Information dimension in fractal structures

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We derive an exact formula for the recently introduced information dimension D_I for random-walk processes in terms of the $V(r,n)$ function, the function that gives the number of sites that have exactly r visits during a random walk on a lattice after n steps. This form is general, and it pertains both to regular lattices and fractal structures. The controlling parameter is S_n, the number of sites visited at least once in an n-step walk. We perform computer simulations on regular lattices and on fractal structures: the Sierpinski gasket, two-dimensional, and three-dimensional percolation clusters exactly at criticality. It is found that D_I has the same numerical value as the spectral dimension as $n \to \infty$, but it takes unusually long times to reach such behavior.

I. INTRODUCTION

Recently[1] we introduced the concept of the information dimension D_I for transport processes on lattices. Since random-walk models have been proved to be very useful in such studies we applied this new idea to random walks and showed that it provides an alternate picture to the set of critical exponents presented during the last five or so years. For a recent review on the multitude of reported exponents and their numerical values see Ref. 2. As its definition implies D_I provides complete information on the history of the transport mechanism, i.e., it not only gives the range of transport but also the frequency of visitation in space as a function of time. Thus D_I is expressed in terms of occupation probabilities of a particle performing a random walk on a specific lattice. It is

$$D_I = I_n / \ln n \ , \tag{1}$$

where

$$I_n = -\sum_{k=1}^{S_n} P_k \ln P_k \ . \tag{2}$$

Here n is the number of discrete steps (i.e., time), P_k is the probability of the particle visiting the kth site on the lattice, and S_n is the number of distinct sites visited at least once in the walk. P_k is given by $P_k = i_k / n$, and i_k is the number of times that site k has been visited. The sum is carried over all sampled sites in the lattice that have at least one visit, i.e., if $i_k = 0$ there is no contributing term. The above should be considered as a general definition provided that $n \to \infty$, in the spirit of all other related exponents.[2] Subsequently[3] we solved exactly the problem of multiple visits on lattices, i.e., we provided analytic solutions for the mean number of sites visited at least a certain number of times (r), $S(r,n)$, and the mean number of sites visited exactly a certain number of times (r), $V(r,n)$. The S and V functions are directly used to calculate the D_I exponent.

The S and V forms (that were originally developed[3] for perfect lattices) are functions of S_n, n, and r only. Their success is due to the fact that we now have very accurate expressions for S_n, both for two-dimensional (2D) and 3D lattices.[3] The question arising is whether they can be used in imperfect lattices and/or fractals provided that we utilize the proper S_n expression. We find below that this is true. We use the known expressions for the spectral dimension to derive the appropriate S_n theoretically, and by using it we find that we recover the whole $V(r,n)$ profile successfully. Thus it is not necessary to resort to the complicated formula of the generating functions for the visitation probabilities. Our preliminary work[1] showed that the D_I exponent is in the same class of exponents as the spectral (fracton) dimension exponents, but showed some differences in its numerical values. Here we establish that these assertions are correct, both theoretically and from the computer experiments. The differences were due to the fact that the asymptotic limit was not reached in these calculations,[1] and it is now established that indeed only after very long times D_I and $d_s/2$ have the same numerical values. The results are verified by extensive computer simulations of these processes.

II. NUMERICAL METHODS

The Monte Carlo simulation techniques are described in detail in our earlier work.[1] Briefly, the Sierpinski gasket is generated to ninth-order (29 526 sites) using a linear cellular automaton with a modified version of Rule 90 (according to Wolfram's notation[4]). We consider a cellular automaton of length $2M-1$, where M is the number of sites that make up the side of the Sierpinski gasket (triangle), and put a one (1) in the middle cell. The gasket consists of the states of the automaton created after M-1 time steps.[5] The 2D lattices have the square lattice geometry (four nearest neighbors), while the 3D lattices have the simple cubic geometry (six nearest neighbors). The lattice sizes were 600×600 and $100 \times 100 \times 100$, respectively. For both lattices we build a percolation cluster exactly at the critical point ($p_c = 0.5935$ for the 2D case and $p_c = 0.315$ for the 3D case, for site percolation)

using the cluster multiple-labeling technique (CMLT).[1] All small clusters are erased and only the largest percolating cluster is maintained. For all generated structures we monitor a random-walk process by using an index (r) on each lattice site, signifying the number of visits for this site at any given instance. This index is initially zero ($r=0$) for all sites. A particle is placed at random on the lattice and starts performing a random walk. Every time it steps on a site the occupancy index is incremented by one for this particular site, and the process is repeated. The value of this index at the end of each realization is used to derive the P_k value. All other details, such as direction of motion, cyclic boundary conditions, random-number generators, etc. are the same as in our past studies of random walks.[1] The average usually is taken after 1000 realizations.

III. RESULTS AND DISCUSSION

The above I_n function requires the sum $\sum_{k=1}^{S_n} P_k \ln P_k$ which is a sum over all lattice sites k. We rewrite this sum as

$$I_n = -\sum_{r=1}^{r_{\max}} V(r,n)\frac{r}{n}\ln\left[\frac{r}{n}\right], \tag{3}$$

where the sum now is over the index r of the number of visits. The factor $V(r,n)$ is introduced to take into account all sites with r such visits. But we recently showed[3] that

$$V(r,n) = n(1-w)^2 w^{r-1}, \tag{4}$$

where $w = 1 - S_n/n$. We substitute into Eq. (3) and get

$$I_n = -(1-w)^2 \sum_{r=1}^{r_{\max}} r w^{r-1} \ln\frac{r}{n}. \tag{5}$$

Taking into account that $\sum_r V(r,n) r = n$

$$I_n = \ln n - (1-w)^2 \sum_{r=1}^{r_{\max}} r w^{r-1} \ln r. \tag{6}$$

Relation (6) may also be written as

$$I_n = \ln n - (1-w)^2 \frac{d}{dw}\left[\sum_{r=1}^{r_{\max}} w^r \ln r\right]. \tag{7}$$

The sum $\sum_{r=1}^{r_{\max}} w^r \ln r$ converges, and a very good approximation of its limit is given by

$$S(w, r_{\max}) = w^2/(1-w). \tag{8}$$

Thus relation (7) takes the form

$$I_n = \ln n - (2-w)w, \tag{9}$$

and

$$D_I = 1 - (2-w)w/\ln n, \tag{10}$$

from where it is obvious that the limit ($n \to \infty$) is $\lim D_I = 1$.

In order to compare with computer simulations we need the $V(r,n)$ data. For perfect lattices these were given in Ref. 3, and they are in excellent agreement with Eq. (4). For example, for the 2D lattice, Eq. (4) gives $V(1,10\,000) = 826.3$, while the simulation result is 824.3; for the 3D lattice Eq. (4) gives $V(1,10\,000) = 4425.7$, while the simulation result gives 4423.2. Thus, using Eqs. (9) and (10) we have a direct way of finding the I_n function and the D_I exponent for perfect lattices.

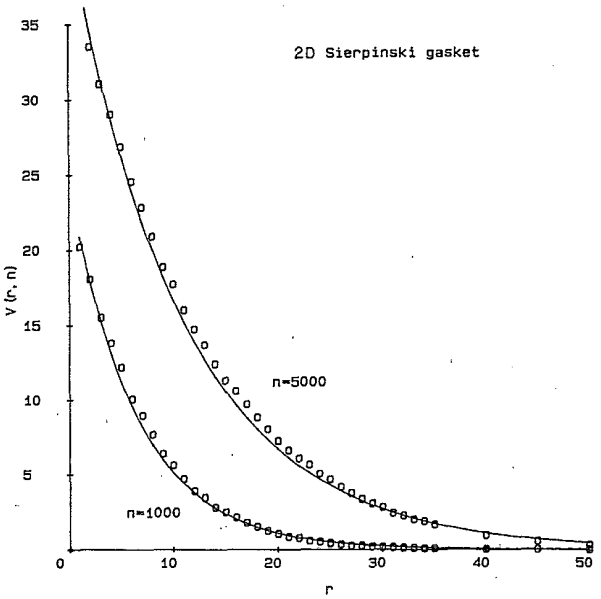

FIG. 1. $V(r,n)$ as a function of n for the 2D Sierpinski gasket for two different n values. The solid lines are solutions of Eq. (4), the circles are results of computer simulations of random walks on the gasket.

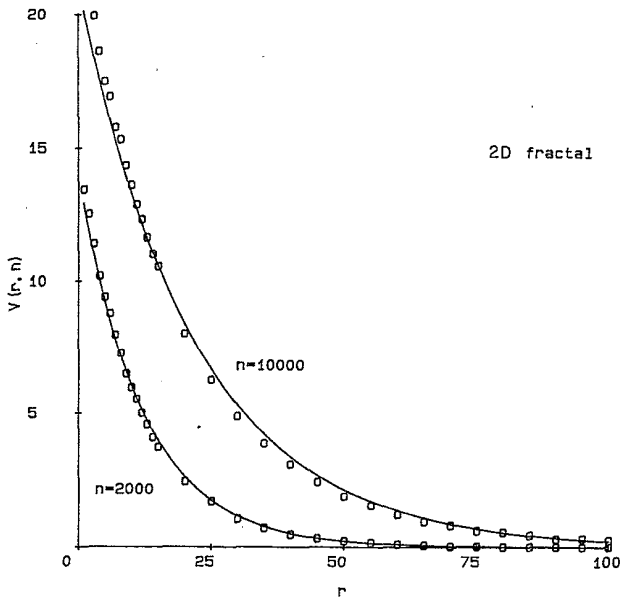

FIG. 2. $V(r,n)$ as a function of n for the 2D fractal lattice (percolation cluster exactly at the critical point) for two different n values. The solid lines are solutions of Eq. (4), the circles are results of computer simulations of random walks on 2D percolation clusters exactly at criticality.

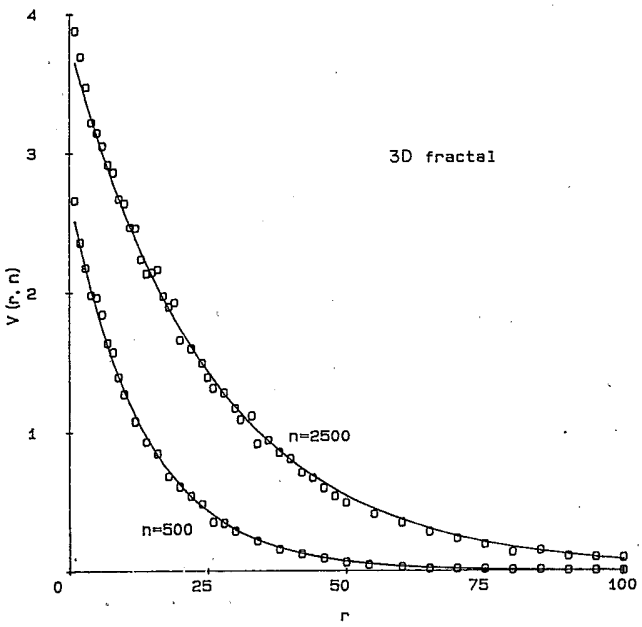

FIG. 3. $V(r,n)$ as a function of n for the 3D fractal lattice (percolation cluster exactly at the critical point) for two different n values. The solid lines are solutions of Eq. (4), the circles are results of computer simulations of random walks on 3D percolation clusters exactly at criticality.

We now turn to the case of fractal lattices. We examine the Sierpinski gasket, the 2D, and the 3D percolation clusters exactly at criticality. In Figs. 1, 2, and 3 we give the $V(r,n)$ functions for the above structures. We now have available a way for calculating S_n for fractals. This is

$$S_n = an^{d_s/2} \tag{11}$$

provided that $d_s < 2$. We use it directly and calculate $V(r,n)$ from Eq. (4). We take the a and d_s values from the literature,[6] since as we know the asymptotic values of a and d_s are reached fairly fast. For the Sierpinski gasket we use $a = 1.282$ and $d_s/2 = 0.684$. Similarly for the 2D lattices we use $a = 1.13$ and $d_s/2 = 0.65$ and for the 3D lattices we use $a = 0.52$, and $d_s/2 = 0.666$. Then we use Eq. (4) and derive the $V(r,n)$ function. The solid lines in Figs. 1–3 represent the solutions of Eq. (4). The circles are simulation results. Good agreement is found for all cases. Some small discrepancies are attributed to the fact that the values of a and d_s used have some uncertainty.

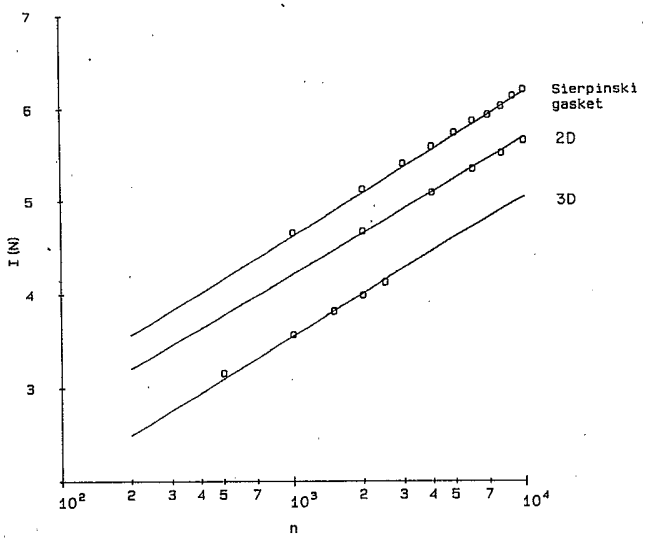

FIG. 4. I_n as a function of time for the fractal structures of the previous three figures. The solid lines are results of calculations using the $V(r,n)$ expressions of the previous figures. The circles are results from computer simulations.

The accuracy of some of these values has been a topic of controversy the last few years. By using Eq. (11) the $V(r,n)$ equation becomes

$$V(r,n) = \left[\frac{an^{d_s/2}}{n}\right]\left[1-\frac{an^{d_s/2}}{n}\right]^{r-1} . \tag{12}$$

After taking logarithms and some algebra we get

$$\ln V(r,n) = \ln\left[\frac{a^2 n^{d_s/2}}{1-an^{(d_s/2)-1}}\right] + r\ln(1-an^{(d_s/2)-1}) . \tag{13}$$

The slope of this equation is $\ln(1-an^{(d_s/2)-1})$. By using a value $d_s = \frac{4}{3}$ for $n = 10\,000$ we receive a slope of 0.053, in good agreement with our previous calculations.[1] Thus, by knowing the fractal parameters we can calculate $V(r,n)$ immediately for any r and n.

A striking feature is the absolute values of the y axes in Figs. 1–3. While for the 2D case (for $n = 2000$) $y \cong 14$, for the 3D case $y \cong 3.5$. This is due to the fact that $S_n = 160.9$ (2D), while $S_n = 83.0$ (3D), so that fewer sites get to be visited in the 3D case. This is because in the 3D case there are a lot fewer open sites, as $p_c = 0.315$ (3D)

TABLE I. $D_I(n)$ exponent for fractals (computer simulation data).

Sierpinski gasket		2D percolation cluster		3D percolation cluster	
n	D_I	n	D_I	n	D_I
10 000	0.659	2000	0.630	1000	0.610
30 000	0.667	10 000	0.638	10 000	0.647
100 000	0.677	100 000	0.641	40 000	0.654
Asymptotic value	0.685	Asymptotic value	6.650	Asymptotic value	$\frac{2}{3}$

and $p_c=0.593$ (2D). This causes a higher degree of revisitation in the 3D case, and thus the $V(r,n)$ function in the 3D case has smaller values for small r and higher values for large r than the 2D case. The same is also observed in the case of the 2D Sierpinski gasket, where (for $n=2000$) $V(r,n)\cong 25$; here S_n is still higher, $S_n=232.2$, showing that there are no bottlenecks, narrow passages, etc. that temporarily hinder the motion but are present to a large degree in the percolation clusters. Here all sites have exactly four neighbors and this facilitates transport.

In Fig. 4 we plot the resulting function I_n as a function of time (n) for all the systems studied. The full lines are the theoretical prediction using Eq. (10), while the circles are results from the computer simulations. Some slight differences in this figure may be also due to some uncertainty in the knowledge of the parameters of Eq. (11), which was used to derive the solid lines.

The interesting feature from these formulae and calculations is that the resulting D_I exponent has a value that only asymptotically with time approaches the $d_s/2$ value. This is shown in Table I, where this exponent is given as a function of time from our computer simulation data. We observe that this trend holds for all systems that we tested here. Usually the opposite holds true, i.e., we approach the asymptotic value at most in a few thousand steps.[6] However, this is not always the case.[7] This point drew some interest recently, when the discrepancies of the calculated D_I exponent and the spectral dimension was questioned. In a Comment[8] de Arcangelis, Coniglio, and Paladin used an approach taken from multifractality[9] and considered the moments $M(q)$ of the measured distribution, which in this case is that of the visitation probability. They calculate these moments by dimensional counting, and by simple comparison with the known expressions of the visitation probability they showed that the cases we considered here are not multifractals. In other words D_I and d_s are not two independent exponents. Actually these thoughts necessitated more calculations (such as the data in Table I) which now resolved this problem. Thus, the values reported here in the above figures and the Table are only *effective exponents* as they have not approached their limiting value yet. This happens only at $n\rightarrow\infty$.

Summarizing, we derived an expression for the entropy-like function I_n, which yields the information exponent for random-walk processes. This was based on the accurate expression that was recently derived for the $V(r,n)$ function of multiple visits on lattices. We performed computer simulations that verified these expressions. The exponent D_I belongs in the same class as the d_s exponent, but unlike the latter it takes much longer times to reach its asymptotic value.

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