Diffusion on One-Dimensional Multifractals

by

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Abstract

Many geophysical and atmospheric fields exhibit multifractal characteristics over wide ranges of scale. These findings motivate a study of transport phenomena in multifractal media, particularly diffusion. In studying the diffusion properties of one-dimensional universal multifractal resistivity fields, a relation for the diffusion exponent d_w is derived and is found to depend only on $K(-1)$, the value of the moment scaling function $K(q)$ of the resistivity field for the $q=-1^{th}$ order statistical moment. This relation is subsequently verified through Monte Carlo simulations of diffusion on these systems. The one-to-one correspondance that exists between statistical moments and orders of singularity suggests that one order of singularity, namely γ_{-1}, is of special importance to diffusion on multifractals, as is confirmed by simulations performed using fields that have been thresholded. Although convergence is quite slow, in the limit of an infinitely large range of scales a dynamical phase transition occurs about this particular singularity. The relation derived for the diffusion exponent breaks down for those multifractals where the $q=-1^{th}$ order moment diverges, which is typical of a multifractal phase transition. In these cases d_w must be estimated by taking into account the sample size.

Résumé

Plusieurs champs atmosphériques et géophysiques possèdent des caractéristiques multifractales valides sur de très grandes gammes d'échelles. Ces faits motivent l'étude des phénomènes de transport dans des milieux multifractals, particulièrement la diffusion. Dans l'étude des propriétés de diffusion de champs de résistivité multifractals uni-dimensionels, une relation est dérivée pour l'exposant de diffusivité d_w. Il appert que cette relation ne dépend que de $K(-1)$, la valeur de la fonction du moment d'échelle $K(q)$ du champ de résistivité pour l'ordre $q=-1$ du moment statistique. Cette relation est subséquemment vérifiée à partir de simulations Monte Carlo de diffusion sur de tels systèmes. Etant donné la correspondence un à un entre les moments statistiques et les ordres de singularité, un seul ordre de singularité, nommément γ_{-1}, est d'importance dans la diffusion sur des champs multifractals; ceci a été confirmé par des simulations sur des champs tronqués. Bien que la convergence ne soit pas rapide, dans la limite d'une gamme d'échelle tendant vers l'infini, une transition de phase dynamique apparaît près de cette singularité. La relation dérivée pour l'exposant de diffusion n'est plus valide pour les multifractals où le moment d'ordre $q=-1$ diverge, typique d'une transition de phase multifractale. Dans ces cas, d_w doit être estimé en tenant compte de la taille de l'échantillon.

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Chapter 1: Introduction

1.1 Motivation

Many disciplines of science are expressing great interest in the problem of diffusion in disordered media, a branch of the more general problem of transport phenomena. The reason that this interest is so widespread, reaching across areas such as geophysics and condensed matter physics as well as a host of others, is that most systems found in nature are disordered in some respect and as a result, transport on these systems cannot be described by classical diffusion laws. Instead, models are constructed in order to represent these systems and through theory and simulation the transport properties of these models are determined. If the models accurately describe real physical systems, then such studies provide insight into the transport that takes place in these systems and in particular may serve as starting points for the development of various types of prediction schemes (in the areas of groundwater flow and oil recovery, for example).

The area of study to which this work pertains is transport in extremely variable media. Many geophysical fields exhibit extreme variability (intermittency) over wide ranges of scale. This variability arises as a consequence of the nonlinear processes involved in the dynamics of these fields.

The important aspect of nonlinear variability is its scaling properties. A geometrical fractal set can be described by a single power law (a single fractal dimension). A multifractal field exhibits multiple scaling and its description generally requires an infinite number of exponents and hence fractal dimensions. Fields that are scale invariant are generally multiple scaling and can therefore be described by multifractals. As an example, recent empirical findings reveal the structure (pore space geometry) of porous rock to be multifractal (see, e.g., Hansen *et al.* [1988], Muller [1992], and Muller and McCauley [1992]).

The process of diffusion is the simplest transport mechanism of interest in random media. Although many other applications are likely, the original motivation for this study was to understand radiative transport in clouds (see, e.g., Lovejoy *et al.* [1990], Gabriel *et al.* [1990], Davis *et al.* [1990]). Over a wide range of scales, the optical density in clouds has a multifractal distribution; under certain conditions, diffusion is an approximation to radiative transfer in the thick cloud limit.

Geophysical multifractals are likely to belong to universality classes that can be characterized by two basic parameters (Schertzer and Lovejoy [1987]). In this study, diffusion is employed in order to investigate the transport properties of one-dimensional universal multifractals. A summary of the preliminary results of the study can be found in Silas *et al.* [1993]. Although many studies have been performed in order to understand diffusion on scaling binary systems (geometric fractals), very few have been performed in order to understand the same on multifractals. The only directly relevant studies of transport properties of multifractals, of which the author is aware, are those by Meakin [1987], which examined the properties of random walks on multifractals generated by discrete cascades in two dimensions, by Weissman and Havlin [1988], which explored diffusion on deterministic multifractals, and by Saucier [1992], which studied the effective transport properties of multifractal permeability fields using renormalization group methods.

1.2 Fractals and multifractals

A fractal is a geometric set of points that obeys the following power law:

$$N(\ell) \sim \ell^{-D_f}, \qquad (1.2.1)$$

where $N(\ell)$ is the number of boxes of size ℓ required to cover the set. A fractal set can therefore be characterized by a quantity D_f, which is independent of scale, termed the *fractal dimension* (generally non-integer). The fractal and its embedding space constitute a binary system.

A quantity more fundamental than the fractal dimension is the *fractal codimension*. The fractal codimension C_f of a particular fractal set is related to the probability of finding a point on the set; it is therefore related to the fraction of the space that is occupied by the set. The codimension is given by

$$C_f = D - D_f; \quad C_f \geq 0, \tag{1.2.2}$$

where D is the dimension of the embedding space and D_f is the fractal dimension of the set. Though the probability space of a stochastic process is infinite ($D \to \infty$), the codimension stays finite and constant.

A scaling field cannot be characterized by a single fractal dimension; when considering sets that exceed various thresholds (exceedence sets), one generally finds that the fractal dimension of the exceedence set decreases with increasing threshold levels. Such a multifractal field exhibits multiple scaling (or multiscaling) and in general must be described by an infinite number of fractal dimensions. In the codimension formalism (Schertzer and Lovejoy [1987]), a multifractal is described by an infinite number of power laws of the form:

$$\rho_\lambda \sim \lambda^\gamma \tag{1.2.3}$$

whose exponents γ are orders of singularity and constitute the singularity spectrum of the field. These orders of singularity indicate the intensity values of the density ρ_λ of the field, where λ is the scale ratio: the ratio of the largest scale of the system (taken to be unity) to the inner scale of homogeneity. The resolution of the field is the reciprocal of the scale ratio; as $\lambda \to \infty$ the resolution of the field becomes infinitely small.

1.2.1 Universal multifractals

The distribution of orders of singularity of a multifractal field is governed by the following probability distribution (Schertzer and Lovejoy [1987])

$$\Pr(\rho_\lambda \geq \lambda^\gamma) \sim \lambda^{-c(\gamma)} \tag{1.2.4}$$

where again λ is the scale ratio, ρ_λ is the value of the multifractal field at resolution $1/\lambda$, γ is the corresponding order of singularity and $c(\gamma)$ is the codimension function. The symbol '$\sim$' indicates equality to within constants and slowly varying factors. When

$c(\gamma) \le D$, where D is the dimension of the embedding space, the codimension has a geometrical interpretation since $D(\gamma) = D - c(\gamma)$ is the fractal dimension of those regions with singularity γ. The codimension of a particular order of singularity describes the probability with which this singularity is to be found on the field (see equation 1.2.4). A singularity is space filling if its codimension is zero. Although in general, $c(\gamma)$ need only be convex, Schertzer and Lovejoy [1987] have shown that due to the existence of stable, attractive generators of multifractal processes, physical multifractals are likely to belong to multifractal universality classes characterized by two basic parameters: α $(0 \le \alpha \le 2)$ and C_1 $(0 \le C_1 \le D$, where D is the dimension of space). The first of these parameters is the Lévy index α, which measures the *degree of multifractality* or the *deviation from monofractality* $(\alpha = 0)$ of the field. The second of these parameters, C_1, is the *codimension of the mean* order of singularity of the field and it describes the deviation of the mean of the process from homogeneity $(C_1 = 0)$. The universal form of the codimension function is

$$c(\gamma) = C_1\left[\frac{\gamma}{\alpha' C_1} + \frac{1}{\alpha}\right]^{\alpha'}, \quad \alpha \ne 1,$$

$$\frac{1}{\alpha} + \frac{1}{\alpha'} = 1, \tag{1.2.5}$$

$$c(\gamma) = C_1 \exp\left[\frac{\gamma}{C_1} - 1\right], \quad \alpha = 1.$$

Equation 1.2.5 describes conserved universal multifractals; nonconserved multifractals can be obtained via fractional integration and differentiation of order H (taken to be zero in what follows). Conserved universal multifractals can be separated into three main, qualitatively different, classes (figure 1.2.1): $\alpha = 2$, $1 < \alpha < 2$ and $0 \le \alpha \le 1$. The extremes of $\alpha = 2$ and $\alpha = 0$ correspond respectively to the lognormal multifractal and the (monofractal) β–model (Frisch *et al.* [1978]). One can see from this figure that lognormal multifractals display only one space filling singularity $\gamma = -C_1$, multifractals with $1 < \alpha < 2$ display infinitely many space filling singularities, the largest of which is $\gamma = C_1/(1-\alpha)$, and multifractals with $0 \le \alpha \le 1$ display no finite space filling singularities; here the singularities are bounded above by $\gamma = C_1/(1-\alpha)$.

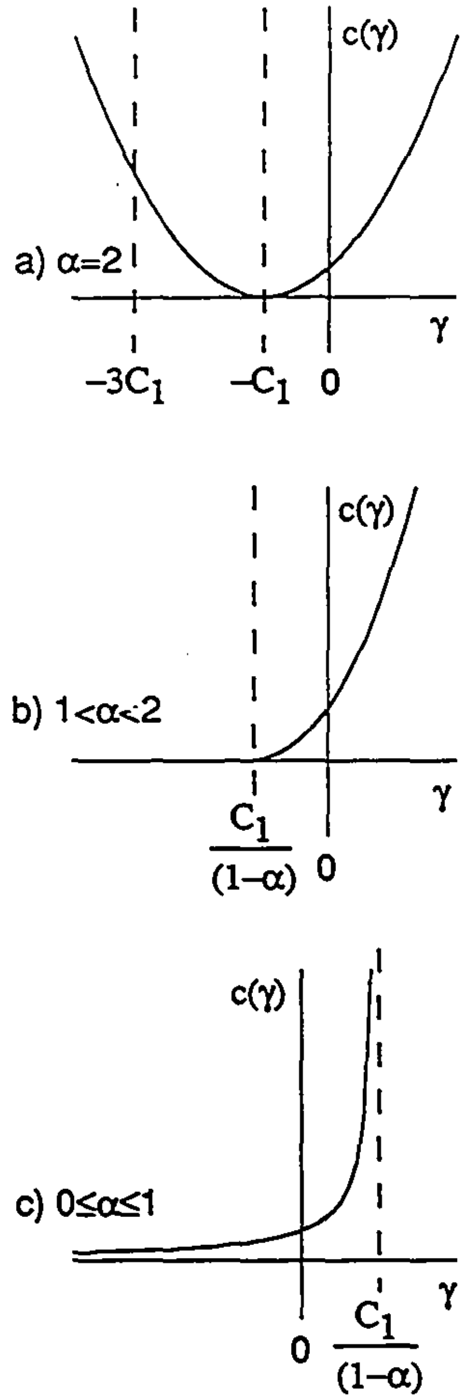

Figure 1.2.1. Codimension function $c(\gamma)$ for the qualitatively different classes of conserved universal multifractals: a) $\alpha = 2$: the lognormal case displays one space filling singularity $\gamma = -C_1$; b) $1 < \alpha < 2$: infinitely many space filling singularities exist, the largest of which is $\gamma = C_1/(1-\alpha)$; c) $0 \le \alpha \le 1$: no finite space filling singularities exist; singularities are bounded above by $\gamma = C_1/(1-\alpha)$.

Just as $c(\gamma)$ describes the multifractal probability distribution, the statistical moments of the multifractal field are described by the *moment scaling function* $K(q)$,

$$\langle \rho_\lambda{}^q \rangle = \lambda^{K(q)}, \tag{1.2.6}$$

where q is the order of the moment and the brackets indicate ensemble averaging. When $K(q)$ is nonlinear in q the moments of the field are said to be multiscaling; this is the signature of multifractality. $K(q)$ and $c(\gamma)$ are related via the Legendre transform (Parisi and Frisch [1985]),

$$\begin{gathered} K(q) = \max_{\gamma}(q\gamma - c(\gamma)) \\ c(\gamma) = \max_{q}(q\gamma - K(q)) \\ \left.\frac{dK(q)}{dq}\right|_{q=q_\gamma} = \gamma_q ; \quad \left.\frac{dc(\gamma)}{d\gamma}\right|_{\gamma=\gamma_q} = q_\gamma , \end{gathered} \tag{1.2.7}$$

where γ_q denotes the order of singularity that maximizes the expression for $K(q)$ and q_γ denotes the order of the moment that maximizes the expression for $c(\gamma)$. The universal form of the moment scaling function is (Schertzer and Lovejoy [1987])

$$\begin{gathered} K(q) = \frac{C_1}{\alpha - 1}\left(q^\alpha - q\right), \quad \alpha \neq 1 \\ K(q) = C_1 q \log q , \quad \alpha = 1 . \end{gathered} \tag{1.2.8}$$

For the β-model ($\alpha = 0$) and the lognormal multifractal ($\alpha = 2$) respectively, the form of the moment scaling function becomes $K(q) = C_1(q-1)$ and $K(q) = C_1 q(q-1)$.

The connection between the codimension formalism of Schertzer and Lovejoy and the dimension formalism (strange attractor notation) of Halsey *et al.* [1986] is as follows. The orders of singularity of the codimension formalism (γ) and of the strange attractor notation (α) are related via $\alpha = D - \gamma$, where D is the dimension of space; α here is not to be confused with the Lévy index α mentioned above. In the strange attractor notation the dimension function is $f(\alpha) = D - c(\gamma)$ and the scaling of the moments is described by $\tau(q) = (q-1)D - K(q)$.

1.2.2 Bare and dressed cascade properties

Universal multifractals can be obtained either via continuous cascade processes or via multiplicative "mixing" of cascade processes (Schertzer *et al.* [1991]). The *bare* quantities of a multifractal field are those that are generated from the cascade process that has proceeded only over a finite range of scales; these are the quantities that obey the equations for universal multifractals for all q and γ. The *dressed* quantities are those that result when the cascade is developed down to an infinitely small scale and the field is subsequently averaged (dressed) to a larger scale. Dressed quantities are indicated by the addition of the symbol ",d" in subscript; in other words, this symbol indicates a spatial average.

The scaling of the statistical moments and singularities of both the bare and the dressed fields are the same for $q < q_D$ and $\gamma < \gamma_D$ $(= K'(q_D))$. For $q \geq q_D$ $(\gamma \geq \gamma_D)$ the moments will diverge (Schertzer and Lovejoy [1987]):

$$\left\langle \left(\rho_{\lambda,d}\right)^q \right\rangle = \lambda^{K(q)} \to \infty \quad \text{for} \quad q \geq q_D. \qquad (1.2.9)$$

where

$$K(q_D) = D(q_D - 1) \qquad (1.2.10)$$

defines q_D and D is the dimension over which the dressing is performed. This bare/dressed distinction is a consequence of the singular behaviour of the multifractal field in the (small scale) limit $\lambda \to \infty$. Furthermore, for all universal multifractals save the lognormal case, all negative statistical moments will diverge for both the bare and the dressed fields. The divergence of moments problem gives rise to a first order multifractal phase transition (Schertzer and Lovejoy [1992], Schertzer and Lovejoy [1993]).

1.3 Random walks and diffusion laws

The numerical simulation of the process of diffusion can be accomplished through the use of random walks. The Monte Carlo method, introduced by Metropolis *et al.* in 1953, is employed in order to perform these random walks on the system of interest. The motion of a random walker in a one-dimensional system is governed by the following master equation:

$$\frac{dP(x,t)}{dt} = T(x+1 \to x)P(x+1,t) - T(x \to x+1)P(x,t) + T(x-1 \to x)P(x-1,t) - T(x \to x-1)P(x,t)\,, \tag{1.3.1}$$

where the T are transition rates for travel between neighbouring sites and $P(x,t)$ refers to the probability with which the walker can be found to be at site x of the system at time t.

The transition rates are related to the diffusive properties of the system; they determine the type of medium being studied. In a uniform system all the transition rates are identical; independent of the dimension, diffusion here is said to be *normal* and follows the *normal diffusion law*:

$$\overline{x^2} \sim t. \tag{1.3.2}$$

In other words, in a uniform system the mean square displacement is linear in time. The bar indicates an average over an ensemble of walkers on an individual realization of a particular system; brackets are reserved for averages taken over an ensemble of realizations.

In disordered media, whether the disorder be structural or physical, diffusion can no longer be described by the normal diffusion law; rather, diffusion becomes *anomalous* and follows the *anomalous diffusion law* (Gefen *et al.* [1983]):

$$\overline{x^2} \sim t^{2/d_w}. \tag{1.3.3}$$

The diffusion exponent d_w characterizes the rate of diffusion in a particular system; diffusion is normal for $d_w = 2$, anomalously slow for $d_w > 2$ and anomalously fast for $d_w < 2$.

1.4 Models of disordered systems

Many models of naturally disordered systems currently exist. In keeping with the theme of this study, the models reviewed here are some of those which seek specifically to reproduce the scaling properties observed in real systems. These and other important models of diffusion in disordered systems, although not relevant to this thesis, can be found in an excellent review article by Havlin and Ben-Avraham [1987].

1.4.1 Fractal models

Anomalous diffusion has been investigated on deterministic fractals such as the Sierpinski gasket (e.g., Given and Mandelbrot [1983]) as well as on (loopless) fractal structures embedded in square lattices and Cayley trees (e.g., Havlin and Weissman [1986]). Expressions for the diffusion exponent in terms of the fractal dimension and other (usually electrical) properties of the substrate have been obtained.

Fractal media exhibit anomalous diffusion as a consequence of the nonuniformity of these binary structures. Diffusion on a fractal proceeds as follows. A random walker may "diffuse" on the fractal only and not in the space which embeds it (the "ant in the labyrinth" problem, de Gennes [1976]). This statement is equivalent to saying that the diffusion coefficient for points on the fractal is one, while that for points off the fractal is zero. In this case the word "nonuniformity" refers to the fact that the random walker cannot reach every point in the system. It must be stressed that this model can only represent binary scaling systems.

1.4.2 Percolation model

In the percolation model for disordered media (Stauffer and Aharony [1992]), sites of a regular lattice are randomly occupied with a probability p. Clusters are formed of nearest-neighbouring occupied sites. At a critical concentration $p = p_c$ an infinite "percolating" cluster appears. The percolation model exhibits anomalously slow diffusion over the entire range of scales *at criticality only*, when the incipient infinite percolation cluster demonstrates fractal characteristics; in fact, this cluster is a random fractal. Because this is so, the incipient percolating cluster can be modeled by an infinite deterministic fractal that is characterized by the same fractal dimension and the same electrical properties.

The slowing of the diffusion process at criticality is due to the dead ends and the bottlenecks and other obstacles of the percolating cluster. Again this system is binary; walkers may move only to occupied sites yet every nearest neighbouring occupied site is assigned the same transition probability. The percolation model therefore is fundamentally geometric.

The incipient infinite percolation cluster does however exhibit some multifractal characteristics. When a unit voltage is applied across a percolating random resistor network, where network bonds are of unit resistance, the moments of the voltage drop distribution are found to be multiscaling (Coniglio [1986]), as are the moments of the current distribution (Fourcade *et al.* [1988], Fourcade and Tremblay [1987]).

1.4.3 Hierarchical structures and (non-universal) multifractals

Hierarchical models of one-dimensional disordered systems are comb-like structures; the "teeth" or potential barriers are meant to act as delays for the transport in these systems. The barriers are distributed in a hierarchical fashion and the transition rates, which satisfy equation 1.3.1, are inversely proportional to the barrier heights and are given by (Havlin and Weissman [1986]):

$$T(x \to x \pm 1) = R^{\ell} . \tag{1.4.1}$$

The x are the sites of the system and the ℓ satisfy the following:

$$x(\mathrm{mod}\, 2^{\ell}) = 2^{\ell-1} . \tag{1.4.2}$$

In other words, the structures are deterministic multifractals where the central point plays a special role. Havlin and Weissman [1986], for example, investigate transport on these hierarchical structures; they find a transition from anomalous diffusion (when $R \leq 1/2$) to normal diffusion (when $R > 1/2$). There is no randomness in this model; it was constructed with the use of a recursive relation. Furthermore, studies of hierarchical structures do not seem to take into account different possible origins for walks that take place in these systems. It will be shown that the lack of even approximate translation invariance in these structures gives them special properties; when starting the particles in the central position, diffusion properties of such systems are quite different from those that result from statistically homogeneous multifractals with particles starting from random origins.

A numerical study of the properties of random walks on two-dimensional discrete non-universal multifractals using Monte Carlo methods was performed by Meakin [1987]. Meakin examined random walks on square lattices (1024X1024) with multifractal distributions of transition rates. These (random) multifractals were obtained via a cascade process; different parameters used in the construction of the cascades resulted in the different multifractal fields that were studied. On every realization of a particular field, 100 walks of 100,000 steps each were performed. The origins of the walks were chosen at random. Six hundred realizations were performed for each of the different multifractal fields. Various statistical exponents were measured and probabilities of return investigated. Diffusion upon these multifractals was found to be anomalously slow (subdiffusion).

Weissman and Havlin [1988] derive a result for diffusion on multifractals that contradicts Meakin's findings. The result states that anomalous diffusion occurs only on multifractals with discrete $c(\gamma)$ spectra. They further apply this result to investigate diffusion on both the hierarchical model and a deterministic multifractal field (both one-dimensional). As before, diffusion on the hierarchical structure leads to a transition in the diffusion exponent indicating that at the critical point, diffusion is no longer anomalous but becomes normal.

Weissman and Havlin conclude that diffusion is normal on normalized multifractals and that subsequently the problem is not an interesting one. They found diffusion to be anomalous only for non-normalized multifractals. Their result can be seen to hold only when averaging over random walkers that all share a common origin; once this averaging is performed over different starting positions, which for the multifractals of interest here are all statistically equivalent, a quite different (anomalous) result is obtained. Unfortunately, interest in the topic of diffusion on multifractals seems to have dwindled following this article.

1.4.4 A universal multifractal model

In the last section some fractal models and the percolation model were discussed; these are scaling systems (the percolation model is scaling at criticality). However, these systems can be described by geometric sets; the diffusion coefficient for these models can only take on one of two values (the systems are binary). The problem of diffusion on scaling fields is of a more general nature. The hierarchical model and the (non-universal) multifractal model, both also discussed in the last section, have as their diffusion coefficient scaling fields rather than scaling sets; the diffusion coefficient is therefore no longer limited to two values. Most systems encountered in nature consist of a continuum of intensity values; when multiscaling, such systems can be modeled using universal multifractals. This study constitutes the first effort made to understand diffusion on universal multifractals.

Chapter 2: Diffusion on a multifractal

2.1 Diffusion on a one-dimensional disordered system

Consider the motion of a number of particles in a one-dimensional n-site system, which is possibly disordered. The average particle concentration is denoted by $J(x,t)$ and the particle flux by $F(x,t)$. Fick's law describes the relationship between the flux of particles and the concentration gradient (Pathria [1972:454-455]),

$$F(x,t) = -D(x)\frac{\partial}{\partial x}J(x,t), \tag{2.1.1}$$

where the spatially dependent coefficient of diffusion $D(x)$ describes any disorder that is characteristic of the medium. The equation of continuity expresses the conservation of the number of particles in the system:

$$\frac{\partial}{\partial t}J(x,t) + \nabla \cdot F(x,t) = 0. \tag{2.1.2}$$

Substituting equation 2.1.1 into equation 2.1.2 yields the one-dimensional diffusion equation:

$$\frac{\partial J(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[D(x)\frac{\partial J(x,t)}{\partial x}\right]. \tag{2.1.3}$$

If the total number of particles contained in the system is denoted by N, the particle concentration can be expressed as

$$J(x,t) = NP(x,t) \tag{2.1.4}$$

where $P(x,t)$ is the probability density. The total number of particles in the system remains constant; hence the diffusion equation can equivalently be written as

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[D(x) \frac{\partial P(x,t)}{\partial x} \right]. \tag{2.1.5}$$

The diffusion equation can only be solved analytically in special instances of systems with a simple $D(x)$; this is not the case in this study where $D(x)$ is a random function.

2.2 The numerical simulation of diffusion on a one-dimensional disordered system

Random walks can be employed in order to model the process of diffusion in a particular system (Chandrasekhar [1943]). The motion of a random walker in the system defined by $D(x)$ can be described by the *master equation* for diffusion in this medium; this master equation is a discretization of the diffusion equation. In a one-dimensional system a particle (or random walker) has the option of proceeding in one of two directions; the master equation that governs the motion of this particle is (from section 1.3):

$$\begin{aligned} \frac{dP(x,t)}{dt} = {} & T(x+1 \to x)P(x+1,t) - T(x \to x+1)P(x,t) \\ & + T(x-1 \to x)P(x-1,t) - T(x \to x-1)P(x,t), \end{aligned} \tag{1.3.1}$$

where the T are transition rates and $P(x,t)$ now refers to the probability with which the walker can be found to be at site x of the system at time t. Equation 1.3.1 is also called the continuous time random walk equation (Zwanzig [1982]). The relationship between the transition rates T and the coefficients of diffusion D is obtained following a method outlined in Aziz and Settari [1979:83-84].

Consider the one-dimensional n-site system displayed in figure 2.2.1 where periodic boundary conditions have been imposed. Note that this system is ergodic; any site can be reached from any other site, no matter whether a particular move can be realized in one step or that several steps are required. In other words, there is no absolute "trapping" possible. It is clear that the probability for a particle to proceed in a single step to a site that

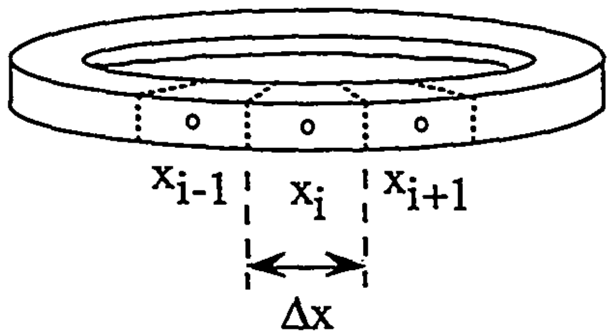

Figure 2.2.1. A one-dimensional n-site system with periodic boundary conditions. To every site x a diffusion coefficient $D(x)$ and particle concentration J_x are assigned (after Aziz and Settari [1979]).

is not its nearest neighbour is zero. This is also the case for a particle wishing to stay still; particles are forced to move at every step of the process: $T(x \rightarrow x) = 0$.

Sites of the system are equally separated by a distance Δx and to each site x a diffusion coefficient $D(x)$ and particle concentration J_x are assigned. Over a region of size on the order of the scale length Δx, each of the diffusion coefficients will be uniform (hence this scale is called the inner scale of homogeneity). Between two such regions one can imagine an interface, located for simplicity midway between the two sites of interest, that is characterized by a discontinuity in the diffusion coefficient. To determine the proper transition rates for travel between sites, consider a discretized version of Fick's law (equation 2.1.1). The flow of particles from site x_i to the interface is given by

$$F_{i \rightarrow \text{int}} = -D(x_i)\frac{[J_{\text{int}} - J_i]}{\Delta x/2} \tag{2.2.1}$$

where $\Delta x/2$ is the distance between the site and the interface and J_{int} is the (unknown) concentration of particles at the interface. Similarly the flux from the interface to site x_{i+1} is

$$F_{\text{int} \rightarrow i+1} = -D(x_{i+1})\frac{[J_{i+1} - J_{\text{int}}]}{\Delta x/2}. \tag{2.2.2}$$

The flow of particles on either side of the interface must be the same, i.e., equal to the flow of particles across the interface and between sites x_i and x_{i+1}:

$$F_{i \rightarrow \text{int}} = F_{\text{int} \rightarrow i+1} = F_{i \rightarrow i+1}. \tag{2.2.3}$$

An explicit relation for $F_{i \rightarrow i+1}$,

$$F_{i \rightarrow i+1} = -\sigma(x_i; x_{i+1})\frac{[J_{i+1} - J_i]}{\Delta x}, \tag{2.2.4}$$

requires the definition of a transmission coefficient $\sigma(x_i; x_{i+1})$, which effectively describes the *conductance* (or some quantity proportional to it) between sites x_i and x_{i+1}. Equations 2.2.1 to 2.2.4 can be used to solve for $\sigma(x_i; x_{i+1})$. Using equations 2.2.1 and 2.2.2

respectively, expressions for J_i and J_{i+1} can be substituted into this last relation (equation 2.2.4):

$$F_{i\to i+1} = \frac{-\sigma(x_i;x_{i+1})}{\Delta x}\left[\left(\frac{-F_{\mathrm{int}\to i+1}}{D(x_{i+1})}\frac{\Delta x}{2} + J_{\mathrm{int}}\right) - \left(\frac{F_{i\to \mathrm{int}}}{D(x_i)}\frac{\Delta x}{2} + J_{\mathrm{int}}\right)\right]. \quad (2.2.5)$$

The interfacial particle concentration J_{int} is cancelled out; using equation 2.2.3 to eliminate the fluxes and then solving for $\sigma(x_i;x_{i+1})$ yields the following:

$$\sigma(x_i;x_{i+1}) = \frac{2D(x_i)D(x_{i+1})}{D(x_i)+D(x_{i+1})}. \quad (2.2.6)$$

Therefore the "conductance" between two adjacent sites is simply the harmonic mean of their individual coefficients of diffusion. The transition rates are then obtained by normalizing the transmission coefficients so that the probabilities, for a single particle, of proceeding to the left and right of a particular site add up to one. In other words the normalized transition rates for a particle at site x_i are

$$T(x_i \to x_{i+1}) = \frac{\sigma(x_i;x_{i+1})}{\sigma(x_i;x_{i+1})+\sigma(x_i;x_{i-1})}$$

$$T(x_i \to x_{i-1}) = \frac{\sigma(x_i;x_{i-1})}{\sigma(x_i;x_{i+1})+\sigma(x_i;x_{i-1})} \quad (2.2.7)$$

$$T(x_i \to x_{i+1}) + T(x_i \to x_{i-1}) = 1.$$

For systems of a dimension greater than one, equation 2.2.7 can be generalized to

$$T(x_i \to x_j) = \frac{\sigma(x_i;x_j)}{\sum_j \sigma(x_i;x_j)}$$

$$\sum_j T(x_i \to x_j) = 1. \quad (2.2.8)$$

These probabilities must be calculated for every site of the system.

Hence before every step taken on the diffusivity field, the random walker must make a choice that is weighted according to the values of the field at sites pertinent to the next move in the walk. Each step that the walker takes is dependent only upon the previous one.

Now that the proper transition rates have been determined, the Monte Carlo simulation may begin. The Monte Carlo method will lead to a determination of the moments of the position $\langle x^q \rangle$ as a function of time. These statistics must be gathered after many random walks have been performed on many different realizations of the diffusivity field.

2.3 Diffusion on a one-dimensional multifractal

In this study the medium is modeled using a one-dimensional multifractal density field $\rho_\lambda(x)$, where λ is the scale ratio. The coefficient of diffusion is taken to be its reciprocal since regions of high resistance to diffusion are likely to correspond to rare, dense (impenetrable) regions of the medium:

$$D_\lambda(x) = \frac{1}{\rho_\lambda(x)}. \qquad (2.3.1)$$

The diffusion approximation to radiative transfer, for example, involves taking $\rho_\lambda(x)$ to be proportional to the (multifractal) optical density and then taking its reciprocal to be the diffusion coefficient. In electrical conductivity problems, $\rho_\lambda(x)$ would be identified with the resistivity; regions of extremely large resistance (large singularities) are expected to be rare and regions of weaker resistance (smaller singularities) are expected to be more common.

Substituting equation 2.3.1 into Fick's law (equation 2.1.1) and noting that at the inner scale of homogeneity all (uniform) regions are the same length, it can be seen that the time it takes to diffuse across a region centred about a particular site is proportional to the value of the field at that site. Hence, in simulating diffusion on a multifractal, time is incremented in units of density; for each step that is taken by the walker, the time increment is determined by the value of the field at the new site.

Also note that, when subtituting equation 2.3.1 into equation 2.2.6, the expression for the transmission coefficients in terms of $\rho_\lambda(x)$ becomes

$$\sigma_\lambda(x_i;x_{i+1}) = \frac{2}{\rho_\lambda(x_i)+\rho_\lambda(x_{i+1})}. \tag{2.3.2}$$

The transition rates remain as in equation 2.2.8, only now using this last expression for the transition coefficients so that the tranport that occurs from site to site is directly related to the values of the density field.

Consider a single random walk performed on a single realization of a random medium. The long time, large distance properties of the walk can be derived analytically by taking Fourier and Laplace transforms of the master equation (equation 1.3.1). Subsequently, the following relation has been shown to hold (Machta [1981], Zwanzig [1982]):

$$\frac{1}{D} = \frac{t}{x^2} = \frac{1}{N_s}\sum_{i=1}^{N_s}\frac{1}{D_i}, \tag{2.3.3}$$

where N_s is the number of distinct sites visited by the random walker and the D_i are the diffusion coefficients associated with those sites. The random walker experiences an effective diffusion coefficient D for that particular walk that is equal to the harmonic mean of the D_i.

This equation will now be applied to a multifractal that has been developed over the range of scales Λ (smallest scale = Λ^{-1}). At some larger scale λ^{-1}, where the scale ratio λ is smaller than the ratio Λ (see figure 2.3.1), the effective diffusion coefficient in the j^{th} interval of length λ^{-1} is

$$D_{\lambda,j} = \left[\frac{\lambda}{\Lambda}\sum_{i=1}^{\lambda}\rho_{\Lambda,i}\right]^{-1} = (\rho_{\lambda,j,d})^{-1}, \tag{2.3.4}$$

where the sum is over all the $\rho_{\Lambda,i}$ for the $N_s = \lambda^{-1}/\Lambda^{-1}$ sites in the interval. The term $\rho_{\lambda,j,d}$ indicates a dressing of the ρ_Λ field: a spatial average of the field taken over the j^{th}

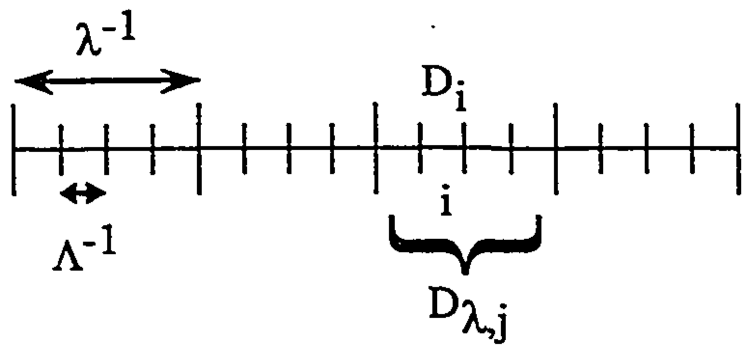

Figure 2.3.1 A one-dimensional multifractal diffusivity field that has been developed over the range of scales Λ. The D_i are the diffusion coefficients assigned to the each site i of the system at the smallest scale Λ^{-1}. The effective diffusion coefficient $D_{\lambda,j}$ that a walker experiences in the j^{th} region of size λ^{-1} $(\lambda < \Lambda)$ is the harmonic mean of all the D_i in that interval.

region of scale $1/\lambda \sim \overline{x^2}^{1/2}$. Therefore, for random walks over distances of $1/\lambda \sim \overline{x^2}^{1/2}$ whose origins are in the j^{th} interval, the corresponding time is estimated by:

$$t_j \sim \frac{D_{\lambda,j}}{x^2}. \qquad (2.3.5)$$

In the limit of longer and longer times, the scale λ^{-1} over which these walks take place is simultaneously increased and will eventually reach the size of the system in a finite time. Seeing that this is the case, one must use equation 2.3.4 for regions of a finite size and then average over all such regions of the field; this procedure further takes into account the diffusion of particles with random origins. Hence, averaging over all intervals of length λ^{-1} yields:

$$\overline{\overline{D}} = \frac{1}{\lambda}\sum_{j=1}^{\lambda} D_{\lambda,j} = \overline{\overline{(\rho_{\lambda,d})^{-1}}}; \qquad (2.3.6)$$

the double bar indicates a spatial average taken over all intervals of the field.

Two properties are now required. The first is the equivalence of the scaling of the bare and dressed moments; this will be true if $q < q_D$ (section 1.2.2) and if the bare moment exists. Here $q = -1$ and since $q_D > 0$, the only requirement for this moment to exist is for $K(-1)$ to be finite. This requirement will hold for most multifractals considered in the literature; however, it will *not* hold for universal multifractals with $\alpha < 2$. The second property required is the equivalence of spatial averaging over a single realization and ensemble averaging over many realizations. This will be true for $\alpha = 2$ and as long as the *sampling dimension* is large enough (see Schertzer and Lovejoy [1989]).

Applying these two assumptions yields:

$$\overline{\overline{(\rho_{\lambda,d})^{-1}}} = \left\langle (\rho_{\lambda,d})^{-1} \right\rangle = \left\langle \rho_\lambda^{-1} \right\rangle = \lambda^{K(-1)}. \qquad (2.3.7)$$

Hence from equations 2.3.6 and 2.3.7,

$$\overline{\overline{D}} = \overline{\overline{\left(\frac{\overline{x^2}}{t}\right)}} = \lambda^{K(-1)}, \qquad (2.3.8)$$

and since $1/\lambda = \overline{\left(x^2\right)}^{1/2}$ it follows that

$$\overline{\left(x^2\right)} \sim t^{2/[2+K(-1)]} \sim t^{2/d_w}; \tag{2.3.9}$$

therefore for diffusion on multifractals,

$$d_w = 2 + K(-1). \tag{2.3.10}$$

For multifractals with $\alpha < 2$, $K(-1) \to \infty$ (corresponding to a multifractal phase transition) and the above result breaks down. In these cases d_w can be estimated by taking into account the sample size (the number of realizations of the field); diffusion on these multifractals will be further investigated elsewhere.

To obtain the results for hierarchical systems and those cited by Weissman and Havlin [1988], the walkers are given a fixed origin and there is no averaging performed over different regions of the field. In this case,

$$\frac{1}{D_{\lambda,j}} = \rho_{\lambda,d} \tag{2.3.11}$$

is (generally) a random variable that depends on the starting point since

$$\rho_{\lambda,d} \sim \lambda^{\gamma_{\rho,d}}, \tag{2.3.12}$$

where $\gamma_{\rho,d}$ is the corresponding (dressed) order of singularity of ρ. Since $D_\lambda = 1/\rho_\lambda$,

$$\gamma_{D,d} = -\gamma_{\rho,d} \tag{2.3.13}$$

and therefore

$$\rho_{\lambda,d} = \frac{t}{x^2} = \lambda^{-\gamma_{D,d}} = \overline{x^2}^{\gamma_{D,d}/2} \tag{2.3.14}$$

so that

$$\overline{x^2} \sim t^{2/[2+\gamma_{D,d}]}. \qquad (2.3.15)$$

Hence when different particle origins are not considered, i.e., when there is no averaging over different intervals of the field

$$d_w = 2 + \gamma_{D,d}. \qquad (2.3.16)$$

The various results for the hierarchical model, as well as those of Weissman and Havlin [1988], correspond to $\gamma_{D,d} > 0$ (subdiffusion) and $\gamma_{D,d} = 0$ (normal diffusion). These results are therefore seen to be direct consequences of considering walks with special origins.

For lognormal universal multifractals, the form of the moment scaling function (equation 1.2.8) is $K(q) = C_1 q(q-1)$; therefore $K(-1) = 2C_1$ and hence from equation 2.3.10

$$d_w = 2 + 2C_1. \qquad (2.3.17)$$

Findings from the simulations that were performed for this study confirm that this indeed is the form of the diffusion exponent for lognormal multifractals. These results will be discussed in the next chapter.

From equation 2.3.10 it is seen that diffusion on (one-dimensional) lognormal multifractals is completely characterized by $K(-1)$. This indicates that only one moment (that of order $q=-1$), and hence only one singularity due to the one-to-one correspondance between moments and orders of singularity, is important for the diffusion process on these systems. The moments and the orders of singularity are related through the Legendre transform (equation 1.2.7); hence the significant order of singularity is $\gamma_{-1} = K'(-1)$. Taking the derivative of the moment scaling function for lognormal multifractals (see above) with respect to q and evaluating it at $q=-1$ yields for the corresponding order of singularity

$$\gamma_{-1} = -3C_1. \qquad (2.3.18)$$

Hence it is anticipated that this singularity will be of special importance to diffusion on lognormal multifractals; it is believed that there will be a dynamical phase transition about this singularity in the limit $\lambda \to \infty$. This last statement will be investigated in the chapter to follow as well.

Chapter 3: Simulation results

3.1 Scaling of the moments of random walks on one-dimensional multifractals

The steady state solution of the one-dimensional diffusion equation (equation 2.1.5) using equation 2.3.1 is

$$\frac{d}{dx}P_{\lambda}(x) = A\rho_{\lambda}(x), \qquad (3.1.1)$$

where A is a constant, which is determined by the boundary conditions. The derivative of the steady state concentration field $P_{\lambda}(x)$ is therefore proportional to the original multifractal density field $\rho_{\lambda}(x)$. Alternatively, $P_{\lambda}(x)$ is an integral of $\rho_{\lambda}(x)$. The integration of the density field is a smoothing operation; it has the effect of degrading the resolution to a larger scale, which does not change the multifractal character of the field. Hence the steady state probability density $P_{\lambda}(x)$ is a (nonconserved) multifractal, with the same α and C_1 as $\rho_{\lambda}(x)$.

Though the steady state probability density is multifractal, requiring in general an infinite number of exponents for its specification, the statistical moments $\overline{x^q}$ will scale with a single exponent (the bar indicates an average over an ensemble of walkers on an individual realization),

$$\overline{x^q} \sim t^{S(q)} \qquad (3.1.2)$$

where

$$S(q) = H_w q; \qquad (3.1.3)$$

$H_w = 1/d_w$ is called the *gap exponent* and for normal diffusion $H_w = 1/2$ (see, e.g., Havlin and Ben-Avraham [1987:711]). This monoscaling of the moments is a consequence of the fact that a random walk is a random *additive* process whereas multiscaling arises from *multiplicative* processes. The only singularity that determines the diffusion on lognormal multifractals is $\gamma_{-1} = -3C_1$ (corresponding to the $q = -1^{th}$ order moment; see section 2.3). The maximum and minimum orders of singularity that can exist on a single realization of a one-dimensional multifractal are such that $c(\gamma_{\max}) = c(\gamma_{\min}) = 1$. Using the universal form of the codimension function for lognormal ($\alpha = 2$) multifractals to solve for these singularities yields $\gamma_{\max} = -C_1 + 2\sqrt{C_1}$ and $\gamma_{\min} = -C_1 - 2\sqrt{C_1}$. The Legendre transform is employed to find the corresponding $q_{\max} = +1/\sqrt{C_1}$ and $q_{\min} = -1/\sqrt{C_1}$. Therefore $q_{\min} < -1$ as long as $C_1 < 1$, so that in this case the $q = -1^{th}$ order moment and hence the γ_{-1} singularity exists for every realization of a lognormal multifractal. Because this is so, averages taken over an ensemble of realizations of these multifractals are equivalent to averages taken over individual realizations: $< x^q > \equiv \overline{x^q}$.

Results from this study confirm that $S(q)$ is linear and hence that the moments of the walk are monofractal. The moments of the position as a function of time are

$$\langle x^q \rangle = \int x^q P(x,t)dx. \tag{3.1.4}$$

Equation 3.1.3 implies that $P(x,t)$ must be of the scaling form

$$P(x,t) \sim \frac{1}{t^{H_w}} \Pi\left(\frac{x}{t^{H_w}}\right). \tag{3.1.5}$$

Figure 3.1.1 displays a plot of $t^{H_w} P(x,t)$ versus x/t^{H_w} for diffusion (random walks) on a multifractal field with $\alpha = 2$, $C_1 = 0.2$ and $\lambda = 1024$. Each curve on this plot represents a different time in the walk. All of these curves collapse onto one, hence the scaling form of equation 3.1.5 holds here. Accordingly, though the steady state field is multiscaling (multifractal), the moments of the walk are indeed monoscaling.

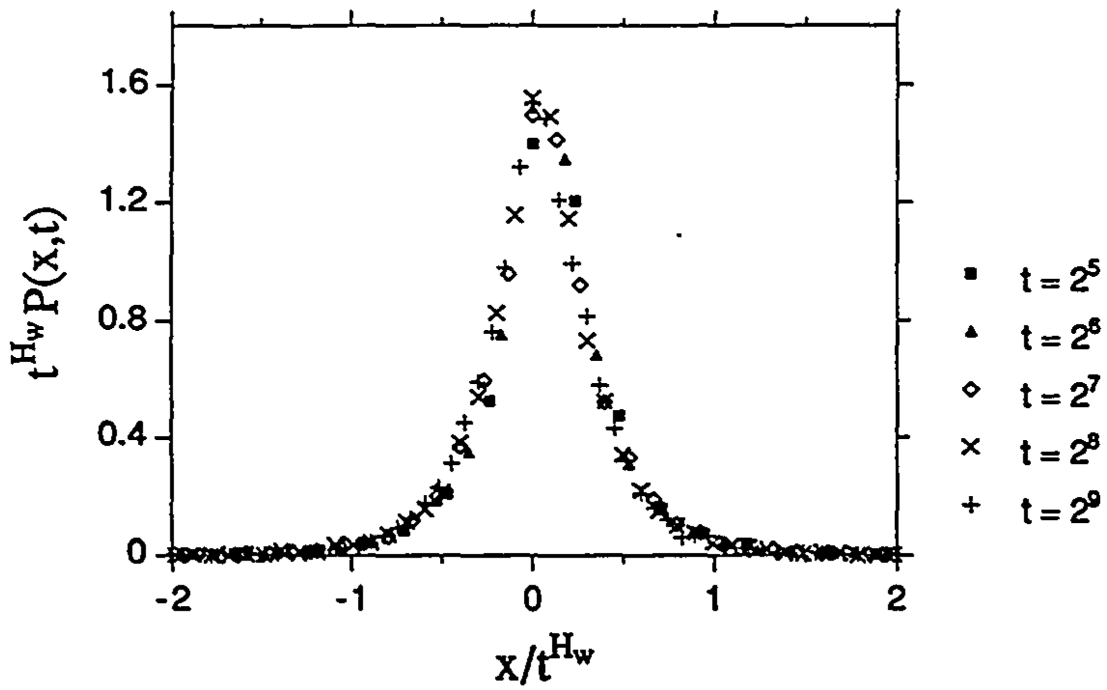

Figure 3.1.1. This plot displays that the scaling form of the probability density $P(x,t)$ for random walks on a one-dimensional multifractal (here using $\alpha = 2$, $C_1 = 0.2$ and $\lambda = 1024$) is $P(x,t) \sim 1/t^{H_w}\,\Pi(x/t^{H_w})$. Each set of data points represents a different time in the walks. The collapse of these curves onto one indicates that the moments of the walks are monoscaling (here $H_w = 0.4167$, see section 3.2).

3.2 Simulations

A typical one-dimensional continuous universal (Schertzer and Lovejoy [1987], Wilson *et al.* [1991], and Pecknold *et al.* [1993]) multifractal field is displayed in figure 3.2.1 with $\alpha = 2$, $C_1 = 0.2$ and $\lambda = 1024$. Consider a particle injected into the center of this field (periodic boundary conditions are imposed); this random walker follows the rules outlined in section 2.2 for random walking on a one-dimensional multifractal. After 121,810 steps the walker is still contained within the inset of figure 3.2.1. Figure 3.2.2 shows a blow-up of the inset with the trail of the walker superimposed upon it. It is clear from this figure that the diffusion is slowed due to the delaying of the walker between large values of the field (low diffusivity regions). The scaling exponent of the second order moment $S(2)$ for diffusion in this medium is determined from figure 3.2.3, which displays the scaling of the mean square distance with time. Statistics for 10,000 realizations of the field upon each of which 10 particles were made to walk for a time of 2^{10} units yield $S(2) \cong 0.837 \pm 0.002$. The scaling exponent and its error have been determined from a least squares fit to the straight line segment. The region of the plot that will be fitted is ascertained in the following manner. The finite size of the system introduces a systematic error into the problem that will be amplified for certain statistics. In particular, statistics for short walks as well as those for long walks will be unreliable. In the first case, the problem with the statistics derives itself from the discreteness of the field. The smallest length scale is the length of the pixel; within this distance the field is uniform. Over larger length scales the field is scaling and hence between these two régimes there will be a scale break in the statistics due to the break in the scaling of the system. In the second case, i.e., long walks approaching the size of the system (the largest scale), any random walkers that cross the boundary will be traveling distances larger than the outer scale of the scaling regime; these statistics will no longer be scaling either. The lengths of the walks performed on the multifractals studied here turn out to be much smaller than the size of the system (walk lenghts are limited by computer running time); hence only short walks must be avoided in the fit for the scaling exponent in order to minimize these finite size effects. The above result for $S(2)$ was found by making a fit between the limits of 2^5 and 2^{10} time units, which corresponded to walks covering about 1.2 to 5.1 percent of the system.

An explicit relation for the diffusion exponent d_w for lognormal multifractals was obtained in section 2.3. Since $d_w = 1/H_w = 2/S(2)$, this expression can be rewritten as

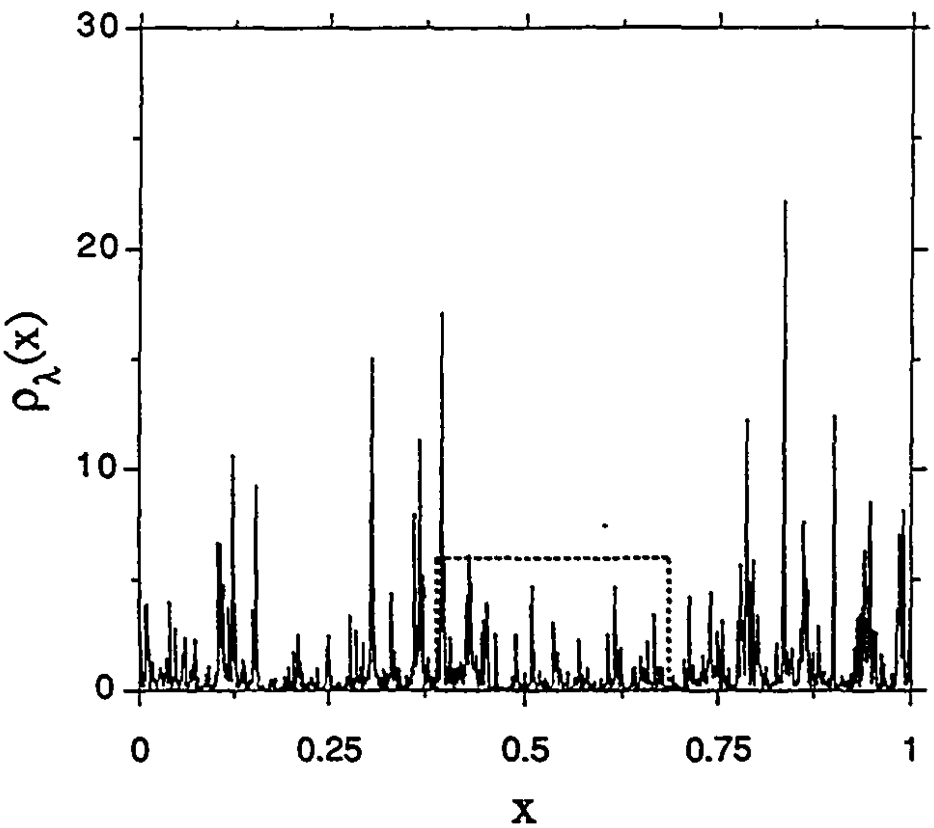

Figure 3.2.1. A one-dimensional multifractal field with $\alpha = 2$, $C_1 = 0.2$ and $\lambda = 1024$.

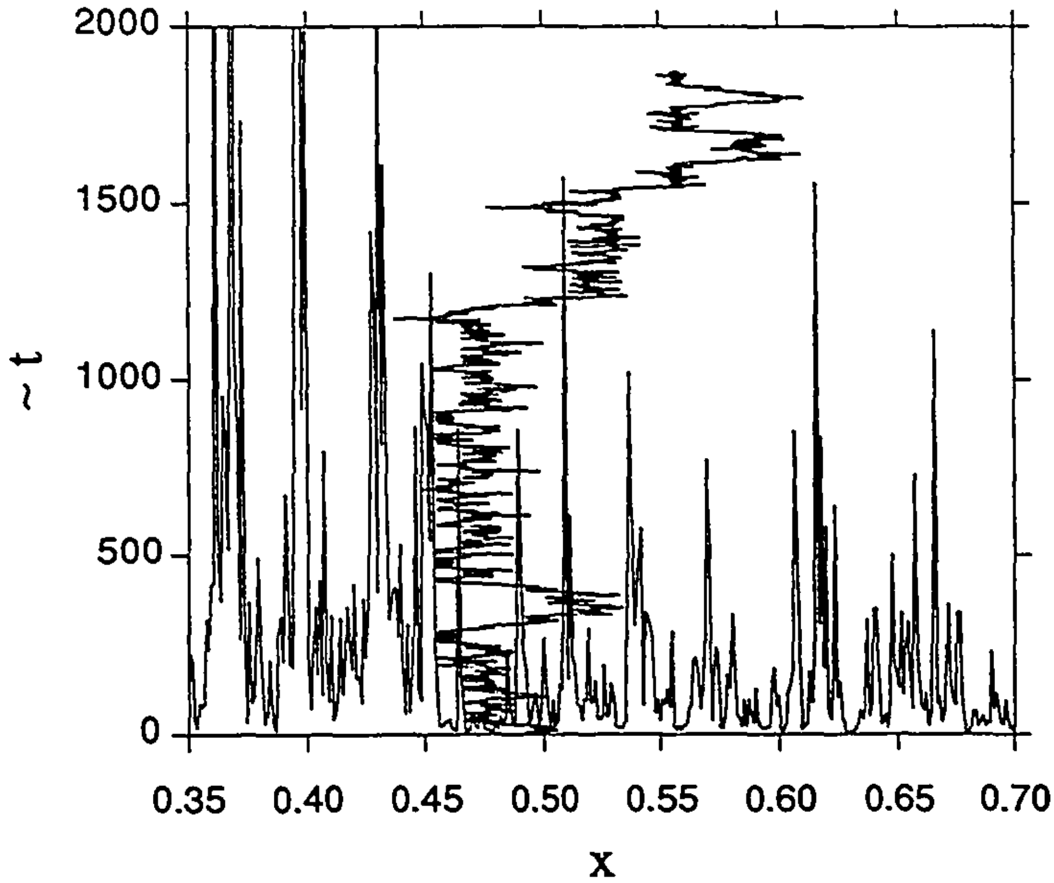

Figure 3.2.2. A random walk performed on a one-dimensional multifractal field with $\alpha = 2$, $C_1 = 0.2$ and $\lambda = 1024$. A superposition of the trail of the walk (121,080 steps taken) upon the region of the field explored by the walker (inset of Figure 3.2.1) is pictured here. The walker is delayed between large values of the field, hence a slow-down of the diffusion process.

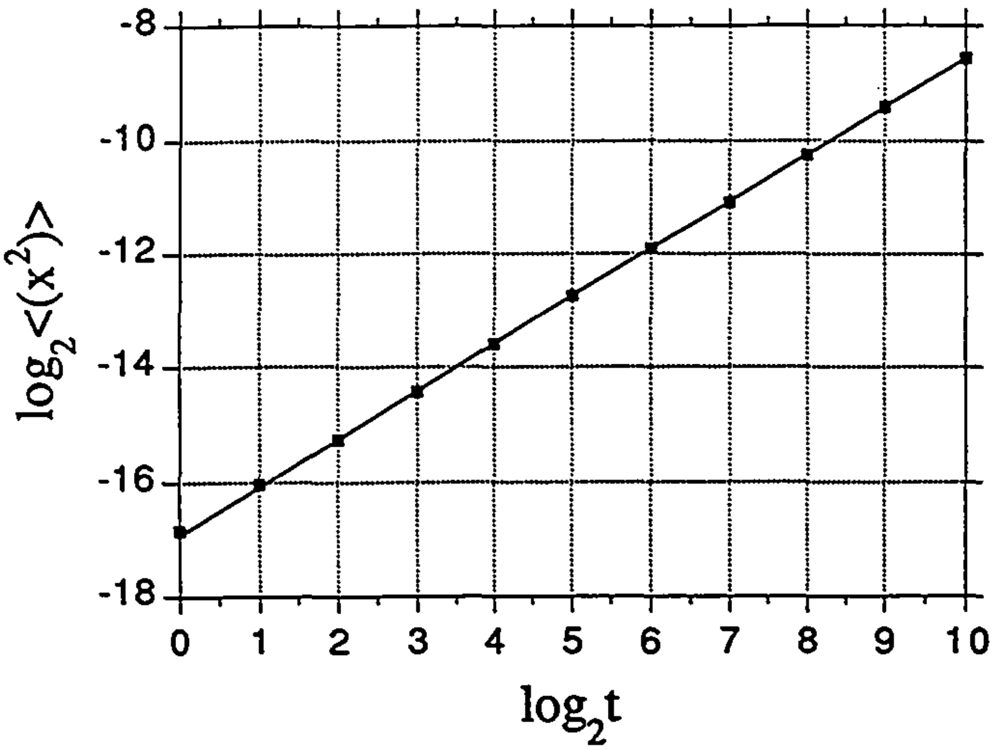

Figure 3.2.3. Determination of the scaling exponent $S(2)$ for the scaling of the mean square distance with time for diffusion on a one-dimensional multifractal with $\alpha = 2$, $C_1 = 0.2$ and $\lambda = 1024$. Here $S(2) = 0.837 \pm 0.002$.

$$S(2) = \frac{1}{1+C_1}. \tag{3.2.1}$$

Using this last relation, the scaling exponent of the second order moment for lognormal multifractals with $C_1 = 0.2$ is $S(2) = 0.833$. These last two results for $S(2)$ fall within 0.4% of each other.

Findings for the scaling exponent $S(2)$ confirm the subdiffusive behaviour of the random walkers as found by Meakin [1987]. Naturally, the variability of the field will differ depending on α and C_1 and subsequently $S(2)$ will vary as well; the diffusion will be slowed at different rates. For instance, the rate of diffusion decreases with increasing C_1; the further away the field from homogeneity, the harder it is for the walker to move about due to the increased chance that there will be delaying between large values of the field. Figure 3.2.4 shows the dependence of $S(2)$ on C_1 for lognormal multifractals. Here, the values for $S(2)$ that were obtained from the simulations were superimposed upon a plot of equation 3.2.1. This figure confirms the validity of equation 2.3.10 in describing diffusion on lognormal multifractals.

The monoscaling of the moments as found in section 3.1 is further illustrated by figure 3.2.5, a plot of the scaling exponents $S(q)$ versus the order of the moment q for these same random walks. The straight line, whose slope is the gap exponent, confirms the monofractal nature of the moments. Here $H_w = 0.412 \pm 0.002$ and this value differs by approximately one percent from the theoretical value of $H_w = 0.41\overline{6}$.

3.3 Thresholding

In section 2.3 it was argued that one singularity will dominate the diffusion process on a lognormal multifractal: that which determines the $q = -1^{th}$ moment of the ρ_λ field. The theoretical predictions were accurately verified in section 3.2. It is of some interest however to have a more direct confirmation of the role of the $\gamma_{-1} = -3C_1$ singularity. To this end, diffusion is studied using a series of thresholded fields. The threshold T is characterized by a threshold order of singularity γ_t such that

$$T = \lambda^{\gamma_t}, \tag{3.3.1}$$

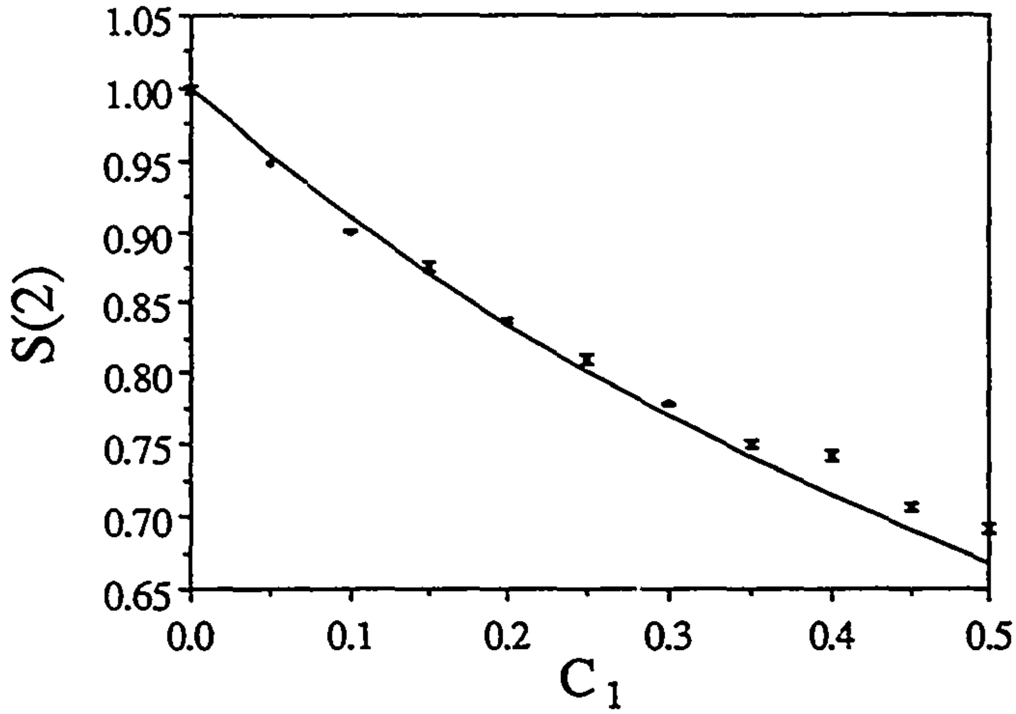

Figure 3.2.4. Dependence of the scaling exponent $S(2)$ of the second order moment of x ($<x^2> \sim t^{S(2)}$) on C_1, the codimension of the mean, for one-dimensional lognormal ($\alpha = 2$) multifractals. The solid line is a plot of equation 3.2.1. The superimposed data points were obtained from simulations.

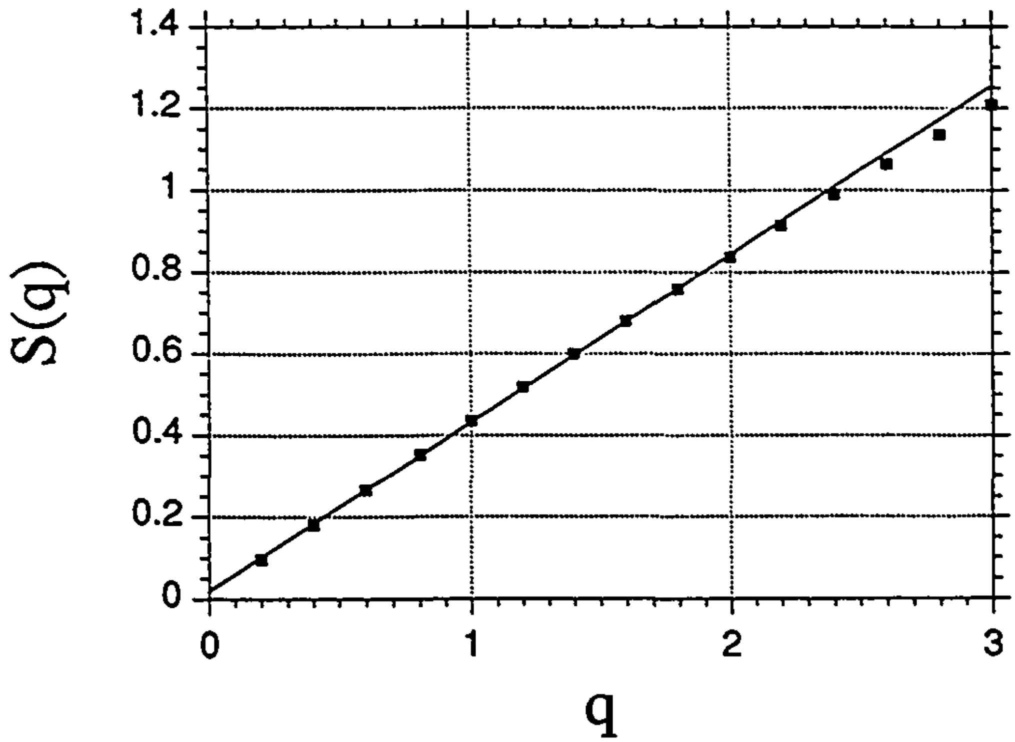

Figure 3.2.5. Scaling exponents $S(q)$ versus order of moment q. The straight line behaviour indicates that the moments $< x^q >$ can all be characterized by a single exponent H_w, where $S(q) = H_w q$. $H_w = 1/d_w$ is called the "gap exponent". Here $H_w = 0.412 \pm 0.002$.

where λ is the scale ratio. Thresholding is a scale breaking operation; therefore, an extremely wide range of scales may be necessary to yield the appropriate dressed behaviour of the fields.

To discover the effect of the various orders of singularity on the diffusion (in the limit of an infinitely large range of scales, $\lambda \to \infty$), the systematic elimination of the individual orders of singularity is performed in either of two ways. The thresholds may be imposed in such a way that the orders of singularity become bounded from above, i.e., singularities of the field are removed, one by one, starting with the largest and progressing to lower ones. Alternately, the orders of singularity may be bounded from below; this is the case when first imposing a threshold at the lowest order of singularity and then progressing to higher ones. Note that this thresholding is performed on each realization of the field and that each time a threshold is imposed the random walk process is repeated so that the statistics at these new thresholds may be monitored. Figure 3.3.1 clarifies the concepts of thresholding the field by bounding the singularities either from above or from below.

The actual thresholding procedure undertaken is the following. Consider the case where on each realization of the field the thresholding is such that the singularities are bounded from above. Once the first threshold has been determined and imposed, any region of the field with a value that exceeds it is assigned the threshold value. Clearly, for different threshold values of a particular field there will be different rates of diffusion and therefore the asymptotic régime, from which the scaling exponents are determined, will be attained at different times. For instance, eliminating large singularities from the field will cause the diffusion to be more rapid. Therefore each time a threshold is imposed and before the random walk process is repeated the field is normalized, for the sake of numerical simplicity, such that $\overline{\rho}_\lambda = 1$. Normalizing the field (multiplying it by a constant) does not affect the diffusion process; it merely shifts the timescale of the problem. Consider the one-dimensional diffusion equation (equation 2.1.5). Make the following change of variables:

$$\begin{aligned} D' &\to aD \\ \rho' &\to \tfrac{1}{a}\rho, \end{aligned} \tag{3.3.2}$$

where $a = <\rho_\lambda>$ is a constant. Substituting this into the diffusion equation one can see

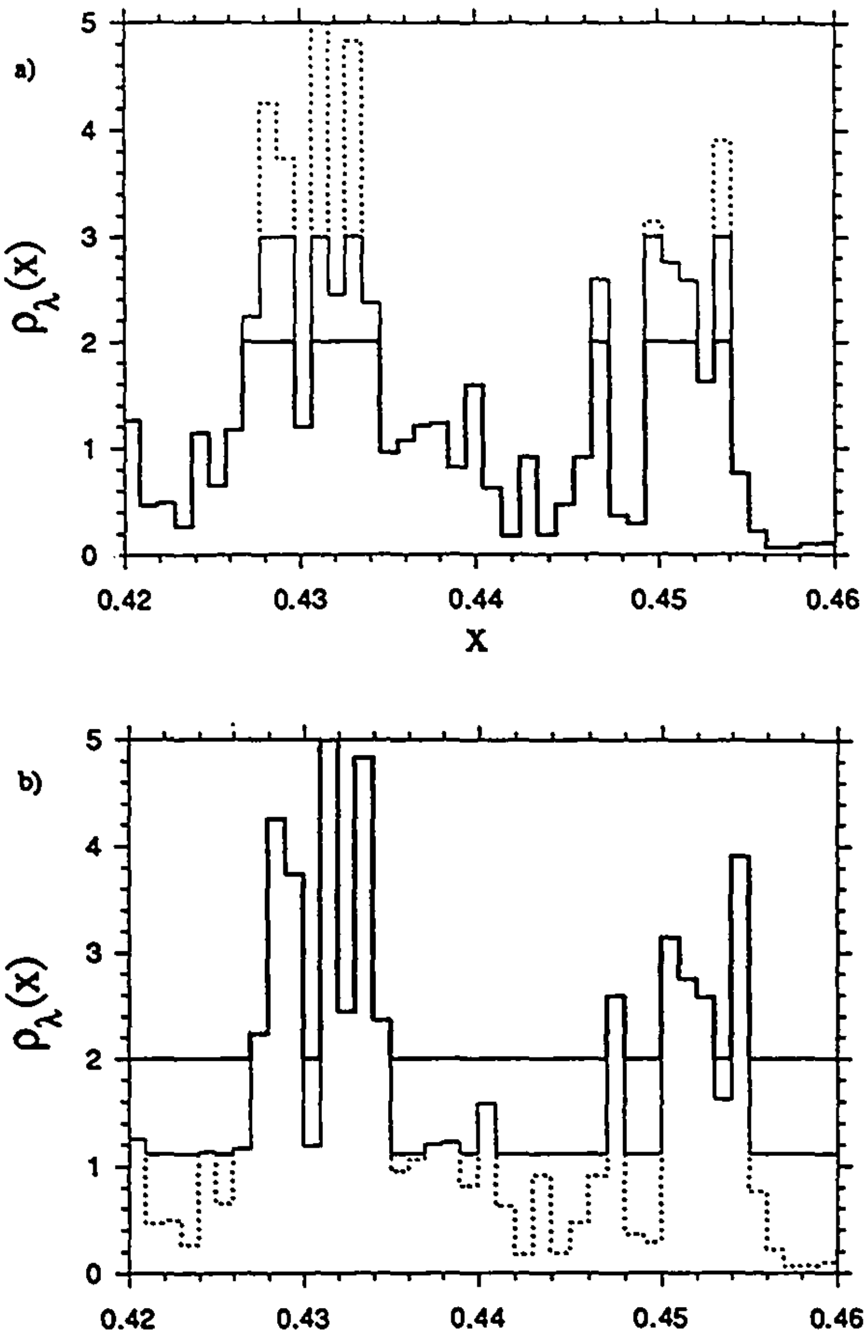

Figure 3.3.1. Thresholding: a) bounding the orders of singularity from above; b) bounding the orders of singularity from below.

that

$$t' = at. \tag{3.3.3}$$

Normalizing the field serves only to standardize the scaling region from which the scaling exponents, which describe the diffusion, are obtained.

In theory, the process of thresholding should not affect the multifractal parameters of the field. To elaborate, the codimension function $c(\gamma)$ is related to the probability of finding a particular singularity of the field to be of an order equal to or greater than γ, or rather, it is related to the probability that a particular singularity of the field will be found to belong to the *exceedence* set that is characterized by the order of singularity γ (see equation 1.2.4). When a threshold characterized by an order of singularity γ_t is imposed (still bounding from above), all singularities which have an order greater than γ_t are eliminated and hence the probability of finding any is zero; the largest order of singularity that will then exist for the field is γ_t. The exceedence set characterized by this same γ_t, however, remains unchanged (and so does $c(\gamma_t)$ and $c(\gamma)$ for $\gamma < \gamma_t$) since all the orders of singularity that were previously larger than γ_t are set equal to γ_t. This idea is illustrated in figure 3.3.2, which indicates how the bare codimension function changes for lognormal multifractals when the singularities are bounded (thresholded) from above. In practice however, thresholding is observed to be a scale breaking operation and therefore care must be taken when looking at the statistics of the new (dressed) field (Hooge [1993:67-70]).

A first glimpse of how this thresholding affects the statistics of the random walks is provided by figure 3.3.3. This graph displays several plots of the scaling of the mean square distance with time for walks that took place on a field with $\alpha = 2$, $C_1 = 0.2$ and $\lambda = 1024$; each plot represents the statistics for walks on the field when a particular threshold was imposed. Here again, the singularities were bounded from above. As the threshold was lowered the extreme singularities were eliminated; this facilitated transport throughout the field; hence the diffusion rates (the scaling exponents) increased.

In order to study more clearly the behaviour of the random walkers, the scaling exponent of the second moment S(2) was plotted as a function of the threshold singularity γ_t. The entire procedure was executed using both methods of thresholding for several different cases of α and C_1. For a given α and C_1, the results for $S(2, \gamma_t)$ that were obtained when the singularities of the field were bounded from above were sumperimposed

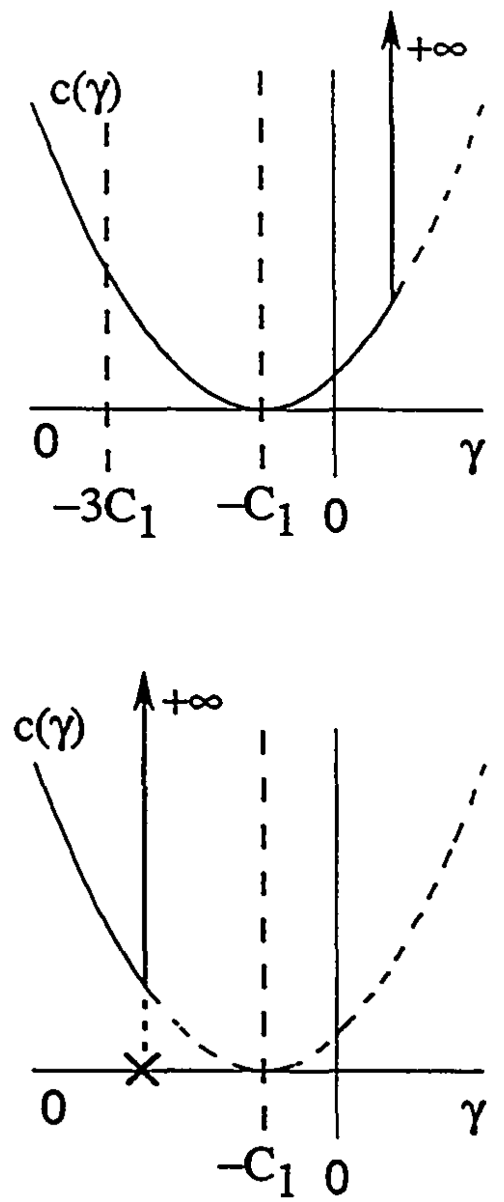

Figure 3.3.2. The effects of thresholding on $c(\gamma)$, the bare codimension function, for lognormal ($\alpha = 2$) multifractals when bounding the orders of singularity from above.

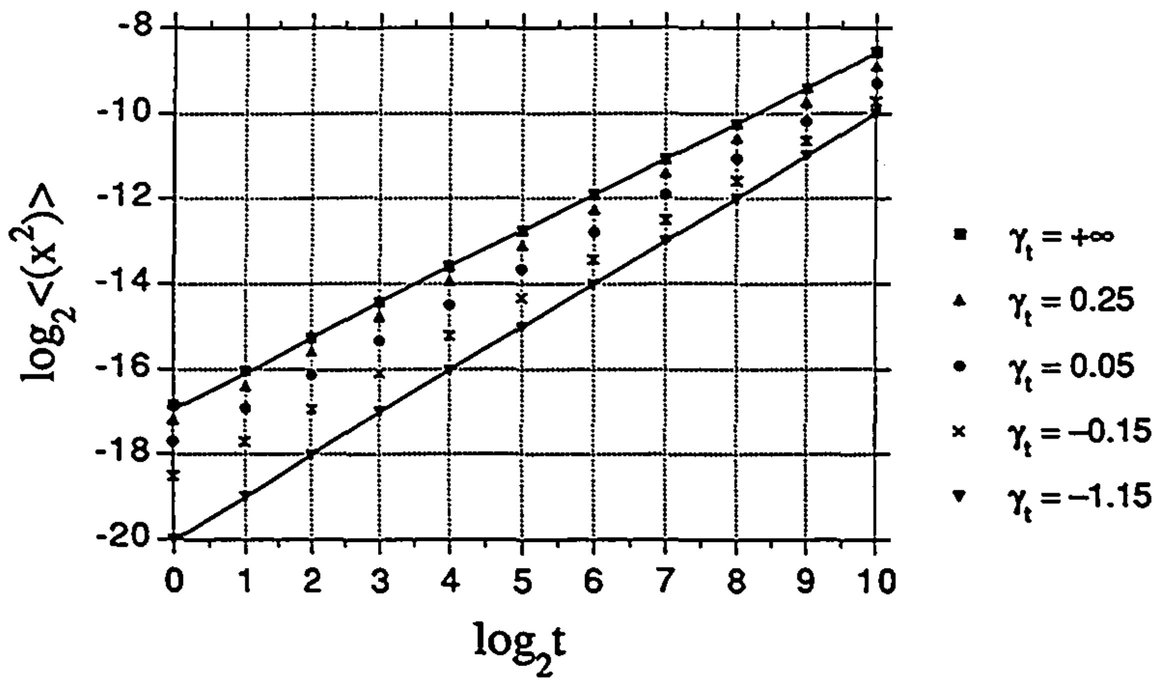

Figure 3.3.3. The effects of thresholding on the scaling of the mean square distance with time for diffusion on a one-dimensional multifractal with $\alpha = 2$, $C_1 = 0.2$ and $\lambda = 1024$, when bounding the orders of singularity from above. The scaling exponent $S(2)$ increases as the threshold T is lowered ($T \sim \lambda^{\gamma_t}$); when $\gamma_t = +\infty$, $S(2) = 0.837 \pm 0.002$ and when $\gamma_t = -1.15$, $S(2) = 1.0031 \pm 0.0007$.

with those obtained when the singularities were bounded from below. Figure 3.3.4 displays the two plots of $S(2,\gamma_t)$ versus the order of singularity γ_t, which characterizes the threshold, for random walks on a multifractal field with $\alpha=2$, $C_1=0.2$ and $\lambda=1024$. These plots indicate a *transition* from anomalous to normal diffusion; the transition region begins roughly about the anticipated order of singularity (see section 2.3), $\gamma_{-1}=-3C_1=-0.6$, and the transition itself is centred roughly about $\gamma=-0.2$. Toward the end of the thresholding process in both plots there occurs a slight fluctuation about $S(2)=1$, the value of the scaling exponent for normal diffusion. These statistical fluctuations could be reduced by allowing longer walks to take place; longer walks would provide more points for the scaling regime, from which the scaling exponent is determined. The transition that is observed in figure 3.3.4 appears smeared. Figure 3.3.5 demonstrates that the smearing is a finite size effect; for systems with smaller λ the transition region is broader and for systems which have larger λ the transition is clearly steeper. Furthermore, as λ is increased, the point at which the transition is centred moves steadily (although the motion is slight) toward smaller order singularities yet the transition region always seems to begin at $\gamma=-0.6$. Therefore, although the convergence is slow, it is plausible that in the limit $\lambda\rightarrow\infty$ there is a "dynamical phase transition" about $\gamma_{-1}=-3C_1$.

In section 2.3 it was found that the singularity $\gamma_{-1}=-3C_1$ must have some special significance for diffusion on one-dimensional lognormal multifractals. Thresholding essentially confirmed this hypothesis; findings indicate that in the limit $\lambda\rightarrow\infty$ the transition should occur about $\gamma_{-1}=-3C_1$. This effect was very slight however, as convergence is quite slow, and could only be made more evident by using an exceedingly large range of scales. It is stressed that although this procedure (thresholding) was used to verify the importance of this singularity, it is a scale breaking operation.

3.4 Extensions to higher dimensions

Meakin [1987] examined random walks on two types of *two-dimensional* random multifractals; they were each constructed using a cascade process characterized by four parameters (or probabilities): P_1, P_2, P_3 and P_4. The first multifractal studied, which he calls "type I", was constructed with $P_1=P_2=1$ and $P_3=P_4=R$. The second multifractal, "type II", was constructed with $P_1=1$, $P_2=R$, $P_3=R^2$ and $P_4=R^3$. Though equation 2.3.10 completely determines diffusion on *one-dimensional* lognormal

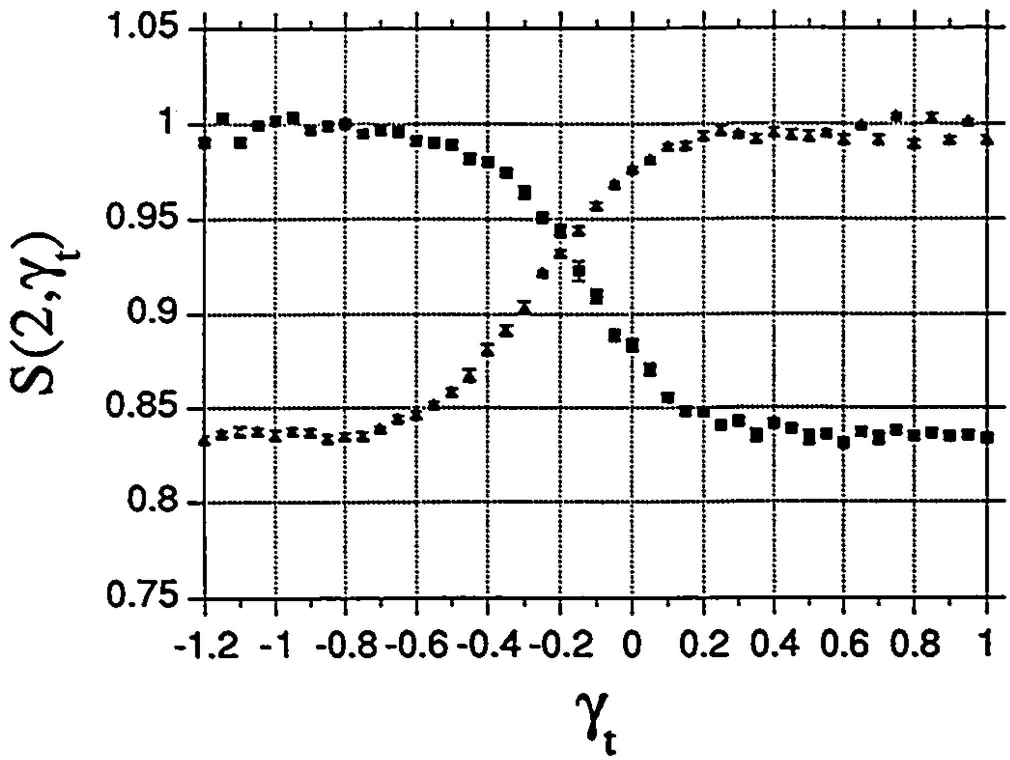

Figure 3.3.4. Scaling exponent $S(2)$ as a function of the order of singularity γ_t, which determines the threshold ($T \sim \lambda^{\gamma_t}$), for $\alpha = 2$, $C_1 = 0.2$ and $\lambda = 1024$. The squares indicate that thresholding began with the removal of the largest singularity and so on to the smaller ones; the triangles indicate that the process began with the removal of the smallest singularity and so on to the larger ones. A transition from anomalous to normal diffusion occurs about $\gamma = -0.2$; the transition region begins roughly about $\gamma = -3C_1 = -0.6$. The smearing of this transition is a finite size effect (see figure 3.3.5).

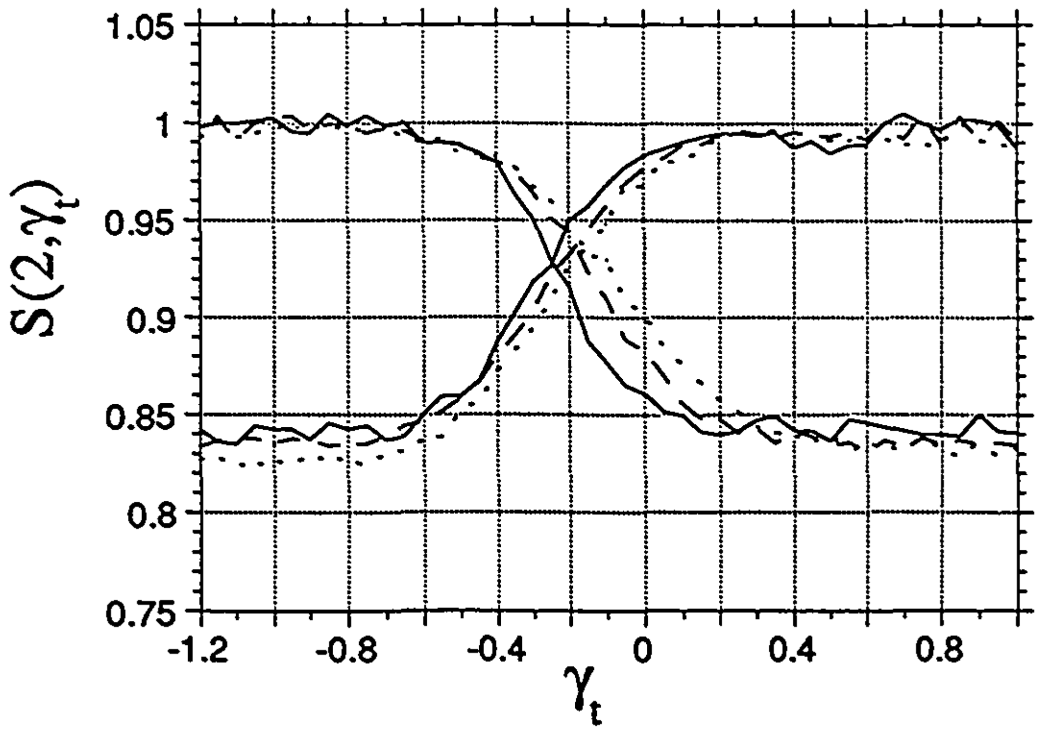

Figure 3.3.5. Scaling exponent $S(2)$ as a function of the order of singularity γ_t for $\alpha = 2$, $C_1 = 0.2$ and different values of λ. Here the transition is smeared most for $\lambda = 256$ (dotted lines) and is sharpest for $\lambda = 16384$ (solid lines); $\lambda = 1024$ (dashed lines) falls between. As λ is increased, the point at which the transition is centred moves steadily (although the motion is slight) toward smaller order singularities yet the transition region always begins at $\gamma = -3C_1 = -0.6$. Errors are on the order of 0.005.

multifractals, it is of interest to apply it to Meakin's multifractals for the sake of comparison. Table 3.4.1 compares these results with the higher dimensional results obtained by Meakin for the scaling exponent of the second moment $S(2) = 2/d_w$ for diffusion on both types of multifractals.

Some simulations of diffusion on higher dimensional lognormal multifractals have been performed by J. Tobochnik (private communication, 1992). The results from these simulations are given in table 3.4.2. The relation $d_w = 2 + K(-1)$ has been shown to hold for one-dimensional multifractals. From these tables one sees that the numbers are different in higher dimensional systems. Nevertheless, the trends are the same; furthermore Tobochnik's results show that increasing the dimension systematically lowers d_w. It is believed that diffusion, even on these higher dimensional multifractals, is dominated by one singularity.

	R	$S(2)$ 2-D (numerics, Meakin [1987])	$S(2)$ 1-D (theory: $S(2)=2/[2+K(-1)]$)
Type I	1/4	0.8641	0.7565
	1/8	0.7514	0.5988
	1/16	0.6447	0.4791
	1/32	0.5534	0.3930
	1/64	0.4926	0.3309
Type II	3/4	0.9694	0.9313
	1/2	0.8373	0.7108
	1/4	0.5830	0.4150
	1/8	0.4079	0.2708
	1/16	0.3008	0.1963

Table 3.4.1. Comparison of results found by Meakin [1987] for the scaling exponent $S(2)$ for two-dimensional multifractals with those from the one-dimensional theoretical $S(2)=2/[2+K(-1)]$ for the corresponding cases. The numbers are different but the trends are the same.

Dimension	Size of system	C_1	$S(2)$	$S(2)$ 1-D (theory: $S(2) = 1/[1 + C_1]$)
2-D	256X256	0.2	0.91	0.833
2-D	256X256	0.5	0.82	0.667
2-D	256X256	0.8	0.77	0.556
3-D	64X64X64	0.2	0.91	0.833
3-D	64X64X64	0.5	0.85	0.667

Table 3.4.2. Results of some simulations of diffusion on higher dimensional lognormal multifractals (J. Tobochnik, private communication, 1992).

Conclusion

A study of the transport properties of multifractals is motivated by findings that indicate that many geophysical and atmospheric fields are multifractal. Multifractals are found theoretically and empirically to belong to universality classes, which are characterized by two parameters (for conserved processes). This study established the first investigation of transport on universal multifractals by examining diffusion on one-dimensional lognormal multifractals.

In this study a multifractal served as the diffusion coefficient and hence the diffusion equation could not be solved analytically; diffusion is anomalous on disordered systems. Therefore, numerical simulations were employed in order to investigate diffusion on multifractal media. The transition rates that were appropriate for diffusion on a multifractal were determined in section 2.2. In section 2.3 a theoretical expression for the diffusion exponent for one-dimensional multifractals was derived: $d_w = 2 + K(-1)$, where $K(-1)$ is the value of the moment scaling function $K(q)$ for the $q = -1^{th}$ order moment. Due to the one-to-one correspondance between orders of singularity and statistical moments, it was further argued that one order of singularity would be of special importance to diffusion on these multifractals: $\gamma_{-1} = K'(-1)$ $(= -3C_1$ for lognormal multifractals).

Although the steady state concentration field was found to be multifractal, the moments of the walks were found to scale with a single (gap) exponent (section 3.1). Simulations of diffusion on one-dimensional lognormal multifractals confirmed this and showed also that the diffusion here was anomalously slow; the subdiffusion was a consequence of the delaying of the random walkers that resulted from the existence of regions of high resistance to flow. These simulations further proved the validity of the relation found in section 2.3, which provided a theoretical description of diffusion on lognormal multifractals. In order to verify that one singularity is particularly important to diffusion on lognormal multifractals, the studies were systematically duplicated for these fields when thresholds of different levels were imposed. Indeed, a transition from anomalous to normal diffusion was observed; although convergence is quite slow, in the limit $\lambda \rightarrow \infty$ a dynamical phase transition will occur at $\gamma_{-1} = -3C_1$.

Diffusion on universal multifractals was found to be much less trivial than formerly thought; previous results were explained in section 2.3 as special cases where no averaging over different particle origins took place. While transport on one-dimensional lognormal universal multifractals is completely determined by equation 2.3.10, this result breaks down for multifractals with $\alpha < 2$ since here $K(-1) \rightarrow \infty$ (indicating a multifractal phase transition); it is still believed in these cases that one order of singularity dominates the diffusion process. The general features of these cases must therefore be deduced; this is to be undertaken in future studies. Future studies will also concentrate on the problem of diffusion on higher dimensional universal multifractals.

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