Iterated function system and diffusion in the presence of disorder and traps

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(Received 21 February 1995)

The escape probability ξ_x from a site x of a one-dimensional disordered lattice with trapping is treated as a discrete dynamical evolution by random iterations over nonlinear maps parametrized by the right and left jump probabilities. The invariant measure of the dynamics is found to be a multifractal. However the measure becomes uniform over the support when the disorder becomes weak for any nonzero trapping probability. Possible implications of our findings to diffusion processes are brought out briefly.

PACS number(s): 05.40.+j, 05.60.+w, 61.43.Hv

Diffusion in the presence of disorder and trapping has become by now a classic field. This is mainly because the problem *per se* is mathematically interesting and is well posed; also it has a tremendous potential for a wide range of applications which include migrations of optical excitations [1], polymer physics [2], and diffusion-limited binary reactions [3]. See, e.g., [4] for an exhaustive review.

The standard approach to this class of problems is to write down a second order master equation for the probability of the particle to be at a lattice site at a given time, and solve it employing analytical or numerical techniques, see, for example, [5]. An alternate approach, based on the first passage time (FPT) formulation, has attracted growing attention in the recent times [6–10]. This approach has an advantage in that the master equation is first order to start with. All the transport properties of the system can also be calculated from the first passage time formulation.

Employing FPT formulation for the Sinai model [11] it was recently shown that the distribution of the mean FPT over the disorder exhibits interesting multifractal scaling [8]. Also the probability to escape from one site of the lattice to the next was found to have self-similar fluctuations [9,10]. The Sinai model however, is a highly idealized, albeit interesting, mathematical model, and whose link to physical reality appears to be rather abstract.

In this work we shall consider a more realistic model for diffusion where a particle diffuses by overcoming random barriers but can also be trapped at various sites with site dependent random probabilities [12]. The main characteristic of this class of models is that the total probability (called the survival probability) is *not* a conserved quantity. It has been shown that the survival probability is an erratical descreasing function of time and leads to interesting and unexpected behavior like enhanced diffusion, breaking of self-averaging and emergence of Lifshitz tails [13].

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We shall show that this model, when disorder is strong leads to self-similar fluctuations of the escape probability, and these can be characterized employing multifractal formalisms. However this feature of multifractality disappears when there is no trapping, whatever may be the strength of disorder. More importantly, when the strength of disorder goes to zero the multifractality disappears even with arbitrary nonzero trapping probability. Purely from methodological point of view, we connect diffusion in a trapping environment to an iterated function system [14]. Such a formulation, connecting random walks and iterated function systems, was proposed very recently in the context of a binary model for Sinai disorder [9,10], where we have two maps for random iterations. Here we extend the formulation to problems of diffusion on a disordered lattice in the presence of trapping, where we have infinity of maps parametrized by the jump probabilities which are chosen randomly from a well specified distribution that models the disorder. We restrict our attention to a one-dimensional lattice since, as is often the case [15], it contains all the essential characteristics of the higher-dimensional systems. Furthermore one-dimensional systems are amenable to relatively easy analytical and numerical work.

Let us consider the master equation for the probability $\hat{G}_{x,x+1}(n)$ that a particle makes a first passage from a site x to a site $x+1$ in n steps on a one-dimensional lattice of length N. At each site $x \geq 1$ we shall indicate by $q_x \in [0,1/2]$ the probability for making a left jump and by $p_x \in [0,1/2]$ the probability of making a right jump (see Fig. 1). The sojourn probability at site x is

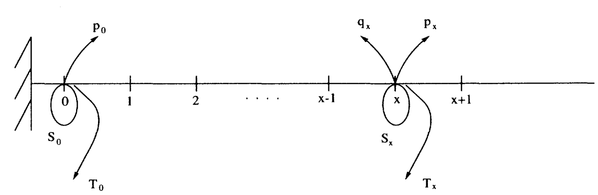

FIG. 1. Definition of the hopping probabilities. At site x the left jump probability is q_x and the right jump probability is p_x. The sojourn probability is $S_x = \gamma(1-q_x-p_x)$ while the trapping probability is $T_x = (1-\gamma)(1-q_x-p_x)$ where $\gamma \in [0,1]$.

given by $\gamma(1-q_x-p_x)$ and the trapping probability is $(1-\gamma)(1-q_x-p_x)$. Here γ is a parameter which can be continuously tuned from 0 (trapping) to 1 (no trapping).

The master equation for $\hat{G}_{x,x+1}(n)$ $(x \geq 1)$ then reads:

$$\hat{G}_{x,x+1}(n) = p_x\delta_{1,n} + q_x\hat{G}_{x-1,x+1}(n-1) + \gamma(1-q_x-p_x)\hat{G}_{x,x+1}(n-1) \quad (1)$$

with the boundary condition that site $x=-1$ is perfectly reflecting:

$$\hat{G}_{0,1}(n) = p_0\delta_{1,n} + \gamma(1-p_0)\hat{G}_{0,1}(n-1) \quad (2)$$

and that $\hat{G}_{x,x+1}(n) = 0$ for $x \leq -1$. We assume that $\{q_x,\ x=1,\ N-1;\ p_x,\ x=0,\ N-1\}$ constitute a set of independent random variables identically distributed in the range $(0-1/2)$, and the common distribution is given by

$$\pi(w) = 2^{1-\beta}(1-\beta)w^{-\beta}\theta(w)\theta(1/2-w) \quad (3)$$

where $w = q$, p and $\beta \in [0,1)$. Here $\theta(\ )$ is the usual Heaviside function. This distribution is known to produce anomalous diffusion for strong disorder ($\beta \to 1$) even with no trapping [5]. For $\beta = 0$, we find that the distribution is uniform in the range zero to half. Thus β can be tuned from 0 (weak disorder) to 1 (strong disorder).

Equations (1) and (2) are readily solved employing generating function technique. We define

$$G_{x,x+1}(z) = \sum_{n=0}^{+\infty} z^n\hat{G}_{x,x+1}(n)\ . \quad (4)$$

Upon the use of convolution theorem,

$$G_{x-1,x+1}(z) = G_{x-1,x}(z)\ G_{x,x+1}(z) \quad (5)$$

we obtain

$$G_{x,x+1}(z) = \frac{zp_x}{1-\gamma z(1-q_x-p_x) - zq_xG_{x-1,x}(z)} \quad (6)$$

for $x \geq 1$ and

$$G_{0,1}(z) = \frac{zp_0}{1-\gamma z(1-p_0)}\ . \quad (7)$$

This solution has earlier been obtained in Ref. [6].

We are interested in the behavior of the *escape probability*, namely the total probability for the first passage from x to $x+1$. This is given by

$$\xi_x \equiv G_{x,x+1}(z=1) = \sum_{n=0}^{+\infty}\hat{G}_{x,x+1}(n)\ . \quad (8)$$

Using Eqs. (6) and (7) it is immediately seen that the escape probability satisfies the following one-dimensional recursion:

$$\xi_x = \frac{p_x}{1-\gamma(1-q_x-p_x) - q_x\xi_{x-1}},\quad x \geq 1 \quad (9)$$

with the initial condition

$$\xi_0 = \frac{p_0}{1-\gamma(1-p_0)}\ . \quad (10)$$

Equation (9) can be interpreted as a dynamical map for a fixed p and q. In fact, since p and q are random, the evolution $\xi_0 \to \xi_1 \ldots \to \xi_x \to \xi_{x+1} \to \ldots$ proceeds by random iteration over the maps parametrized by p and q, which are chosen independently and randomly from the disorder distribution give by Eq. (3) at each stage of iteration. This constitutes an iterated function system, see Barnsley [14].

It is immediately seen that when $\gamma = 1$, which corresponds to a lattice with no trapping Eqs. (9) and (10) lead to $\xi_x = 1$, for all x *regardless* of the choice of $\{p_x, q_x\}$.

Let us now consider the nonconserved case, for which γ is less than 1. For given values of q and p the fixed point of the map (9) is

$$\xi^* = \frac{[1-\gamma(1-q-p)] - \sqrt{[1-\gamma(1-q-p)]^2 - 4pq}}{2q} \quad (11)$$

and it is stable. It lies (see Fig. 2) in the region delimited by $\xi^* = 0$ corresponding to $p = 0$, $q > 0$ (only left jump) and $\xi^* = p/[1-\gamma(1-p)]$ corresponding to $q = 0$, $p > 0$ (only right jumps).

We now show that the escape probability exhibits self-similar fluctuations and these can be characterized employing multifractal formalisms [16]. From numerical point of view, it proves convenient to rescale ξ_x in such a way that the domain is the interval $[0,1]$. To this end we employ the standard rescaling:

$$\frac{\xi - \xi_{\min}}{\xi_{\max} - \xi_{\min}} \to \xi\ . \quad (12)$$

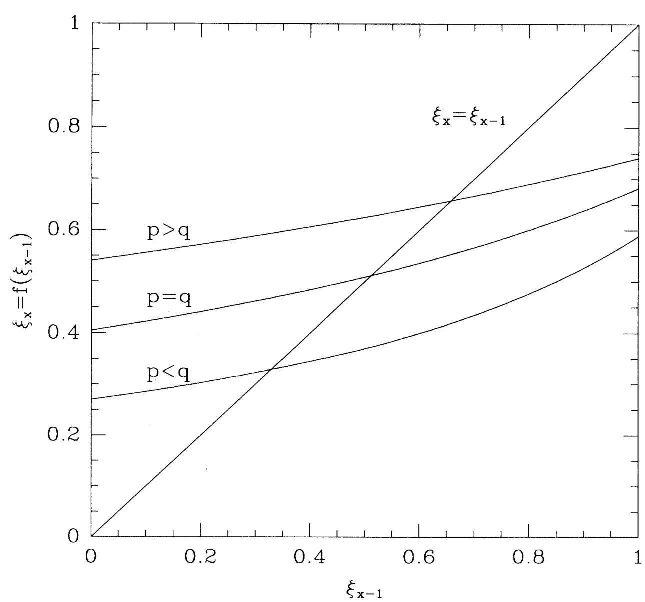

FIG. 2. The map $\xi_x = f(\xi_{x-1})$ for $p = 0.2$, $q = 0.1$, $p = q = 0.15$ and $p = 0.1$, $q = 0.2$. Fixed points are the intersections of the maps with the $\xi_x = \xi_{x-1}$ line.

We denote by $\rho_i(\epsilon)$, the fraction of the total number of ξ values that belong to the ith interval of size $\epsilon = 1/N$. Then the *partition function* is given by

$$Z(Q,\epsilon) = \sum_{i=1}^{N} \rho_i^Q(\epsilon) \tag{13}$$

where the sum is taken over nonempty intervals only. Here, in analogy with conventional statistical mechanics, the *partition function* $Z(Q,\epsilon)$ represents the total contribution of the *measures* $\{\rho_i(\epsilon), i = 1, \ldots N\}$, each of which goes to zero in the $\epsilon \to 0$ limit. Here $-\infty < Q < +\infty$ is a real parameter that highlights the contributions of the different magnitude of the measure to the sum represented by the partition function. The way in which the partition function scales with the dimension of the *ruler* ϵ, is governed by the following standard [16] scaling ansatz [17],

$$Z(Q,\epsilon) \overset{\epsilon \to 0}{\sim} \epsilon^{\tau(Q)} \tag{14}$$

from which we obtain the scaling exponents as

$$\tau(Q) = \lim_{\epsilon \to 0} \frac{\ln[Z(Q,\epsilon)]}{\ln \epsilon} \ . \tag{15}$$

Figure 3 shows a log-log plot of $Z(Q,\epsilon)$ versus $\epsilon (= 1/N)$ for N ranging from 10 to 3×10^6. The linearity of the curves establishes unambiguously the scaling ansatz (14). From the scaling exponents we calculate the generalized Renyi dimensions, given by $D(Q) = \tau(Q)/(Q-1)$, for $Q \neq 1$. Legendre transform of $\tau(Q)$, defined as

$$f(\alpha) = \alpha Q - \tau(Q) \ , \tag{16a}$$

$$\alpha = \frac{d}{dQ}\tau(Q) \tag{16b}$$

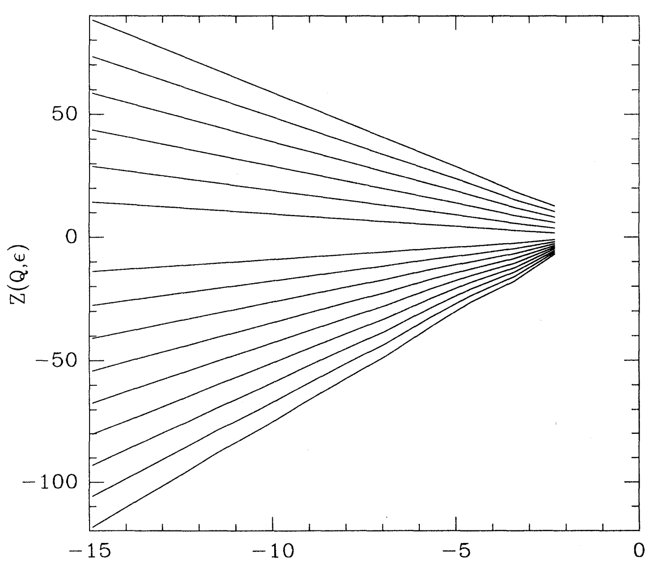

FIG. 3. Behavior of the partition function $Z(Q,\epsilon)$ vs ϵ in a log-log plot for $\beta = 0.3$ and $\gamma = 0.99$. Q varies from -5 (top curve) to $+10$ (bottom curve) in units of 1 with $Q \neq 1$.

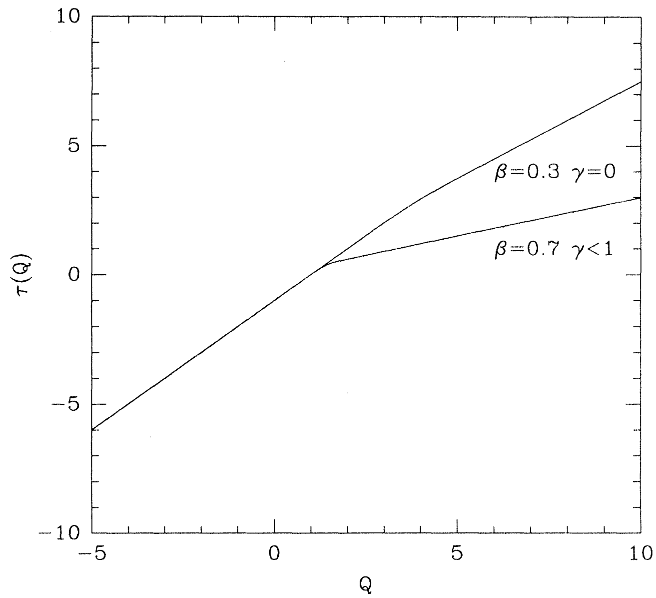

FIG. 4. Plot of $\tau(Q)$ vs Q.

yields the spectrum of singularities denoted by $f(\alpha)$.

Figure 4 depicts the scaling exponents $\tau(Q)$. It is well defined and exhibits clear change in slope, establishing that the underlying measure is multifractal. Figure 5 depicts the spectrum of Renyi dimensions $D(Q)$ for various strengths of disorder (β) and trapping (γ). We observe that when the disorder is strong ($\beta \to 1$), $D(Q)$ remains the same for all values of $\gamma \neq 1$. In other words, the strength of trapping does not influence the fractal measures of the escape probability, when the disorder in the lattice is strong. However when the disorder is weak ($\beta \to 0$), the spectrum of Renyi dimensions changes from

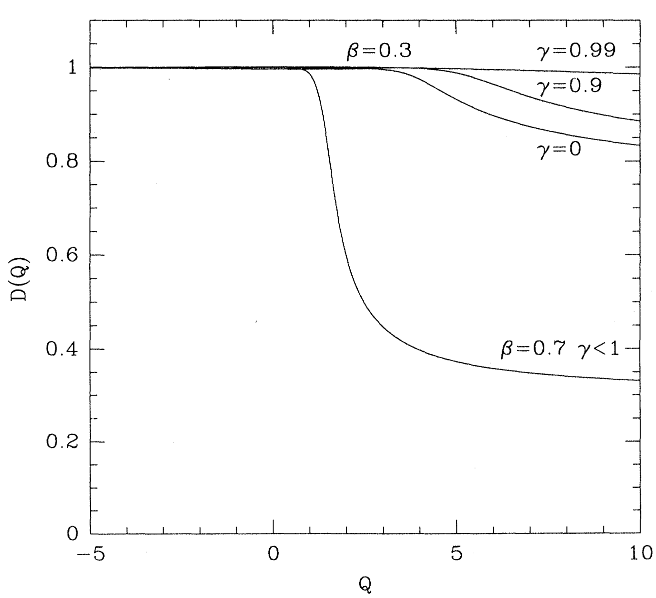

FIG. 5. Spectrum of the Renyi dimensions $D(Q)$ vs Q.

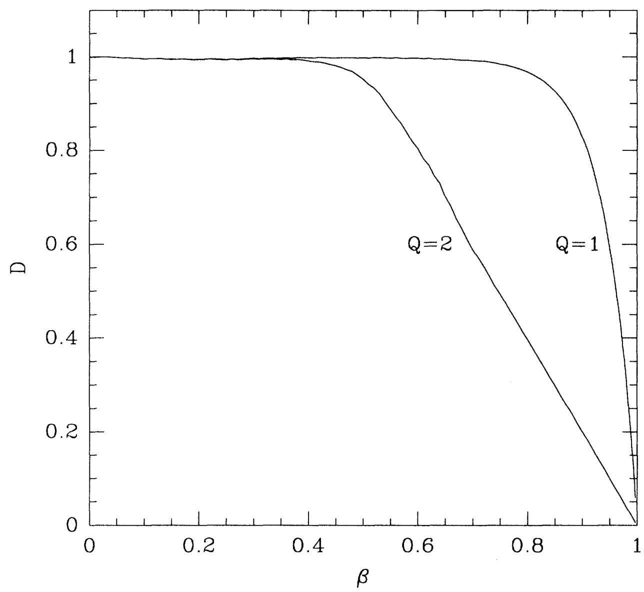

FIG. 6. The information dimension $D(1)$ and the correlation dimension $D(2)$ as a function of the strength of the disorder β, for $\gamma = 0$.

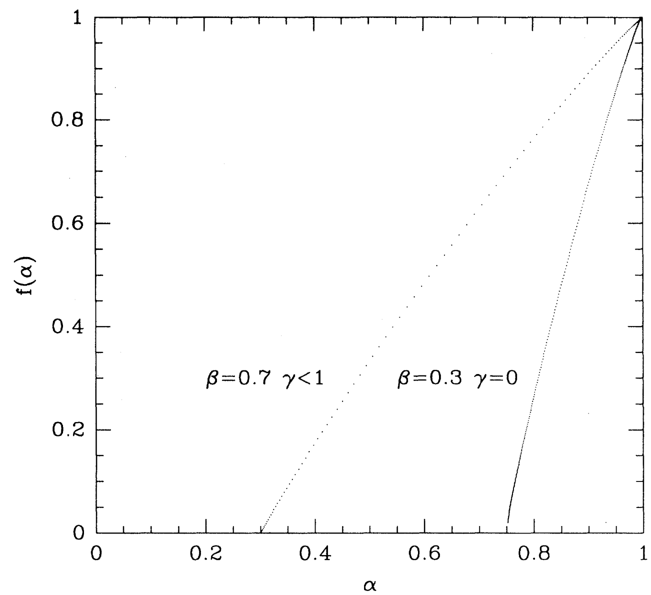

FIG. 7. The spectrum of singularities for $\beta = 0.7$, γ arbitrary and $\beta = 0.3$, $\gamma = 0$.

one trapping rate to the other. Also in the limit of $\beta \to 0$, the $D(Q)$ curve becomes flat with unit intercept, for all values of $\gamma \neq 1$, implying that the measure is space filling. To capture in a simple fashion the dependence of the fractal measure on the strength of disorder, we depict in Fig. 6 the variation of the information dimension $D(1)$ and the correlation dimension $D(2)$, as a function of β for a fixed value of $\gamma = 0$. We find that both $D(1)$ and $D(2)$ decrease with increasing strengths of disorder. We plot in Fig. 7 the f-α curve. It is worthwhile noticing that since the slope of $\tau(Q)$ for $Q \to -\infty$ saturates at unity, the side of $f(\alpha)$ for $\alpha > 1$ does not exist.

A natural question that arises in this context relates to the implications of our findings to the transport properties of the disordered systems. More specifically we ask the question: Is there a connection between anomalous diffusion and fractal fluctuations? For example we find that when the disorder is strong ($\beta \to 1$), the escape probability exhibits multifractal fluctuations for arbitrary nonzero trapping rate. For weak disorder ($\beta \to 0$), the fluctuations become regular and are not multifractal [18].

It has been shown earlier [5] that this model of disorder exhibits anomalous diffusion when $\beta \to 1$. Also, when the disorder is weak ($\beta \to 0$) there is no anomaly in the diffusion process.

However it should be noted that in our analysis an interplay of trapping and disorder is the one that leads to fractal measures of fluctuations in the escape probability.

In view of the results presented here, we feel it would be extremely interesting to extend the approaches of Ref. [5] to the case where trapping is also present. Numerical and analytical investigations in this direction are underway and will be reported soon.

It is a pleasure to thank K. W. Kehr for illuminating discussions and for a critical reading of the manuscript. K.P.N.M. would like to thank IFF of KFA-Jülich for hospitality and financial support. He also thanks M. C. Valsakumar and R. Indira for many discussions and collaboration on related work. A.G. acknowledges support from the HCM program under Contract No. ERB4001GT932058.

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