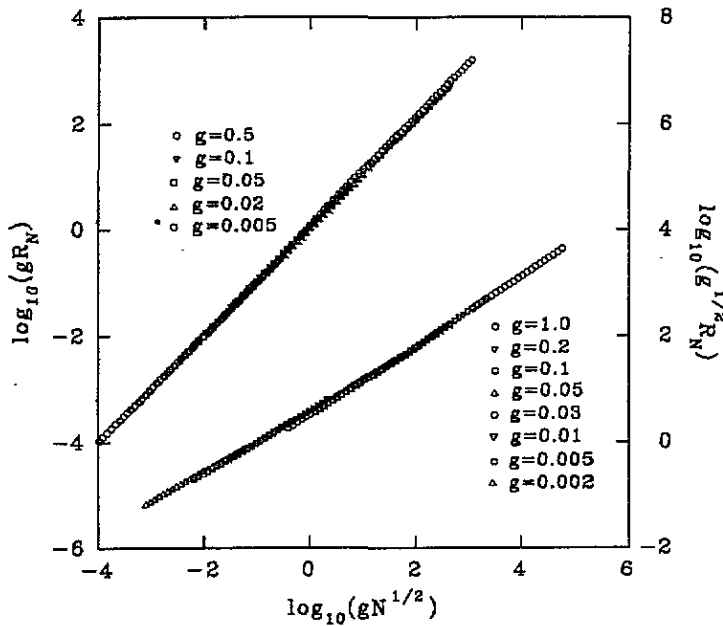
$$R_N = N^{\nu_{pc}} f(N|p - p_c|^{\nu_{perc}/\nu_{pc}}) \quad (11)$$

where  $\nu_{pc}$  is the Flory exponent of TSAW at  $p_c$ . In the two extreme limits of scaling variable  $x \equiv N|p - p_c|^{\nu_{perc}/\nu_{pc}}$ , the scaling function  $f(x)$  satisfies

$$f(x) = \begin{cases} \text{constant} & \text{as } x \rightarrow 0 \\ x^{\nu_1 - \nu_{pc}} & \text{as } x \rightarrow \infty. \end{cases} \quad (12)$$

Assuming that TSAW crosses over from fractal to Euclidean lattices,  $\nu_1$  can be considered as the regular lattice value. However, if TSAW crosses over from  $p_c$  to a new critical behaviour controlled by a new fixed point at  $p^*$  between  $p_c$  and 1, as suggested for SAW on diluted lattices [18],  $\nu_1$  would be the exponent at  $p^*$ .

We have studied scaling analyses for both 3D and 4D. However, since the scaling argument is similar in both cases, we will present 3D results only. We fixed  $g = 0.1$  and generated walks for various values of  $p$  near  $p_c$ ,  $0.312 \leq p \leq 0.40$ . Shown in figure 6 is the scaling function obtained using  $\nu_{perc} \simeq 0.9$  [25] and  $\nu_{pc} = 0.328$ . For small  $N$  for each  $p$ -value data do not collapse. This is because the walk does not reach the asymptotic region if  $N$  is relatively small. (As the convergence behaviour of TSAW is relatively slow as we mentioned before, our data indicated that  $N$  should be over  $10^3$  steps.) However, as is clear from the figure, data for sufficiently large  $N$  for each  $p$  appear to converge onto a single curve. Although the overlapping of the data for different  $p$ 's was not observable for small  $x$ , one can reasonably expect from the plot that they would overlap if the longer walks are obtained. This suggests that data would indeed scale in the asymptotic limit of  $N \rightarrow \infty$ .



**Figure 7.** RW-to-TSAW cross-over scaling function of TSAW on a SC lattice (above) and on a percolation cluster at  $p_c$  (below). The left ordinate is for the data on a SC lattice and the right ordinate for the data on a infinite percolation cluster at  $p_c$ .

Data for both  $x \ll 1$  and  $x \gg 1$  show correct limits. For  $x \ll 1$  and  $N \gg 1$ , the plot is flat as expected in equation (12), indicating our value of  $\nu_{p_c} \simeq 0.33$  to be correct. For  $x \gg 1$ , the slope of the plot is about 0.17, which is close to the expected value of  $\nu_1 - \nu_{p_c}$  if  $\nu_1 = \frac{1}{2}$ . This indicates that TSAW crosses over from fractal at  $p_c$  directly to the full lattice behaviour as  $x$  increases, unlike the case of SAW where the cross-over is expected from  $p_c$  to  $p^*$  between  $p_c$  and 1 (but this is still inconclusive, as far as we are aware). From this, we conclude that no fixed point between  $p_c$  and 1 exists for TSAW and, therefore, the critical behaviour of TSAW on a percolation cluster is clearly different from that of SAW.

The cross-over scaling can also be considered as the parameter  $g$  varies. When  $g \ll 1$ , since the walk can visit the same lattice site many times, the TSAW behaves like RW if  $N$  is not large enough. However, as  $N$  increases, all walks for any  $g > 0$  are expected eventually to cross over to TSAW. Therefore, one can expect the RW-to-TSAW cross-over as both  $N$  and  $g$  increase.

Such a cross-over was previously discussed in one dimension and the scaling function was suggested as [5]

$$gR_N = \phi(z)z^{2\nu} \tag{13}$$

with the scaling variable  $z = gN^{1/2}$  and  $\phi(z)$  being of the form

$$\phi(z) = 1 + a_1z + a_2z^2 + \dots \tag{14}$$

We have studied similar scaling in 3D. In figure 7 we show plots of scaling functions for TSAW on an SC lattice (above) and on a percolation cluster at  $p_c$  (below). For TSAW on an SC lattice, data for the scaling function in equation (13) for various values of  $g$ , plotted against  $z$  on a double logarithmic scale, collapse onto a single straight line of slope 1. This implies that the scaling relation for higher dimensions is also similar to that in one

dimension, although the scaling function might be different. The straightness of the plot is obvious since the critical behaviour of TSAW is identical to that of RW on a regular lattice, as expected above  $d_c$ , and thus no cross-over region between TSAW and RW exists. On the other hand, for TSAW on a percolation cluster, the result is different. We found that the scaling function in equation (13) is no longer valid for TSAW on a percolation cluster. The lower plot in figure 7 is the data for  $g^{1/2}R_N$  against  $z$ , as specified on the right ordinate (not as in equation (13)). For all  $g$ 's, data for the first 500 steps were discarded in the plot because we believe that they were not in the asymptotic scaling region. The Monte Carlo data show fairly good data collapsing for all  $g$ 's.

The scaling function plotted was found merely by numerical investigation and was not predicted before. The origin of such variation in scaling function might be due to the fact that the self-avoidance constraint affects the RMS distances much more for TSAW on a percolation cluster than on a regular lattice. This can be supported from the plot in figure 1, where the difference between the data for  $g = 0.1$  and  $g = \infty$  are more pronounced on a percolation cluster than on a regular lattice. (Note that multiplying  $g^{1/2}$  (instead of  $g$ ) on  $R_N$  for each case reduces this difference).

The RW-to-TSAW cross-over is evident from the plot. The slope for  $z \gg 1$  is about 0.66 which is twice our estimate  $\nu_{pc}$ , as expected. On the other hand, the slope for  $z \ll 1$  is about 0.55, which is slightly larger than the expected value  $2\nu_{RW} \simeq 0.52$ . We believe this is a reflection of the fact that the convergence behaviour of RW on 3D and 4D percolation clusters are relatively slow and the RMS distance might have strong non-analytic correction terms, as we discussed earlier. This could be supported since half of the slope is just the value we could obtain by a simple eyeball extrapolation of  $\nu_N$  for  $g = 0$  in figure 2.

We have also studied the same scaling analysis in 4D and found that results are qualitatively similar to those in 3D. In both dimensions, data exhibited clear RW-to-TSAW cross-over as  $z$  increases.

#### 4. Summary

We studied by way of Monte Carlo simulations the critical behaviour of TSAW on fractal lattices of fractal dimension larger than the upper marginal dimension of TSAW. We estimated the Flory exponent for TSAW on infinite percolation clusters in 3D and 4D and on a DLA cluster in 3D. We found, as results, that the upper marginal dimension  $d_c = 2$  of TSAW does not have any specific role on fractal lattices, and the Flory exponent was found to be generally smaller than that on a regular lattice. In addition, all of our estimates of  $\nu$  were in good agreement with the predictions by Bouchaud and Georges and by one of the present authors. In particular, that of the latter, although simple in its form, appears to be just as good as the former, and it can describe fairly well the critical behaviour of TSAW on any fractal lattices.

We have also studied the cross-over scaling of TSAW. We found that the fractal-to-Euclidean cross-over scaling does indeed hold for our estimate of  $\nu_{pc}$  in the appropriate scaling region: however, we found that the scaling region is rather narrow, in the sense that data for relatively small  $N$  ( $N \leq 10^3$ ) deviated from the asymptotic curve.

We have also studied the RW-to-TSAW cross-over scaling for TSAW both on an ordinary SC lattice and on a critical percolation cluster. For both cases, data exhibited fairly good collapsing with valid limiting slopes in the two extreme limits. On a percolation cluster, RW-to-TSAW cross-over scaling was evident, but the scaling relation appears to be modified in an appropriate way.

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## References

- [1] Amit D J, Parisi G and Peliti L 1983 *Phys. Rev. B* **27** 1635
- [2] de Gennes P G 1979 *Scaling Concepts in Polymer Physics* (Ithaca, NY: Cornell University Press)
- [3] Pietronero L 1983 *Phys. Rev. B* **27** 5887
- [4] Family F and Daoud M 1984 *Phys. Rev. B* **29** 1506
- [5] Rammal R, Angles d'Auriac J C and Benoit A 1984 *J. Phys. A: Math. Gen.* **17** L9
- [6] Bernasconi J and Pietronero L 1984 *Phys. Rev. B* **29** 5196
- [7] For 1D see, e.g., [5] and for fractal lattices, we have confirmed by direct simulations (unpublished)
- [8] For a review, see, e.g. Vicsek T 1989 *Fractal Growth Phenomena* (Singapore: World Scientific)
- [9] Angles d'Auriac J C and Rammal R 1984 *J. Phys. A: Math. Gen.* **17** L15
- [10] Rammal R 1984 *J. Stat. Phys.* **36** 547
- [11] Alexander S and Orbach R 1982 *J. Physique Lett.* **43** L625
- [12] Lee S B and Lee M J 1990 *J. Phys. A: Math. Gen.* **23** 3263
- [13] Lee S B 1992 *Phys. Rev. A* **45** 7098
- [14] Bouchaud J P and Georges A 1989 *Phys. Rev. B* **39** 2846
- [15] Vanimenus J, Nadal J P and Martin H 1984 *J. Phys. A: Math. Gen.* **17** L351
- [16] For some loopless fractals such as Eden trees or DLA this scaling relation is found to breakdown; see, e.g. Dhar D 1985 *Phys. Rev. Lett.* **54** 1346, and also see [27]
- [17] Obukhov S P 1990 *Phys. Rev. A* **42** 2015
- [18] Le Doussal P and Machta J 1991 *J. Stat. Phys.* **64** 541
- [19] Lam P M 1990 *J. Phys. A: Math. Gen.* **23** L831
- [20] Heermann D W and Stauffer D 1981 *Z. Phys. B* **44** 339
- [21] Meir Y and Harris A B 1989 *Phys. Rev. Lett.* **63** 2819
- [22] Majid I, Ben-Avraham D, Havlin S and Stanley H E 1984 *Phys. Rev. B* **84** 1626
- [23] de Gennes P G 1976 *La Recherche* **7** 919
- [24] Havlin S and Ben-Avraham D 1987 *Adv. Phys.* **36** 695
- [25] Stauffer D and Aharony A 1992 *Introduction to Percolation Theory* (London: Taylor and Francis)
- [26] Grassberger P 1986 *J. Phys. A: Math. Gen.* **19** 1681
- [27] Jacobs D J, Mukherjee S and Nakanishi H 1994 *J. Phys. A: Math. Gen.* **27** 4341
- [28] Kremer K 1981 *Z. Phys. B* **45** 149
- [29] Lee S B and Song Y J 1992 *AIP Conf. Proc.* **256** 529