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LETTER TO THE EDITOR

Mapping between hopping on hierarchical structures and diffusion on a family of fractals

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Abstract. We present a simple analytical approach to studying diffusion on hierarchical and fractal structures. We show that hopping on one-dimensional hierarchical structures can be mapped onto diffusion on a family of loopless fractals.

The problem of diffusion on hierarchical and fractal structures has recently been of considerable interest [1-8]. In many disordered systems (glasses, spin glasses, proteins, etc), anomalously slow relaxation has been observed and attributed to the hierarchical or fractal space structure of the system.

In this letter, we study the relation between two types of diffusion: *hopping* and *walking* on hierarchical (see figure 1) and fractal structures (see figure 2). The *hopping* process is the diffusion of a particle hopping from cell to cell on the backbone of the structure with hierarchical energy barriers determining the transition rates. The *walking* process is a nearest-neighbour random walk on the entire structure including backbone and dead ends. We find that both types can be studied by the same analytical approach and that hopping on a one-dimensional hierarchical structure can be mapped onto diffusion on a family of loopless fractals.

We first consider hopping on a one-dimensional lattice with energy barriers distributed in a hierarchical way as shown in figure 1. A particle can hop from site k to site $k\pm1$ with transition rates $w_{k,k\pm1}=w_{k\pm1,k}$ which are inversely proportional to the barrier heights:

$$\begin{aligned} &w_{k,k\pm1}=R^l \qquad 0<R\leqslant 1\\ &k(\text{mod}\, 2^l)=2^{l-1} \qquad l>0,\ \text{integer}. \end{aligned} \tag{1}$$

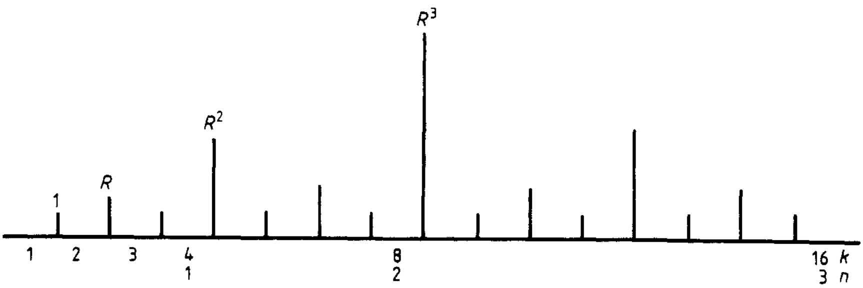

Figure 1. Hierarchical barrier structure. The particle can hop from a cell to its nearest-neighbour cell with transition rates inversely proportional to the height of the barrier, R^{-l}. The index k represents the cell number and n represents new cells determined by $k=2^{n+1}$. This hierarchical structure is generated from an ultrametric tree with two sons, $m=2$.

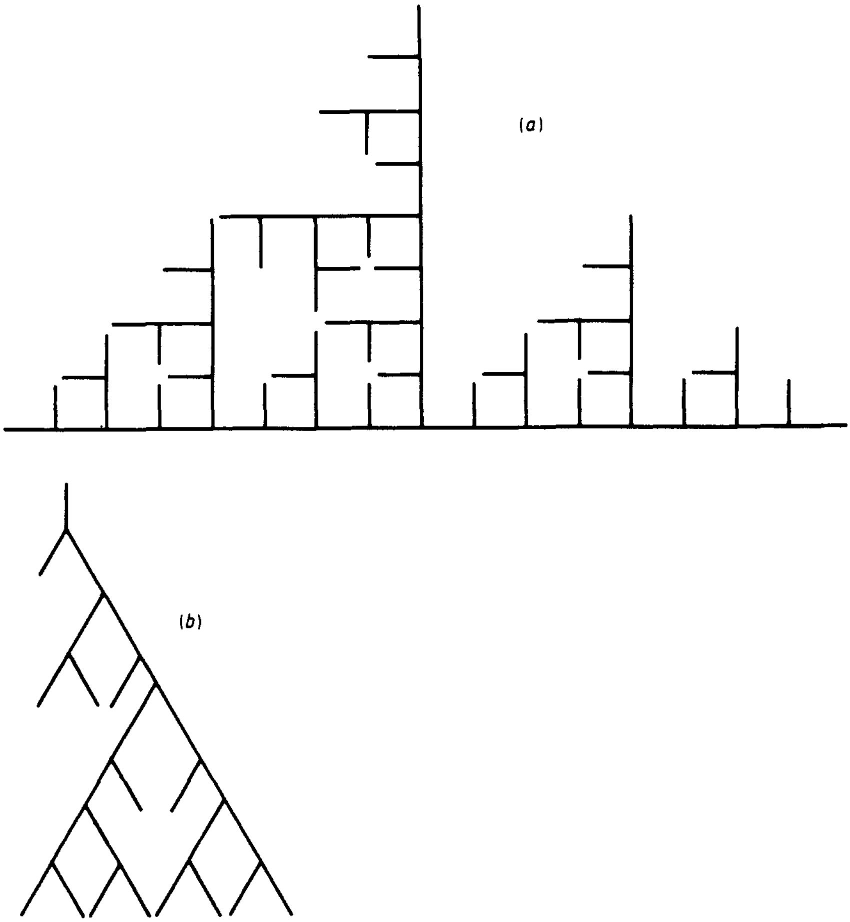

Figure 2. A loopless fractal embedded (*a*) on a square lattice and (*b*) on a Cayley tree lattice. The coordinate number is $z=3$ and the fractal dimension is $d_f = \log 3/\log 2$.

This model has recently been studied using renormalisation group techniques [2–4]. Here we use a simple analytical derivation to calculate the diffusion exponent d_w defined by $\langle x^2\rangle \sim t^{2/d_w}$ where $\langle x^2\rangle$ is the mean square displacement of the random walker on the hierarchical structure.

Following Zwanzig [9], the diffusion constant D can be written as

$$t/\langle X^2\rangle \equiv D^{-1} = \frac{1}{N}\sum_{k=1}^{N}\frac{1}{w_{k,k\pm1}} \tag{2}$$

where N is the number of distinct sites visited by the random walker. New cells are denoted by n and defined by $k=2^{n+1}$ (see figure 1). For the new cells, one can write a recursion relation

$$\frac{1}{w_n} = \frac{2}{w_{n-1}} + \frac{1}{R^n} \tag{3}$$

where

$$\frac{1}{w_n} = \sum_{k=1}^{2^{n-1}-1}\frac{1}{w_{k,k+1}}. \tag{4}$$

Equations (2)-(4) lead to

$$D^{-1}=\frac{1}{2}\sum_{n=0}^{n_{max}}\frac{1}{(2R)^n} \tag{5}$$

where n_{max} is related to $x\equiv k\sim\langle X^2\rangle^{1/2}$ by $X\sim 2^{n_{max}+1}$. In the limit of large x, i.e. $n_{max}\gg 1$, one may distinguish two cases [3]:

$$\begin{aligned} &t/X^2=D^{-1}=R/(2R-1) && R>\tfrac{1}{2}\\ &D^{-1}=\tfrac{1}{2}(1/2n)^{n_{max}-1} && R\leqslant\tfrac{1}{2} \end{aligned} \tag{6}$$

from which follows

$$\begin{aligned} &d_w=2 && R>\tfrac{1}{2}\\ &d_w=1+\frac{|\ln R|}{\ln 2} && R\leqslant\tfrac{1}{2}. \end{aligned} \tag{7}$$

These results are consistent with the exponent $\nu=1/d_w$ found for the autocorrelation function $P_0(t)\sim t^{-\nu}$ by several authors [2, 3]. Note that similar results are obtained in one dimension with random barriers [3, 10] distributed as $P(w)\sim w^{-\alpha}$ where $\alpha=1-\ln 2/|\ln R|$. In this case, $d_w=(2-\alpha)/(1-\alpha)$; writing α in terms of R yields (7).

Next we consider walking on the hierarchical structure where the barriers represent dangling ends, and a random walker can walk (unit steps) on the entire structure, including backbone and dangling ends. The size of the dangling ends is given by the height of the barrier, i.e. R^{-l}. It was shown [11] that the average time spent on a dead end is inversely proportional to its length. Therefore, $w_{k,k+1}$ will represent the inverse of the average time a random walker spends on the dead end between cells k and $k+1$. Equation (5) can be rederived by similar arguments, the only difference being the value of n_{max}. The value of n_{max} is now determined by the span of the diffusion along the y direction. The diffusion in the x and y directions are related by

$$t\sim y^2\sim x^{d_w}. \tag{8}$$

This result stems from the fact that the only anomaly occurs along the x direction. The effective diffusion span in the y direction is related to n_{max} by $y\sim R^{-(n_{max}+1)}$ which yields from (8)

$$R^{-(n_{max}+1)}\sim X^{d_w/2}. \tag{9}$$

Substituting (9) into (5) leads to $d_w=2$, for $R>\frac{1}{2}$, and the following self-consistent equation for d_w for $R\leqslant\frac{1}{2}$ and $n_{max}\gg 1$,

$$d_w=2+\frac{d_w}{2}\frac{\ln(2R)}{\ln R} \tag{10}$$

which leads to

$$d_w=4\ln R/\ln(R/2). \tag{11}$$

This result agrees with its analogue—diffusion on a *random* comb with a power law distribution $p(l)\sim l^{-(1+\gamma)}$, $(0\leqslant\gamma\leqslant 1)$ of the dead-end length. In this case, it was found [12] that $d_w=4/(1+\gamma)$. The relation $\gamma=\log 2/|(\log R)|$ then leads to (11). It should be noted that it follows from (8) and (9) that the random walker does not visit all sites along the dead ends. This is the reason for the difference between (7) and (11) (see also [12]).

It is seen that hopping and walking on hierarchical structures are of a similar nature, with the only difference resulting from a different cut-off in (5). In order to map between the processes of hopping and walking (such that both cut-offs will be the same), we introduce the fractal structures shown in figure 2. This fractal is embedded in the square lattice with coordination number $z=3$ and with fractal dimension $d_f = \log 3/\log 2$. Note the similarity in the structure between the teeth and the backbone. We will show that diffusion on this fractal can be regarded as a particular case of hopping on hierarchical structures.

The self-similarity property of the fractal shown in figure 2 yields that the average time the random walker spends on the n tooth scales in the same way as the time spent on the fractal until reaching that tooth when starting from the left-hand corner of the fractal. Thus,

$$\frac{1}{w_n} = \sum_{k=1}^{n} \frac{1}{w_{k,k+1}} \qquad k = 2^{n+1}. \tag{12}$$

Using (3) and (12) leads to the following recursion relation:

$$\frac{1}{w_n} = \frac{3}{w_{n-1}}. \tag{13}$$

This equation can be interpreted as hopping on a hierarchical structure with $R = \frac{1}{3}$. Therefore, diffusion on the above fractal can be mapped onto hopping on a hierarchical structure with $R = \frac{1}{3}$.

In contrast to the previous case, because of the self-similarity nature of the fractal the random walker now visits *all* sites on the dead ends of the fractal, and (8) is no longer valid. Hence we expect $n_{\max}$ to scale with x as $2^{n_{\max}+1} \sim x$. Using (5), we obtain (7) and, for our particular case $R = \frac{1}{3}$,

$$d_w = \ln 6/\ln 2. \tag{14}$$

This mapping can be generalised to other values of R and to their corresponding coordination number z. In figure 3, we present a fractal with coordination number

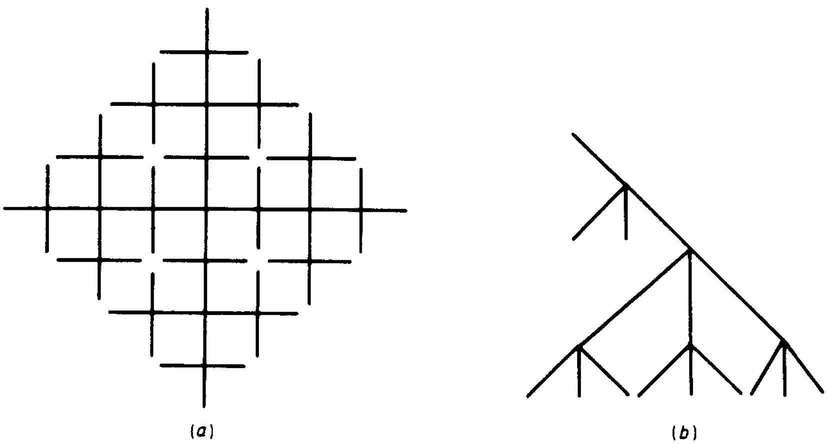

Figure 3. A loopless fractal embedded (a) on a square lattice and (b) on a Cayley tree lattice. The coordination number $z=4$ and the fractal dimension $d_f = 2$. Note that the fractal is compact. Fractals with higher coordination numbers can be embedded only in higher dimensions or on a Cayley tree.

$z=4$. In this case, the similarity between the teeth and backbone yields

$$\frac{1}{w_n}=2\sum_{k=1}^{n}\frac{1}{w_{k,k+1}} \qquad k=2^{n+1} \tag{15}$$

leading to

$$\frac{1}{w_n}=\frac{4}{w_{n-1}} \tag{16}$$

which identifies R to be $\frac{1}{4}$ and thus

$$d_w=1+\frac{|\ln R|}{\ln 2}=3. \tag{17}$$

For a general value of z, the diffusion exponent d_w for this family of fractals is

$$d_w=1+\frac{\ln z}{\ln 2}. \tag{18}$$

This result can also be obtained [13] using the Einstein relation for the diffusion on loopless aggregates, $d_w=d_f(1+1/d_l)$. Since $d_f=d_l=\ln z/\ln 2$ for these families, (18) follows immediately. Equation (18) was also tested numerically for $z=3$ and 4 using exact enumeration methods [14]. Results are shown in figure 4. From these plots we find $d_w=2.60\pm0.05$ and $z=3$, and $d_w=3.0\pm0.1$ for $z=4$ in excellent agreement with (17).

It should be noted that whereas the diffusion exponent d_w is identical for hopping on a one-dimensional hierarchical structure and diffusion on the above fractal, the properties of the autocorrelation function $P_0(t)$ are different. This is due to the fact that the fractal dimension plays an important role [15] in determining $P_0(t)$. Indeed, $P_0(t)\sim t^{-d_s/2}$ where $d_s/2=1/d_w$ for the hopping case and $d_s/2=d_f/d_w$ is the diffusion on the fractal case. It is also interesting to note that for the case of walking on heirarchical structures, $d_s/2$ is neither $1/d_w$ nor d_f/d_w but takes the value [12] $d_s/2=(3-\gamma)/4=(3|\log R|-\log 2)/4|\log R|$.

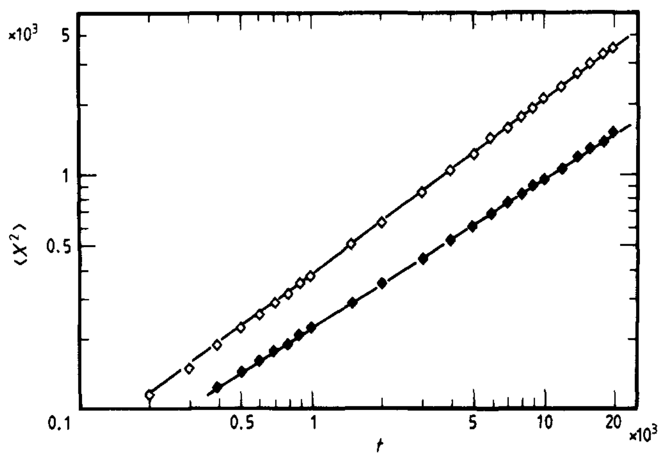

Figure 4. Plot of $\langle x^2\rangle$ as a function of t for diffusion on the fractals shown in figures 2 and 3 with coordination numbers $z=3$ (◇) and $z=4$ (◆).

Our results for diffusion on hierarchical structures can be extended to diffusion on a generalised family of hierarchical structures. This family is obtained from ultrametric trees with coordination number $m+1$ (or m sons). In this case $\alpha = 1 - \ln m/|\ln R|$ and (3), (7) and (11) read, respectively,

$$\frac{1}{w_n} = \frac{m}{w_{n-1}} + \frac{m-1}{R^n} \qquad k = m^{n+1} \tag{19}$$

$$d_w = 1 + \frac{|\ln R|}{\ln m} \tag{20}$$

$$d_w = \frac{4 \ln R}{\ln(R/m)}. \tag{21}$$

It is seen that the anomaly decreases with m, as expected, since the relative number of low barriers increases in these structures.

To summarise, we have shown that hopping on hierarchical structures is identical to walking on a family of certain fractals. We have also presented a simple derivation for the diffusion exponent for hopping on hierarchical structures (equation (7)) and have shown that walking on a hierarchical structure can be treated similarly.

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