Information Dimension in Random-Walk Processes

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Energy transport in disordered media is studied by use of random walks, through a new entropylike function I_N which results in an information dimension D_I of a random-walk process. D_I is calculated and compared to the fractal dimension for two-dimensional square lattices. It is found that a fractal lattice has a much broader (by a factor of 5) site-visitation distribution than a perfect lattice. The above parameters contain more information than the usual random-walk parameters, and provide a new picture and characteristic quantities where random walks are used to simulate transport properties.

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In recent years a large interest has been developed in the properties of disordered lattices, mainly because they provide the most plausible model for amorphous and technologically oriented materials.[1] A random two-component binary lattice to a good approximation possesses this property because of the inherent randomness introduced in its preparation. Moreover, such lattices have been shown to have a structure that is described by a critical fractal exponent, while a dynamic effect on such structures, such as a random-walk process by a particle, is described by the spectral dimension (exponent), with considerable effort being devoted (and justifiably so) to their exact numerical values.[2]

The fractal dimension of a percolation cluster is found by the consideration of several sections of the lattice with a different linear size λ each time, and then by the calculation of the number of sites M that belong to this cluster in each section.[1-3] The fractal (Hausdorff) dimension is defined as

$$D_f = \ln[M(\lambda)]/\ln(\lambda). \tag{1}$$

For a particle performing a random walk of N steps on a percolation cluster, the spectral (fracton) dimension D_s is defined as

$$D_s = 2\ln(S_N)/\ln N, \tag{2}$$

where S_N is the number of distinct sites visited at least once in the walk. The quantity S_N gives an overall measure of the spread or the range of the particle motion. Thus, it has been used in the past to simulate exciton transfer in guest-host and guest-trap systems,[4] in the chlorophyll action in photosynthetic units of plants,[5] in chemical reactions,[6] and other solid-state applications.[1] In all these cases the parameter of interest was the overall range of the random walk, since this range is directly related to a trapping probability, a cross-section probability for reaction, etc., while it makes no difference how many times a particle has visited the same site. To collect this new information one introduces the quantity i_k, which is the number of times that site k has been visited in this walk. The range of k will be $1 \le k \le S_N$, so that all visited sites are accounted for. Also $\sum_k i_k = N$. Then the probability P_k of visiting the kth site is $P_k = i_k/N$. Then,

$$D_I = I_N/\ln N, \tag{3}$$

where

$$I_N = -\sum_{k=1}^{S_N} P_k \ln P_k. \tag{4}$$

D_I is called the information dimension. Its definition is based on the new function I_N which, because of the form $P\ln P$, bears out an entropylike character. I_N is a measure of the relative probability that each site is accessed at some time in the walk. More generally, the information dimension is a property of any random variable with a probability measure implied in it. If all sites have exactly the same probability of visitation then $P_k = 1/S_N$ and

$$I_N = -\sum_{k=1}^{S_N} (1/S_N)\ln(1/S_N) = \ln S_N, \tag{5}$$

and therefore Eq. (4) is reduced to Eq. (2), i.e., $D_I = D_s$. Also in the trivial case of $P_k = 0$ the product $P_k \ln P_k$ is taken to be 0. It is expected that I_N will show characteristic scaling for these processes.

The functions and distributions are calculated by monitoring random-walk simulations as a function of time. Lattices are generated in two-dimensional square topology, first perfect and then random according to a given occupational probability p, where p ranges from $p_c \le p \le 1.00$, p_c being the critical percolation threshold. For the square lattice, I use $p_c = 0.593$ (site percolation problem), I isolate the largest cluster using a cluster multiple labeling technique (CMLT),[2] and all subsequent work is performed on this cluster. I monitor several random-walk properties, such as S_N, the number of distinct sites visited at least once, and R_N^2, the mean-square displacement, which are found to be in very good agreement with past studies.[2,7] I also monitor here i_k, the number of times that site k has been visited as a function of time, for each and all lattice sites. I use both the myopic- and the blind-ant models.[8] In the blind-ant model when the particle is on the perimeter of the percolation cluster an attempt to move outside this cluster consumes one time step. In the myopic-ant model such an attempt consumes no time at all, a new attempt is made until the particle moves to a regular cluster site. Since this is a study of multiple visitations by a single particle, I felt it important to investigate both models.

In Figs. 1 and 2 I plot the site-visitation distributions for the perfect lattice and for the percolating lattice, respectively, curves a. The x axis labeled i is the number of occupations (visits) i on the lattice sites. The y axis is the number of sites w_i with the corresponding i occupations. I call this the w_i distribution. This result is derived as follows: For each realization, first the i_k function is calculated and then the w_i distribution is formed. Finally, the average of 1000 distributions from 1000 separate realizations is taken. We notice that curves a have exponential line shapes; when plotted on semilogarithmic paper, they yield exact straight lines with slopes -0.34 ($p=1.0$) and -0.05 ($p=p_c$). We observe that all visited sites do not have the same visitation probability; instead, sites with a small number of visits abound, while sites with a large number are scarce. These distributions are qualitatively the same for any N I tried. We also observe that w in the perfect lattice falls off much more rapidly than in the fractal lattice (in spite of the change of scales). These curves give an average "$1/e$" value of $i \simeq 3$ (perfect lattice), and $i \simeq 15$ (fractal lattice). Therefore, I conclude that not only does S_N drastically decrease as one approaches p_c, but at the same time the w distribution becomes about 5 times broader. Physically, this means that around p_c, even though S_N is smaller than it is on the perfect lattice as a result of the effective geometrical restrictions (lower dimensionality), the particle motion is spread more evenly on the visited sites than on the perfect lattice, where the degree of frequent revisitation is much higher.

The total probability of visiting a site i times, Q_i, is given by

$$Q_i = W_i/N, \qquad (6)$$

where $W_i = iw_i$. The W_i distribution is shown in Figs. 1 and 2, curves b. We observe that at $p=p_c$, the curve is broader than at $p=1.0$ by about a factor of 7. A maximum appears at $i \simeq 3$ (perfect lattice) or at $i \simeq 18$ (fractal lattice).

With the definition (4), I expand as follows:

$$I_N = -(1/N)\sum_i Z_i + \ln N, \qquad (7)$$

where $Z_i = iw_i \ln i$. The Z_i distribution is also given in Figs. 1 and 2, curves c. We see that Z depends on both i

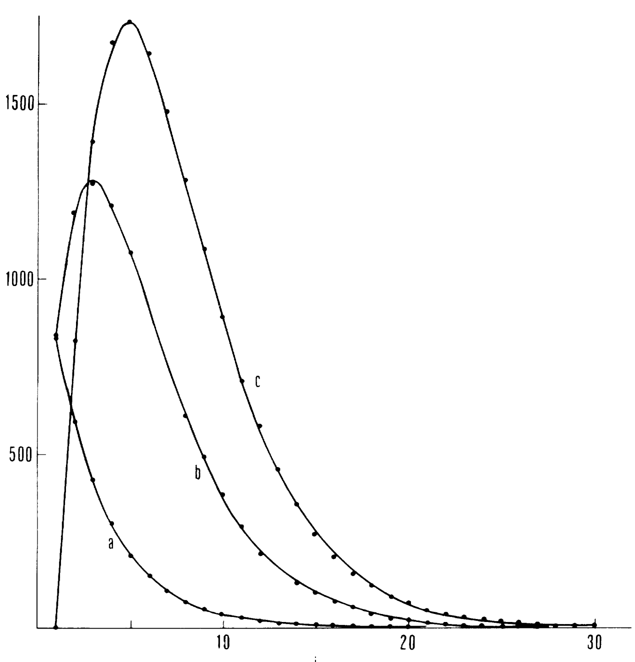

FIG. 1. Site-visitation distribution for a perfect square two-dimensional lattice ($p=1.00$). Data are for $N=10000$ steps, on a 300×300 lattice, averaged after 1000 realizations. The lines are only visual aids. Curve a, w distribution ($\times1$); curve b, W distribution ($\times1$); and curve c, Z distribution ($\times1$).

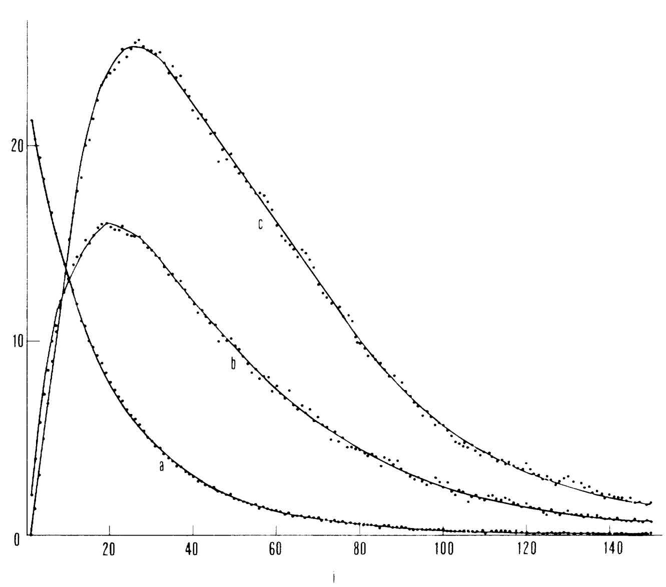

FIG. 2. Site-visitation distribution for a square two-dimensional lattice at the critical percolation threshold ($p=p_c$), for the myopic-ant model. Data are for $N=10000$ steps, on a 300×300 lattice, averaged after 1000 realizations. The lines are only visual aids. Curve a, w distribution ($\times1$); curve b, W distribution ($\times10$); and curve c, Z distribution ($\times20$).

and w_i, i.e., on W_i. Because of the shape of the W distribution, only sites with relatively few visits (small i) contribute appreciably to Z and, therefore to I_N. From the maxima in Figs. 1 and 2, we see that this happens at about $i \simeq 5$ (perfect lattice) and at about $i \simeq 30$ (fractal lattice), i.e., there is a difference by a factor of 6 between the two cases.

In Fig. 3 we have an information plot of I_N as a function of time for the perfect lattice and at $p = p_c$. The least-squares values of the slopes of the straight lines give $D_I = 0.89 \pm 0.02$ (perfect lattice) and $D_I = 0.62 \pm 0.02$ (fractal lattice). We see that in the latter case the blind- and myopic-ant models give identical slopes, leading to the same dimension. This agreement is in accord with previous studies,[7,8] where these two models result in the same exponent, as a result of the fact that the exponent is derived from ratios of the S_N quantities (or slope of the S_N plot), and not from the S_N absolute values, which are certainly different in the two models. I now compare these with values derived with different methods. For a perfect lattice as a result of the logarithmic and the other correction terms,[9]

$$S_N = a_1 N / \ln(a_2 N) + a_3. \quad (8)$$

From this equation the perfect lattice dimension $D = 0.89$, for the range of N studied here. For the fractal lattice (at $p = p_c$)[7,10] for $d = 2$ the spectral dimension $D_s = 1.30$, but $D_s = \frac{4}{3}$ for $d \geq 3$. The random-walk exponents are $D_s/2$ [Eq. (2)], i.e., 0.65 ($d = 2$) and $\frac{2}{3}$ ($d \geq 3$). We thus see that for the perfect lattice the two methods coincide, while for the fractal lattice the information dimension D_I is somewhat lower than the spectral dimension D_s. Intuitively, there is no reason for these sets of exponents to coincide to the same value, but it is certainly a striking feature that this happens in the case of a perfect lattice while a small deviation is observed in the fractal lattice.

A similar type of approach with an entropylike function was recently introduced[11] in related work for growth models, diffusion-limited–aggregation and Eden models. The exponents resulting from the entropy function of the generated clusters were also found to be lower than the usual fractal exponents, but no random walks were reported in these structures.

Summarizing, this work has shown that the information dimension D_I, through the function I_N, presents an alternate approach to the well-known sets of fractal exponents [Eqs. (1) and (2)] in studies of random walks and their applications. It is a function that is used in dynamical systems in many areas of physics.[12] In addition to S_N, which was first derived[7] through D_s, we recover now the w_i and W_i functions, and thus quantitatively explain the decrease of S_N as one goes from the perfect to the fractal lattice. D_I scales surprisingly well for all lattices (Fig. 3), thus resulting in exponent values

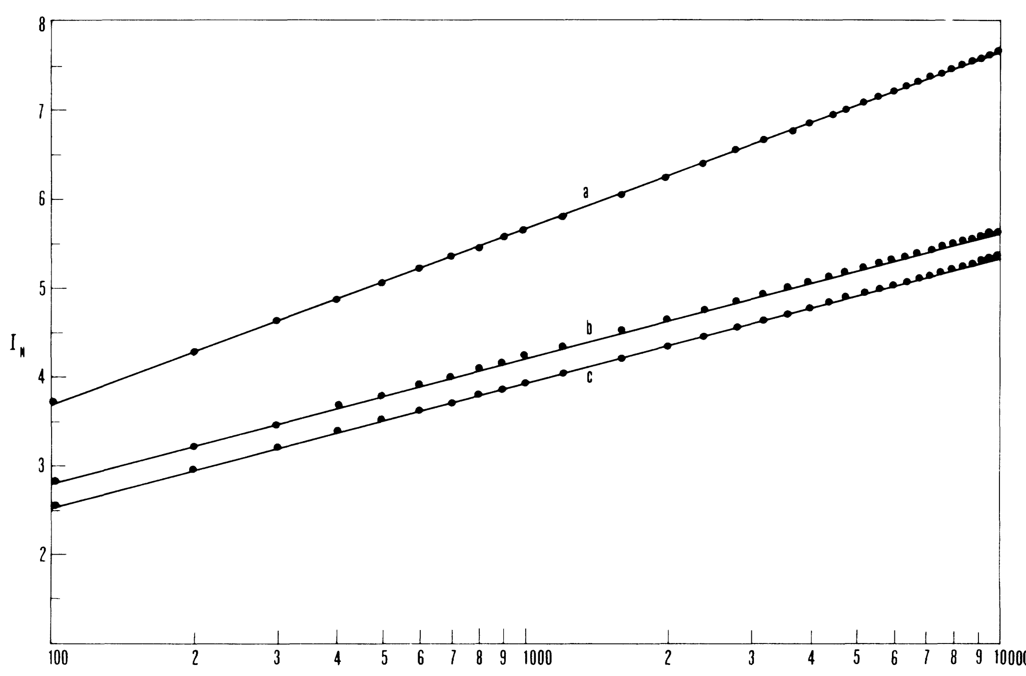

FIG. 3. I_N as a function of time (logarithmic form) for the same data as in the previous figures. The lines are the best fit from a linear least-squares method. Here curve a is for the $p = 1.00$ lattice, curve b is for the $p = p_c$ lattice, myopic-ant model, and curve c is for the $p = p_c$ lattice, blind-ant model.

comparable to the fractal exponents. Also, the exponential function w_i (Figs. 1 and 2) is found to obey scaling laws, both in the perfect and in the fractal lattice cases. The analytical behavior of the w_i function and the problem of multiple visits in all dimensionalities is an extended but old[13] problem. It is more tractable in the case of perfect lattices, but just as interesting in the case of disordered lattices at the critical point, as well as in the crossover (fractal-to-classical) region. It is far from being solved in all contexts discussed here. Work is currently in progress along these lines, and the results will be published elsewhere.

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