Random Walk and the Ideal Chain Problem on Self-Similar Structures

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Random walks and ideal chains (equally weighted trajectories) on self-similar structures are shown to have, in specific examples, drastically different asymptotic behaviors. In certain instances localization effects let the end-to-end distance of an ideal chain of length n grow like $\exp[\alpha(\log n)^{\phi}]$ $(\phi < 1)$ or $(\log n)^{\psi}$ for large n. The renormalization-group analysis and the fixed point, giving these behaviors, are of a new type. These results could be of experimental relevance for the migration properties of excitations on fractal structures in the presence of a trapping environment.

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Random walks (RW) on self-similar structures are well known and have been studied extensively[1] both because their properties are related to transport phenomena[2] and because they are directly connected with linear dynamics on the same structures. This problem is defined by a master equation governing its time evolution. On a lattice S, where the concept of neighborhood has been introduced among sites, the probability $P_{x_0x}(n)$ to be at site x after an n-step walk, starting at x_0, satisfies the following equation:

$$P_{x_0x}(n+1) = P_{x_0x}(n) + \sum_y [w_{xy} P_{x_0y}(n) - w_{yx} P_{x_0x}(n)] , \quad (1)$$

where w_{xy} is the probability to jump from the site y to the site x. We shall consider the case where w_{xy} is different from zero only when x and y are nearest neighbors and is independent of x. Two simple choices have been considered in the literature: $w_{xy} = w/z_y$, where z_y is the number of nearest neighbors of y, and $w_{xy} = w$, corresponding to the myopic and blind ant problems,[1,3] respectively. Following the suggestion coming from numerical simulation[4] it has been rigorously proved[5] that asymptotically these two problems define the same exponents governing the long-time behavior of the end-to-end distance. In the case of the myopic ant performing an n-step random walk W which visits sequentially sites with coordination $z_0, z_1, \dots, z_n$, one easily sees that the associated statistical weight is $\prod_i z_i^{-1}$.

The ideal chain (IC) problem is defined on the same ensemble of walks of the previous problem. However, now the statistical weight of a walk depends only on its length and not on the type of sites it visits. In other words, the IC problem is the equilibrium statistical problem of an ideal polymer in solution.[6]

Clearly for structures where the coordination z_x is independent of x, like regular lattices, the two problems are equivalent. Probably due to this equivalence it has been implicitly assumed that for self-similar structures some type of relation (like the one between the myopic and the blind ant) continues to hold and no surprise should be present.

If the structure S is embedded on a regular lattice with coordination z (e.g., an incipient infinite cluster in a percolation model on a d-dimensional hypercubic lattice), one can also define another type of random walk with trapping environment (RWTE):[7,8] The ant moves randomly among all its nearest-neighbor sites and it dies if it jumps on a site not belonging to S. This type of walk could be of experimental interest, for example, in the migration properties of excitations in mixed organic crystals.[8] The environment acts on the excitations like a fast decay channel. It is not difficult, however, to see that the RWTE is equivalent to the IC if the average in the former is restricted only to the surviving ants.

In Ref. 7 some types of fractal lattices have already been studied and indeed different asymptotic behaviors have been predicted for the RW and the RWTE as well as for the IC due to the above remark. However, since there are no substantial differences among the fractal structures studied in Ref. 7 none of the localization effects[9] we are going to present has been found.

Both the RW and IC problems can be studied simultaneously in a unique "phase diagram" using a Gaussian field theory with Hamiltonian

$$\mathcal{H}(\{a_x\}) = \tfrac{1}{2} \sum_x a_x \varphi_x^2 - \sum_{\langle xy \rangle} \varphi_x \varphi_y \equiv \tfrac{1}{2} \sum_{x,y} \varphi_x M_{xy} \phi_y , \quad (2)$$

where the second summation is over nearest-neighbor sites and $a_x = z_x(1+\omega/w)$, $z_x(1+\omega/wz_x)$, and K^{-1} for the myopic ant, blind ant, and ideal chain problems, respectively. We have introduced ω as the discrete Laplace transform parameter of $P_x(n)$, i.e., $\tilde{P}_{x_0x}(\omega) = \sum_{n=0}^{\infty} P_{x_0x}(n)(1+\omega)^{-n-1}$, and the fugacity K per step in the ideal chain problem. In this last case the counterpart of $\tilde{P}_{x_0x}(\omega)$ is the generating function $G_{x_0x}(K) = \sum_{n=0}^{\infty} C_{x_0x}(n) K^n$ of $C_{x_0x}(n)$, the number of n-step walks joining x_0 to x. In any case $\tilde{P}_{x_0x}$ and G_{x_0x} are proportional to the expectation value $\langle \varphi_{x_0} \varphi_x \rangle = M_{x_0x}^{-1}$ with respect to the Boltzmann factor $\exp(-\mathcal{H})$, where $\mathcal{H}$ is defined by Eq. (2) with the above choice of a_x's. The equivalence of random walks and Gaussian models is well known for regular lattices.[10(a)] Generalization to fractal lattices is straightforward[10(b)] and can be used in many other related contexts.[10(c)]

In order to better understand the origin of the localization properties of the IC we begin with the rather simple example of the T fractal which is also useful for some interesting remarks.

Figure 1(a) shows the first two steps, T_1 and T_2, of the infinite sequence $\{T_n\}$ defining it. The resulting fractal dimension is $\bar{d}=\log_2 3$. The renormalization-group (RG) strategy for studying this type of fractal is well known[11] and consists of eliminating the subset of field variables φ_x in T_n with Hamiltonian (2) in order to go back to T_{n-1} with Hamiltonian $\mathcal{H}(\{a_x'\})$. The result is a rescaling of the system by a factor 2. Since there are only two types of coordination the RG procedure requires only two parameters $a_x=a_1,a_3$ for $z_x=1,3$, respectively, which renormalize according to the following recursions:

$$a_1'=a_1a_3-2\,, \qquad (3a)$$

$$a_3'=a_3^2-a_3/a_1-3\,. \qquad (3b)$$

The resulting phase diagram is shown in Fig. 2. The unphysical region is the set of initial conditions which under recursions make a_1 and/or a_3 negative, making the "energy" (2) unbounded from below (i.e., the matrix M_{xy} exhibits negative eigenvalues). The curves m, b, and c represent the set of initial conditions for the myopic ant, blind ant, and the ideal chain, respectively. The curves m and b of the ants intersect the fixed point $W=(a_1^*=1,a_3^*=3)$ as $\omega\to 0$ [see the expressions for the a_x's following Eq. (2)]. This means, as we expect,[5] that the asymptotic behavior of the ants is determined by the same (unstable) fixed point W. There are two eigenvalues, $\lambda=6$ and 2, of the matrix associated with the linearized recursions (3) around W. The highest one, $\lambda_w=6$, gives the exponent $d_w=\log_2\lambda_w$ governing the behavior of the mean-square distance of an n-step RW in the large-n limit; i.e.,

$$\langle R^2(n)\rangle_w \sim n^{2/d_w}\,. \qquad (4)$$

In this case $d_w=\log_2 6=2.585\ldots$, implying a spectral dimension[12] $d_s=2\bar{d}/d_w=2\log 3/\log 6$ describing the scaling of the density of states for harmonic oscillations on the same structure. This result can also be obtained from resistivity arguments. If we associate a unit resistance to each link of the fractal then the resistance between sites at Euclidean distance r behaves like r^ζ, where scaling arguments[12] predict $\zeta=d_w-\bar{d}$. For the T fractal it is evident that $\zeta=1$ which implies $d_w=\log_2 6$. The m curve, i.e., $a_3/a_1=3$, is invariant under recursions (3) and it is also the eigendirection associated with λ_w. The second eigenvalue $\lambda=2$ is associated with the eigendirection which is tangent to the critical line $\mathcal{C}$ joining the fixed point W to another fixed point $C=(a_1^*=\infty,a_3^*=(1+\sqrt{13})/2)$ which attracts the whole line $\mathcal{C}$ (the existence of this line comes both from numerical evidence and from perturbative expansion for the equation of this line around the fixed points W and C).

The asymptotic behavior of the IC is described by the fixed point C since the line c of the initial conditions $a_1=a_3=K^{-1}$ intersects $\mathcal{C}$ at $K_c^{-1}=2.536\ldots$ which by recursions (3) flows to C. For $K<K_c$ the generating function $G_{x_0x}\propto M_{x_0x}^{-1}$ is finite and becomes singular at K_c where zero eigenvalues are present. At C there is only one relevant eigenvalue, λ_c, of the matrix associated with the linearized recursions, giving the equation analogous to (4) for the mean-square end-to-end distance of the IC with d_w substituted by $d_c=\log_2\lambda_c$. In this case $d_c=\log_2(1+\sqrt{13})=2.203\ldots$ which is different from d_w. The second relevant eigenvalue $\lambda=2$ at W describes the crossover between the asymptotic behaviors of the RW and IC. The γ exponent for the IC problem is defined through the average number of n-step chains per lattice site which should behave asymptotically like $K_c^{-n}n^{\gamma-1}$ or, which is the same, through the divergence of the susceptibility χ of the model (2) near K_c; i.e., $\chi=\sum_{xy}G_{xy}(K)/N\sim(K_c-K)^{-\gamma}$, where N is the number of sites of the lattice. If the fractal we are considering is embedded on a regular structure with coordination z

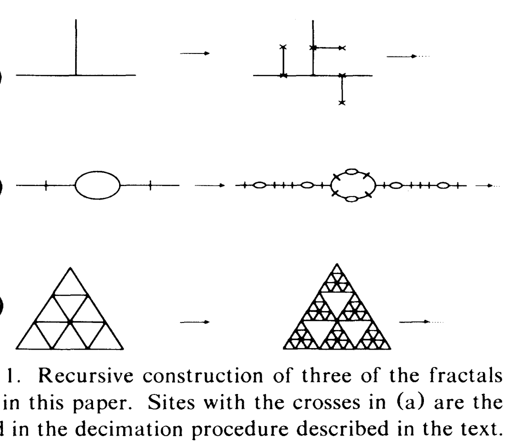

FIG. 1. Recursive construction of three of the fractals considered in this paper. Sites with the crosses in (a) are the ones involved in the decimation procedure described in the text.

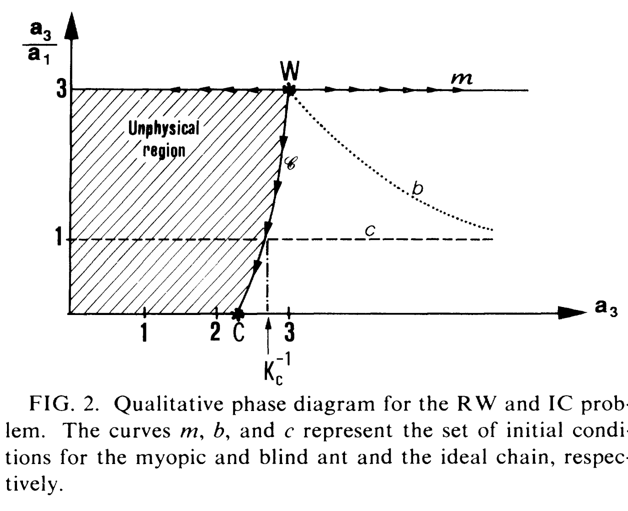

FIG. 2. Qualitative phase diagram for the RW and IC problem. The curves m, b, and c represent the set of initial conditions for the myopic and blind ant and the ideal chain, respectively.

then the survival probability for the RWTE behaves like $(zK_c)^{-n}n^{\gamma-1}$ for large n. For the RW problem the counterpart of χ is $\sum_x \tilde{P}_{x_0x}$ which is equal to ω^{-1} due to the probability conservation $\sum_x P_{x_0x}(n)=1$, thus implying $\gamma=1$.

In order to calculate γ one has to add to the Hamiltonian (2) a coupling with an external "magnetic field" of the type $\sum_x h_x \varphi_x$ [see, e.g., Ref. 11(a)]. The previous renormalization still applies and it is easy to see that one needs only two magnetic fields $h_x = h_1, h_3$ for $z_x = 1,3$, respectively. The recursion equations are linear in the fields h's and the highest eigenvalue $\lambda_H = 2^{y_H}$ gives the γ exponent through the standard relation $\gamma=(2y_H-\bar{d})/d_c$. At the C fixed point we get

$$\gamma=\log[(5+2\sqrt{13})/3]/\log(1+\sqrt{13})=0.919\ldots,$$

while at W we find correctly $\gamma=1$. Thus the two problems belong to different universality classes.

Analogous things occur also for the branching Koch curve.[13] Here we have still two types of coordinations $z_x=2,3$ and one needs two coupling constants $a_x=a_2,a_3$ for $z_x=2,3$, respectively. The phase diagram is qualitatively the same as the one in Fig. 2 with a_1 substituted by a_2. Now we find $W=(a_2^*=2, a_3^*=3)$, $C=(a_2^*=\infty, a_3^*=\sqrt{5})$, $K_c^{-1}=2.755\ldots$ while the critical exponents are $d_w=\log_3\frac{40}{3}=2.357\ldots$ and $\gamma=1$ at W and $d_c=\log_3 11=2.182\ldots$ and $\gamma=\log[(47+21\sqrt{5})/10]/\log 11=0.934\ldots$ at C. γ and $d_c/\bar{d}$ define two new intrinsic exponents of the considered fractals in addition to the spectral dimension d_s.[14]

From both previous examples one learns that near the critical region $\mathcal{C}$ the parameter a_i, associated with the lowest coordination, iterates toward infinity after a few recursions while the other one remains finite. Since from Eq. (2), the statistical weight for visiting site x is $1/a_x$, the leading contribution to G_{x_0x} comes from ideal chains that, at a coarse-grained level, try to avoid sites at low coordination.

The next two examples are such that the sites of highest coordination do not form an infinite cluster of nearest-neighbor sites.

The first structure has been introduced to model the backbone of the incipient infinite cluster in percolation[15] and it is shown in Fig. 1(b). With the same notation as above we find the following recursion equations:

$$a_2' = a_3^2 a_2(a_2^2-2)/2 + a_3(1-a_2^2) - 2a_2^3 + 9a_2/2\,, \qquad (5a)$$

$$a_3' = a_3^2 a_2(a_3a_2-5)/2 + 2a_3(1-a_2^2) + 6a_2\,; \qquad (5b)$$

the corresponding rescaling factor, l, is some unspecified parameter (greater than 1 of course). Apart from the fixed point $(a_2^*,a_3^*)=(2,3)$ describing the asymptotic behavior of the RW, for which $d_s=2\bar{d}/d_w=\log 36/\log 27$, it seems that there is no other fixed point describing the scaling limit for the IC. [The above value of d_s can also be obtained from the same resistivity arguments as for the example of Fig. 1(a).]

What we really find is that indeed there is no other physically important fixed points of (5) but there is an invariant line joining the fixed point (2,3) with "the point" $(\infty,2)$ which is the domain of attraction of this last one. A simple example catching the essential ingredients of the recursions (5) is represented by the following two-dimensional map:

$$X' = XY/(1-X), \quad Y' = Y^2\,. \qquad (6)$$

The ordinary fixed points of (6) are (0,0) and (0,1). Furthermore, it is easy to see that the line $X(Y)=[\sum_{n=0}^{\infty} Y^{2^n-1}]^{-1}$ is invariant under the recursion (6), that it joins the fixed point (0,1) with the point (1,0), and that it is attracted by this last one. The line invariant under the recursions (5) can be obtained recursively starting from $(\infty,2)$ and its first terms are[16]

$$a_3(a_2) = 2 + \frac{1}{a_2} + \frac{5}{4}\frac{1}{a_2^2} + O\left(\frac{1}{a_2^3}\right); \qquad (7)$$

along this line a_2 renormalizes like

$$a_2' = \tfrac{5}{2}a_2 + \tfrac{7}{10} + O(1/a_2)\,. \qquad (8)$$

The intersection of this line with $a_2=a_3=K^{-1}$ occurs at $K_c^{-1}=2.635\,22\ldots$. The phase diagram is similar to the one of Fig. 2 with a_1 substituted by a_2.

The point $(\infty,2)$ is not an ordinary fixed point since it is infinitely repulsive and the recursion equations cannot be linearized around it. In order to derive the scaling of the average end-to-end distance one has to proceed in the following way. Since after n iterations of the RG procedure the length is rescaled by a factor l^n Eqs. (5), (7), and (8) imply that, if we start near $a_3=a_2=K_c^{-1}$ with $a_3=a_3(a_2)+\delta$, the end-to-end distance $R(\delta)$ behaves like

$$R(\delta) \sim l^n R(\lambda^{n^2} k^n c\delta)\,, \qquad (9)$$

where $\lambda=\frac{5}{2}$, while k and c are finite constants depending on the initial conditions. Equation (9) holds as long as n is large and the argument on the right-hand side is equal to some fixed $\delta_0 \ll 1$. We thus obtain for $K \to K_c^-$

$$R(K_c-K) \sim \exp\{|\log(K_c-K)|^{1/2}\log l/(\log\tfrac{5}{2})^{1/2}\}\,, \qquad (10)$$

implying an average end-to-end distance for the ensemble of n-step IC of $\langle R(n)\rangle \sim \exp[\log l(\log n/\log\frac{5}{2})^{1/2}]$, i.e., $d_c=\infty$. The γ exponent in this case is 1. Similar results are obtained also for the Sierpinski gasket based on a generator of side 3 [see Fig. 1(c)], where again two parameters a_4 and a_6 have to be introduced corresponding to the two types of coordination $z_x=4$ and 6, respectively. The fixed point for RW is $a_4^*=4, a_6^*=6$ with $d_w=\log_3\frac{90}{7}$ and $\gamma=1$ in agreement with the result of Ref. 17. For the IC the calculation, straightforward but rather tedious, gives $K_c^{-1}=4.402\,41\ldots$ and for large n,

$$\langle R(n)\rangle \sim (\log n)^{\log 3/\log 2}\,, \qquad (11)$$

i.e., $d_c=\infty$ again. One also finds $\gamma=\frac{3}{2}$. This time the fixed point is such that $a_6^* a_4^* = 6 + 2\sqrt{3}$ and $a_4^* = \infty$. From the position of the fixed points governing the asymptotic behavior of the IC in the last two cases we learn that the cause for the localization effect[9] is just due to the highest coordination sites that act as "entropic traps," preventing the swelling of the ideal chain.

One could ask if similar effects are present whenever the sites with the highest coordination are not connected to form an infinite cluster and are uniformly distributed over the structure. It would be extremely interesting to know if something analogous also occurs for statistical fractals like the incipient infinite cluster in percolation. Of course diffusion is normal on periodic lattices with nonuniform coordination. The localization found here is due essentially to the combined effect of self-similarity and of the nonconstant value of the coordination.

The RWTE can also be generalized to the case where the ant at site x has a different probability between the event to remain in the structure, z_x/z, and that to go out and then die, $p(z - z_x)/z$ with $p \leq 1$. For $p = 0$ and 1 we get the blind ant and the IC, respectively. For the cases studied here one can see that as soon as $p > 0$ the asymptotic behavior is the one of the IC; i.e., there is universality with respect to the parameter p.

Other types of surprises, connected with the entropy of self-avoiding branched polymers on a Sierpinski gasket, like the one used here, have been found in Ref. 18.

Localization effects on RW, due to external forces have also been studied in the recent literature. Two important examples are the one-dimensional RW in a random bias field on each site[19] and the motion of a quantum particle in a hierarchical potential.[20]

It should be mentioned that a RG analysis of the type employed in the present paper allows one to discuss[21] also the localization of RW on fractal lattices with topological or Euclidean bias[22] as well as diffusion on a chain with a heirarchical distribution of bias fields.[21]

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