Violation of the des Cloizeaux relation for self-avoiding walks on Sierpinski square lattices

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The statistics of self-avoiding walks (SAWs) on deterministic fractal structures with infinite ramification, modeled by Sierpinski square lattices, is revisited in two and three dimensions using the reptation algorithm. The probability distribution function of the end-to-end distance of SAWs, consisting of up to 400 steps, is obtained and its scaling behavior at small distances is studied. The resulting scaling exponents are confronted with previous calculations for much shorter linear chains (20 to 30 steps) based on the exact enumeration (EE) technique. The present results coincide with the EE values in two dimensions, but differ slightly in three dimensions. A possible explanation for this discrepancy is discussed. Despite this, the violation of the so-called des Cloizeaux relation, a renormalization result that holds on regular lattices and on deterministic fractal structures with finite ramification, is confirmed numerically.

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I. INTRODUCTION

Self-avoiding random walks (SAWs) constrained to occupy the sites of a fractal structure, the latter defined either in two or in three spatial dimensions, constitute interesting models of linear polymers embedded on irregular surfaces or in porous media displaying spatial scale invariance (see, e.g., Ref. [1,2]). Many theoretically challenging issues remain to be understood, among which we draw our attention here to the shape of the probability distribution function (PDF) of the end-to-end distance.

Fractal structures are classified into two categories, i.e., deterministic and random fractal substrates. Examples of the former are the Sierpinski fractals [3], which are further subdivided into structures with finite or infinite ramification [3,4]. A typical example within the category of random fractals is the incipient percolation cluster at criticality [5,6].

In this work, we reconsider the case of a deterministic fractal with infinite ramification [3,4], in both two and three spatial dimensions. The structures we study are represented by the Sierpinski square lattices (sometimes called Sierpinski carpets in $d=2$ and Sierpinski sponges in $d=3$), to be defined below. Our interest in such a type of scale invariant substrate is motivated by earlier studies of SAWs on these structures [7–9], and in particular by our previous study on the corresponding PDF of the end-to-end distance [10]. In that work, we estimated the scaling form of the PDF by using the exact enumeration (EE) technique, which permits to evaluate all SAW configurations on Sierpinski square lattices up to a (relatively small) maximum number N of SAW steps ($N=30$ in $d=2$ and $N=20$ in $d=3$), limited by the available computer resources. We found that the so-called des Cloizeaux relation [11] does not hold for this type of deterministic fractal, in contrast to the behavior on deterministic fractals with finite ramification. The question, however, remains open whether such small N values, that suggest the breakdown of the des Cloizeaux relation, are sufficient to elucidate the truly asymptotic behavior of the PDF expected for $N \gg 1$.

In order to get further numerical evidence from which one can better judge this intriguing scenario, we present additional results based on the use of the reptation algorithm [12,13]. The latter, although not being exact, allows us to study much longer chains than with the EE method, here up to $N \cong 400$ limited by the size of the fractal lattice that can be generated. It should be emphasized that there exist other, relatively more involved, accurate algorithms for studying very long SAW chains, as for instance the method by Berretti and Sokal [14] or the pruned-riched-Rosenbluth method by Grassberger [15]. Although these methods can in principle be implemented to our present problem, we consider here the much simpler (constant chain length) reptation approach. To better assess the validity of our results, we apply first the method to the case of regular square lattices in both two and three dimensions, for which the corresponding scaling exponents are well known. From this test we will conclude that reptation yields accurate results in the case of uniform systems, indicating among other things that possible nonergodic configurations are not important for the present problem. Based on these results, we expect that reptation can also perform well on infinitely ramified fractals, in the sense that the truly asymptotic behavior of SAWs can be detected with sufficient accuracy for our present purposes. To give further support to our numerical results, specially in three dimensions, we combine reptation with Pivot moves, finding that

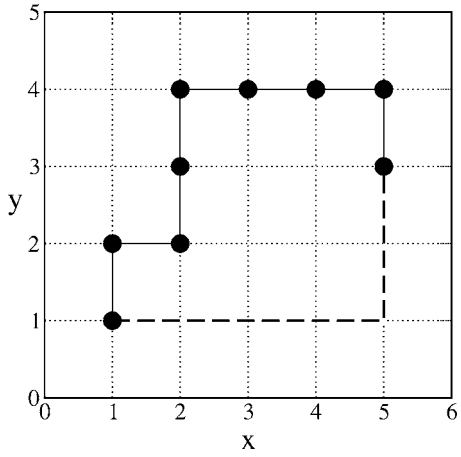

FIG. 1. The l metric on the square lattice. In this example, we show a SAW of $N=8$ steps (thin straight lines connecting nearest-neighbor circles), corresponding to $N+1=9$ monomers (full circles). The l distance between the end monomers at (1, 1) and at (5, 3) is $l=|1-5|+|1-3|=6$, corresponding to the length of the dashed line (in units of the lattice constant).

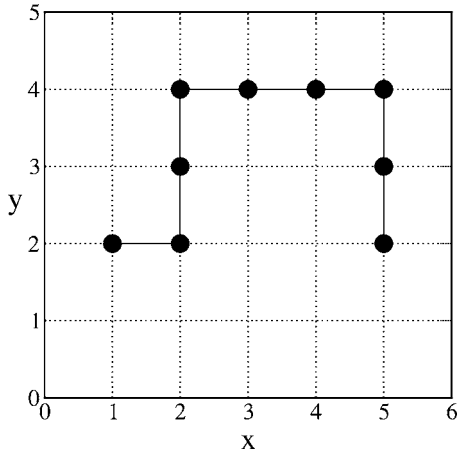

FIG. 2. Illustration of the reptation method. The end monomer at position (5, 3) shown in Fig. 1 has moved to its new location at (5, 2), carrying the whole chain with it along its track.

the corresponding critical exponents of interest remain unchanged.

The paper is organized as follows. In Sec. II, we summarize the quantities of interest and their scaling functions we are considering, and discuss the rules of the reptation algorithm employed. The method is tested for the case of SAWs on regular lattices both in two and three dimensions. The fractal lattices are discussed in Sec. III, for the two and three dimensional cases. The conclusions are summarized in Sec. IV.

II. SAWS ON REGULAR LATTICES

To characterize the spatial extent of SAWs on a given structure, such as the square lattice, we consider the topological end-to-end distance l after N steps of the walk. In particular, for square and simple cubic lattices, the l distance between two points located at coordinates $\{x_1,y_1,z_1\}$ and $\{x_2,y_2,z_2\}$ is defined as

$$l = |x_1 - x_2| + |y_1 - y_2| + |z_1 - z_2|. \tag{1}$$

An illustrative example in $d=2$ is shown in Fig. 1. The present l metric is equivalent to the more standard Euclidean or r metric [i.e., $r=\sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2}$], but has the advantage that fluctuations are minimal permitting a more accurate determination of the configurational exponents defined below.

The end-to-end distance $l(N)$ averaged over all SAW configurations of N steps, denoted as $\bar{l}(N)$, obeys the scaling relation [16]

$$\bar{l}(N) \sim N^{\nu} \quad \text{for } N \gg 1, \tag{2}$$

which defines the critical exponent ν. The latter depends on the dimensionality d of the lattice. The probability distribution function for the end-to-end distance $P(l|N)$, normalized according to $\int P(l|N)dl=1$, obeys also a scaling form given by

$$P(l|N) = \frac{1}{l} F_d\left(\frac{l}{\bar{l}(N)}\right), \tag{3}$$

where $F_d(x)$ is the scaling function. Here, we are interested in the asymptotic behavior of F_d at small x values, which is expected to be given by

$$F_d(x) \sim x^{g+d} \quad \text{for } x \ll 1. \tag{4}$$

The exponent g is expected to obey the so-called des Cloizeaux relation [11]

$$g = \frac{\gamma - 1}{\nu}, \tag{5}$$

where γ is the enhancement exponent. Note, that the exponent g in Eq. (4) has been denoted as g_1 in Ref. [10]. In two dimensions, $\nu=3/4$, $\gamma=43/32$, and $g=11/24$, while in $d=3$ one has $\nu=0.58758$, $\gamma=1.1575$, and $g=0.268$ [2].

A. Reptation algorithm

The reptation algorithm used here consists of two steps: (a) picking up at random one of the two ends of the chain, say the monomer at position (5, 3) in Fig. 1 and (b) choosing one of its nearest-neighbor lattice sites at random as its possible new location. If the nearest-neighbor site is empty [e.g., the one at (5, 2) in the figure] the reptation is performed, and the whole chain is moved along its track, as illustrated in Fig. 2. Otherwise, if the nearest-neighbor site is occupied, the chain remains at its actual position, and the process is repeated from step (a) all over again. In the special case where the occupied nearest-neighbor site corresponds to the other end of the chain, the reptation move is accepted since the occupied lattice site becomes free once the chain moves as a whole.

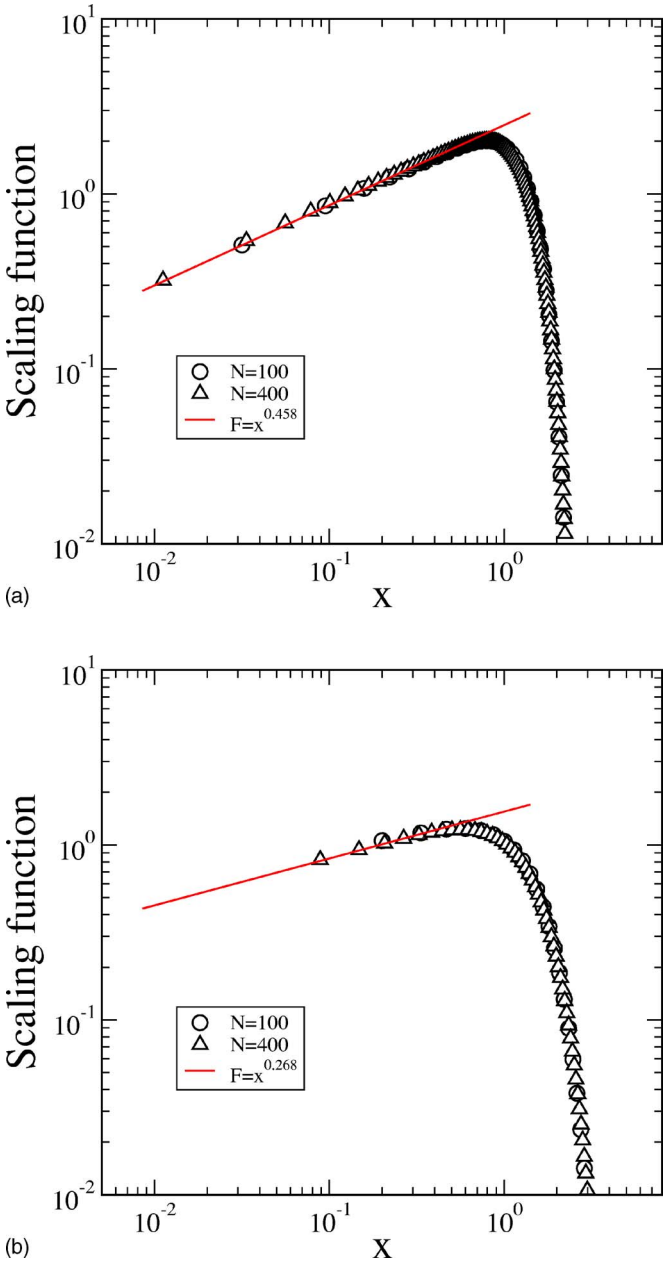

FIG. 3. (Color online) The scaling function $F_d(x)/x^d$ vs x, for the PDF of the end-to-end distance of SAWs: (a) in $d=2$ on the square lattice and (b) in $d=3$ on the simple cubic lattice, for $N=100$ (circles) and 400 (triangles). The straight lines have the expected slopes, Eq. (5), $g=11/24\approx 0.458$ in $d=2$ and $g=0.268$ in $d=3$.

B. Numerical results in two and three dimensions

The lattice sizes L employed were $L=2000$ in $d=2$ (square lattice) and $L=500$ in $d=3$ (simple cubic lattice). The initial SAW configuration was taken as a straight line. In $d=3$, it has an U-shape for the largest N values considered (i.e. $N=400$). A sufficient number of preliminary reptation steps are performed to achieve a completely random SAW configuration. The evaluation of the end-to-end distance PDF is started when the actual chain configuration has left all the lattice sites it occupied at the initial configuration, has attained a random shape, and hence has lost memory of the initial configuration. Typically, the number of reptation steps performed is of the order of 10^7 to 10^8, and the whole process is stopped when the behavior of the PDF has reached a stationary shape (typically after 10^2 independent runs). All resulting chain configurations are taken into account when performing the statistical average of the PDF, including those for which no move of the chain has taken place (see, for instance, Ref. [13]). Since the SAW chain also diffuses on the lattice, there is the problem that it touches the lattice borders. To avoid such finite size effects, we apply periodic boundary conditions.

The numerical results for the scaling function $F_d(x)/x^d$ as a function of x are displayed in Fig. 3(a) for $d=2$ and in Fig. 3(b) for $d=3$. The straight lines display the expected values of the scaling exponents g. The good agreement of the numerical results with the latter gives us confidence that the present approach can be applied also to fractal structures for which exact values of the exponents are not known.

It should be noted that Pivot (or Verdier) algorithms, extensively used on regular lattices, cannot be efficiently applied on their fractal counterparts since in such diluted lattices many moves are rejected as they violate the geometrical constraints and the chain gets easily stuck, making the conformational sampling virtually impossible. On the contrary, in the case of reptation bottlenecks can be easily overcome and the chain can "diffuse" on the lattice, thus exploring essentially all accessible conformations. This has to be contrasted with the problem of ergodicity known for regular lattices, where certain chain conformations are impossible to occur with a reptation scheme [17]. However, the results shown in Fig. 3 seem to indicate that the undersampling of such chain conformations is not playing an important role in determining the exponent g. We have performed also simulations combining reptation with Pivot moves (tail and corner flips and crankshaft moves), the latter allow the chain to reach some configurations which can not be obtained with reptation alone, thus mitigating to some extent the lack of ergodicity of the method. The results however do not differ from those shown in Fig. 3.

In the case of diluted lattices, we expect such non-ergodic chain conformations to play an even less important role than on regular lattices, being the scale invariant dilution of the lattice on large length scales the dominant effect that determines the asymptotic shape of SAWs at vanishing end-to-end distances.

III. SAWS ON SIERPINSKI SQUARE LATTICES

The Sierpinski square lattices considered in this work are illustrated in Fig. 4 in two and three dimensions, at their second generations (we use the translationally invariant structure with the smallest lacunarity [10]). These deterministic fractals are said to be infinitely ramified, since one needs to remove an infinite number of sites (asymptotically) to isolate any given subset of the structure [3,4].

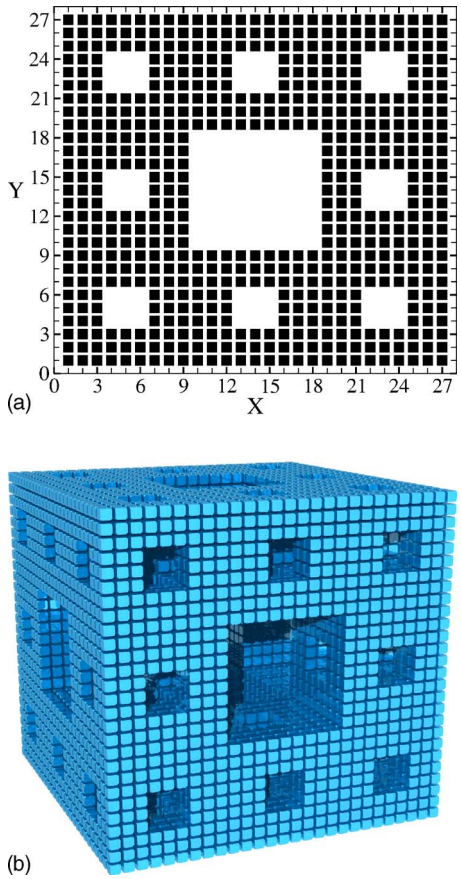

FIG. 4. (Color online) The Sierpinski lattice in (a) two and (b) three dimensions at their second generation. The lattice size is then $L=3\times3^2=27$ in both cases. The SAWs can occupy only those points of the fractal depicted by the full squares and by the full cubes, respectively.

In this work, we have considered lattices of sizes $L=3\times3^6=2187$ (i.e., the sixth fractal generation) in $d=2$ and $L=3\times3^5=729$ (i.e., the fifth fractal generation) in $d=3$. The initial SAW configurations were taken as straight lines, located around the central hole of the fractal lattice, having an U shape for large N. Here, we considered N up to about 400. Preliminary reptation steps are performed as discussed for regular lattices, such that the SAW chain gets completely out of its starting track, has attained a random shape, and hence has lost memory of the initial configuration. Since the SAW chain diffuses on the Sierpinski lattice, there is the problem that it might touch the lattice borders. If the SAW touches any of the sites located at the external border of the fractal, the run is stopped. Even though the chain explores large areas of the Sierpinski lattice, this happened only a very small number of cases. In such an event, only the chain configurations before touching the boundary enter the averaged PDF, so that the PDF is not expected to be altered. The number of reptation steps performed is of the order of 10^7 to 10^8, and the whole process finished when the end-to-end PDF takes a stationary shape (typically after 10^2 to 10^3 independent runs).

For these fractal structures, the scaling function $F_d^S(x)$ obeys, for small x, the relation

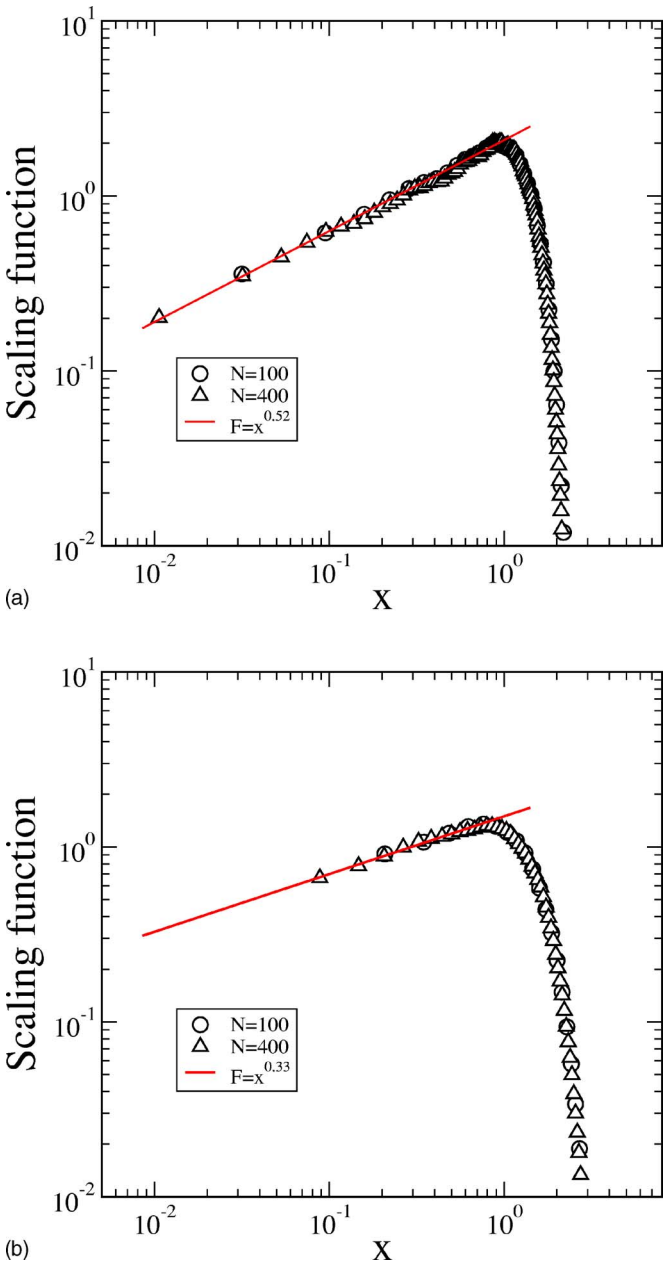

FIG. 5. (Color online) The scaling function $F_d(x)/x^{d_f}$ vs x, for the PDF of the end-to-end distance of SAWs on the Sierpinski lattice: (a) in $d=2$ and (b) $d=3$, for $N=100$ (circles), and 400 (triangles). The straight lines have the slopes $g_S^{\mathrm{rep}}=0.52\pm0.05$ in $d=2$ and $g_S^{\mathrm{rep}}=0.33\pm0.05$ in $d=3$.

$$F_d^S(x) \sim x^{g_S+d_f} \quad \text{for } x \ll 1, \tag{6}$$

where d_f is the fractal dimension of the underlying structure. In $d=2$, one has $d_f=\ln 8/\ln 3\cong1.893$, while in $d=3$, $d_f=\ln 20/\ln 3\cong2.727$. The corresponding SAW scaling exponents (denoted with the subindex S) take the approximate values $\nu_S=0.75\pm0.05$, $\gamma_S=1.23\pm0.04$, and $g_S\approx g_S^{\mathrm{EE}}=0.54\pm0.03$ (EE results [10]) in $d=2$, and $\nu_S=0.58\pm0.03$, $\gamma_S=1.36\pm0.03$, and $g_S\approx g_S^{\mathrm{EE}}=0.16\pm0.05$ (EE results [10]) in $d=3$.

The present numerical results are displayed in Fig. 5(a)

for $d=2$ and in Fig. 5(b) for $d=3$. The data collapse is good in both cases, and values for the exponents g_S can be extracted from the slopes of the straight lines depicted in the plots. In $d=2$, we get $g_S^{\mathrm{rep}}=0.52\pm0.05$, confirming the EE result [10], $g_S^{\mathrm{EE}}=0.54\pm0.03$, in two dimensions. We note that the value $g_S^{\mathrm{EE}}=0.54\pm0.03$ is not consistent with the des Cloizeaux relation (5) which predicts $g_S^C=(\gamma_S-1)/\nu_S=(0.23\pm0.04)/(0.75\pm0.05)=0.31\pm0.07$.

In $d=3$, we get $g_S^{\mathrm{rep}}=0.33\pm0.05$, to be compared with the EE value [10] $g_S^{\mathrm{EE}}=0.16\pm0.05$. It should be noted that g_S^{rep}, although larger than g_S^{EE}, is still inconsistent with the des Cloizeaux relation (5), which predicts $g_S^C=(\gamma_S-1)/\nu_S=(0.38\pm0.03)/(0.58\pm0.03)=0.62\pm0.09$. Further numerical support to the present data has been obtained by mixing reptation with Pivot moves, as explained above for regular lattices. Again, no difference between the results obtained with the two methods has been detected. We hence argue that our 3D results should be free of problems related to ergodicity and accurate enough to draw conclusions about the violation of the renormalization rule considered here.

Actually, the discrepancy between the two numerical values g_S^{rep} and g_S^{EE}, can be attributed to the different chain lengths considered in each calculation. In fact, the present results are consistent with those of the EE method for intermediate values of x, corresponding to shorter chain lengths. Thus, in three dimensions the asymptotic behavior seems to be reached for larger chains lengths as compared to the two dimensional case.

IV. CONCLUSIONS

We have studied the statistics of SAWs on deterministic fractal structures with infinite ramification modeled by Sierpinski square lattices. The different SAW configurations have been generated using the reptation algorithm. The motivation of the present study was to elucidate whether violations of the known des Cloizeaux relation, obtained previously for these systems using exact enumeration techniques for rather short chains, can be considered at least qualitatively correct. Our present results, based on extensive reptation simulations (complemented by combining reptation with Pivot moves) on much longer SAW chains turn out to be in support of the EE conclusions. Only in three dimensions our new value for the exponent $g_S^{\mathrm{rep}}=0.33\pm0.05$, describing the asymptotic shape of the end-to-end PDF at small distances, turns out to be a bit larger than its EE counterpart $g_S^{\mathrm{EE}}=0.16\pm0.05$ but both are inconsistent with the des Cloizeaux prediction $g_S^C=0.62\pm0.09$. We think that the EE results in 3D lack of sufficient chain length, being the truly asymptotic regime attainable for much longer SAW chains. We find that our reptation results are consistent with the EE ones for shorter chains. The problem remains open regarding the actual value of g_S in three dimensions. We can conclude, however, that whatever this value would be, it is likely that it will be bounded by the EE value from below and by the present reptation value from above, thus permitting to argue that the des Cloizeaux relation is indeed violated on infinitely ramified fractal lattices.

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