Iterated Function System and Diffusion in the Presence of Disorder and Traps

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Abstract

The escape probability $\xi_x$ 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 non-zero trapping probability.

Implications of our findings in terms of diffusion are discussed.

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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 [3] and diffusion-limited binary reactions [2]. 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 [6,7,8,9,10]. 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 an 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 highly fluctuating function of time and these fluctuations lead to interesting and unexpected behaviour like enhanced diffusion, breaking of self-averaging and emergence of Lifshitz tails [13].

We shall show that this model, when disorder is strong leads to self-similar fluctuations of the escape probability, and these can be characterised employing multifractal formalisms. However this feature of multifractality disappears when there is no trapping, what ever may be the strength of disorder. More importantly, when the strength of disorder goes to zero
the multifractality disappears even with arbitrary non-zero trapping probability. Purely from methodological point of view, we connect diffusion in a trapping environment to an Iterated Function System (IFS) [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 often the case [15], it is 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 given by $\gamma(1-q_x-p_x)$ and the trapping probability is $(1-\gamma)(1-q_x-p_x)$. Here $\gamma$ 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:

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

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

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

$$\pi(w) = 2^{1-\beta}(1-\beta)w^{-\beta}\theta(w)\theta(1/2-w)$$  \hspace{1cm} (3)
where \( w = q, p \) and \( \beta \in [0, 1) \). Here \( \theta(\cdot) \) is the usual Heaviside function. This distribution is known to produce anomalous diffusion when the disorder is strong \( (\beta \to 1) \) and there is no trapping \[5\]. For \( \beta = 0 \), we find that the distribution is uniform in the range zero to half. Thus \( \beta \) can be tuned from 0 (weak disorder) to 1 (strong disorder).

Equations \[1\] and \[2\] are readily solved employing generating function technique. We define

\[
G_{x,x+1}(z) = \sum_{n=0}^{+\infty} z^n \hat{G}_{x,x+1}(n) \tag{4}
\]

Upon the use of convolution theorem,

\[
G_{x-1,x+1}(z) = G_{x-1,x}(z) G_{x,x+1}(z) \tag{5}
\]

we get:

\[
G_{x,x+1}(z) = \frac{zp_x}{1 - \gamma z(1 - q_x - p_x) - q_x G_{x-1,x}(z)} \tag{6}
\]

for \( x \geq 1 \) and

\[
G_{0,1}(z) = \frac{zp_0}{1 - \gamma z(1 - p_0)} \tag{7}
\]

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

We are interested in the behaviour of the escape probability, namely the total probability for the first passage from \( x \) to \( x + 1 \). This is given by:

\[
\xi_x \equiv G_{x,x+1}(z = 1) = \sum_{n=0}^{+\infty} \hat{G}_{x,x+1}(n) \tag{8}
\]

Using eqns. \[3\] and \[4\] it is immediately seen that the escape probability satisfies the following one-dimensional recursion:

\[
\xi_x = \frac{p_x}{1 - \gamma(1 - q_x - p_x) - q_x \xi_{x-1}} \quad x \geq 1 \tag{9}
\]

with the initial condition

\[
\xi_0 = \frac{p_0}{1 - \gamma(1 - p_0)} \tag{10}
\]
Eq. (9) can be interpreted as a dynamical map for a fixed \( p \) and \( q \). In fact, since \( p \) and \( q \) are random, the evolution \( \xi_0 \to \xi_1 \to \cdots \to \xi_x \to \xi_{x+1} \to \cdots \) proceeds by random iteration over the maps parametrized by \( p \) and \( q \), which are chosen independently and randomly from the disorder distribution given by eq. (3) at each stage of iteration. This constitutes an iterated function system (IFS), see Barnsley \[14\].

It is immediately seen that when \( \gamma = 1 \), which corresponds to a lattice with no trapping eqns. (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 non-conserved case, for which \( \gamma \) is less than 1. For given values of \( q \) and \( p \) the fixed point of the map (9) is

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

and it is stable. It lies (see Fig 2) in the region delimited by \( \xi^* = 0 \) corresponding to \( p = 0 \), \( q > 0 \) (only left jumps) 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 \( \xi_x \) in such a way that the domain is the interval \([0,1]\). To this end we employ the standard rescaling:

\[
\frac{\xi - \xi_{\text{min}}}{\xi_{\text{Max}} - \xi_{\text{min}}} \to \xi
\]

We denote by \( \rho_i(\epsilon) \), the fraction of the total number of \( \xi \) values that belong to the \( i^{th} \) interval of size \( \epsilon = 1/N \). Then the partition function is given by,

\[
Z(Q, \epsilon) = \sum_{i=1}^{N} \rho_i^Q(\epsilon)
\]

(13)

where the sum is taken over non-empty intervals only. We make the following scaling ansatz,

\[
Z(Q, \epsilon) \propto \epsilon^{\tau(Q)}
\]

and obtain the scaling exponents \( \tau(Q) \) as:
\[ \tau(Q) = \lim_{\epsilon \to 0} \frac{\ln[Z(Q, \epsilon)]}{\ln \epsilon} \] (15)

Fig. 3 shows a log-log plot of \( Z(Q, \epsilon) \) versus \( \epsilon = 1/N \) for \( N \) ranging from 10 to \( 3 \times 10^6 \). The linearity of the curves establishes unambiguously the scaling ansatz (13). From the scaling exponents we calculate the generalized Renyi dimensions, given by \( D(Q) = \tau(Q)/(Q - 1) \).

Legendre transform of \( \tau(Q) \), defined as

\[ f(\alpha) = \alpha Q - \tau(Q) \] (16a)
\[ \alpha = \frac{d}{dQ} \tau(Q) \] (16b)

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

Fig. 4 depicts the scaling exponents \( \tau(Q) \). It is well defined and exhibits clear change in slope, establishing that the underlying measure is multifractal. Fig. 5 depicts the spectrum of Renyi dimensions \( D(Q) \) for various strengths of disorder\((\beta)\) and trapping\((\gamma)\). 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 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 uniform and 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 \( \beta \) 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 \( f - \alpha \) 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
It has already been shown analytically that even in the absence of trapping, the system exhibits anomalous diffusion when the disorder is strong ($\beta \to 1$). However when the disorder is weak, the anomaly in the diffusion process disappears. On the other hand, our finding is that when the disorder is strong, for arbitrary trapping rate, (so long it is non zero), the escape probability exhibits multifractal fluctuations. However, when the disorder becomes weak ($\beta \to 0$), the multifractal features disappear. More studies with different disorder models are required to shed more light on the issues raised here. We hope this work would spur some activities along these directions. In any case we believe, it would worth the effort to investigate the intriguing connection between anomalous diffusion and fractal fluctuations in random and trapping environments.

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FIGURES

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 $\gamma \in [0,1]$.

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.

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

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

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

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

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