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Heterogeneous diffusion in comb and fractal grid structures

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ABSTRACT

We give exact analytical results for diffusion with a power-law position dependent diffusion coefficient along the main channel (backbone) on a comb and grid comb structures. For the mean square displacement along the backbone of the comb we obtain behavior $\langle x^2(t)\rangle \sim t^{1/(2-\alpha)}$, where α is the power-law exponent of the position dependent diffusion coefficient $D(x) \sim |x|^{\alpha}$. Depending on the value of α we observe different regimes, from anomalous subdiffusion, superdiffusion, and hyperdiffusion. For the case of the fractal grid we observe the mean square displacement, which depends on the fractal dimension of the structure of the backbones, i.e., $\langle x^2(t)\rangle \sim t^{(1+\nu)/(2-\alpha)}$, where $0 < \nu < 1$ is the fractal dimension of the backbones structure. The reduced probability distribution functions for both cases are obtained by help of the Fox *H*-functions.

1. Introduction

In many physical systems, such as transport in inhomogeneous media and plasmas [1], and diffusion on random fractals [2], the diffusion coefficient is not a constant but depends on the particle position, like in turbulent diffusion [3,4], including turbulent two-particle diffusion [5]. The heterogeneous diffusion equation has been investigated within the continuous time random walk (CTRW) theory in [6–8], and the mean first passage time of such systems was analyzed in [9]. Lévy processes in inhomogeneous media [10] and ergodicity breaking in heterogeneous diffusion processes [11] including isothermal Langevin dynamics with spatially dependent friction [12] have been investigated, as well as the influence of external potentials on heterogeneous diffusion processes was recently considered in [13]. Time and power-law position dependent diffusion coefficient were also considered in the literature [14] in analysis of *N*-dimensional diffusion equation.

The displacement $x(t)$ of a particle in a heterogeneous medium with space dependent diffusivity $\mathcal{D}(x)$ is described by the Langevin equation

$$\frac{d}{dt}x(t) = \sqrt{2\mathcal{D}(x)}\zeta(t), \tag{1}$$

where $\zeta(t)$ is a white Gaussian noise with $\langle\zeta(t)\zeta(t')\rangle = \delta(t-t')$ and zero mean $\langle\zeta(t)\rangle = 0$. In the Stratonovich interpretation this Langevin equation corresponds to the diffusion equation for the probability distribution function (PDF) [11]

$$\frac{\partial}{\partial t}P(x,t) = \frac{\partial}{\partial x}\left[\sqrt{\mathcal{D}(x)}\frac{\partial}{\partial x}\left(\sqrt{\mathcal{D}(x)}P(x,t)\right)\right]. \tag{2}$$

It is supplemented with the initial condition $P(x,t=0) = \delta(x)$, and the boundary conditions are set to zero at infinities. The diffusion coefficient has the power-law position dependent form

$$\mathcal{D}(x) = \mathcal{D}_x|x|^{\alpha}, \qquad \alpha < 2. \tag{3}$$

The solution of Eq. (2) is obtained in the stretched exponential form [11]

$$P(x,t) = \frac{|x|^{-\alpha/2}}{\sqrt{4\pi\mathcal{D}_x t}}\exp\left(-\frac{|x|^{2-\alpha}}{(2-\alpha)^2\mathcal{D}_x t}\right), \tag{4}$$

and the mean square displacement (MSD) has the power-law dependence on time

$$\langle x^2(t)\rangle = \int_{-\infty}^{\infty} dx\, x^2 P(x,t) \simeq \frac{t^{\frac{2}{2-\alpha}}}{\Gamma\left(1+\frac{2}{2-\alpha}\right)}. \tag{5}$$

This expression describes different diffusive regimes, where for $\alpha < 0$ one observes subdiffusion, normal diffusion for $\alpha = 0$, superdiffusion for $0 < \alpha < 1$, ballistic motion for $\alpha = 1$ and hyperdiffusion for $1 < \alpha < 2$. The case with $\alpha = 2$ leads to exponentially

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fast spreading [6,15]. The case with $\alpha > 2$ yields localization[1] with the decay MSD $t^{-\frac{2}{\alpha-2}}$.

A random walk in a simple comb structure consisting of main diffusion channel (backbone) and trapping fingers leads to anomalous diffusion with a transport exponent equal to 1/2 [16]. It can be described by the two-dimensional diffusion equation [17]

$$\frac{\partial}{\partial t}P(x,y,t)=\mathcal{D}_x\delta(y)\frac{\partial^2}{\partial x^2}P(x,y,t)+\mathcal{D}_y\frac{\partial^2}{\partial y^2}P(x,y,t), \quad (6)$$

where $P(x, y, t)$ is the probability distribution function (PDF), $\mathcal{D}_x\delta(y)$ is the diffusion coefficient in x direction with dimension $[\mathcal{D}_x]=\mathrm{m}^3/\mathrm{s}$, and $\mathcal{D}_y$ is the diffusion coefficient in y direction with dimension $[\mathcal{D}_y]=\mathrm{m}^2/\mathrm{s}$. The δ-function in Eq. (6) means that the diffusion along the x direction occurs only at $y=0$ (the backbone) and the fingers play the role of traps. The comb model (6) is used to describe diffusion in low-dimensional percolation clusters [17,18]. Comb models can further be generalized to grid and fractal grid structures [19] in which the diffusion along the x direction may appear in many backbones, even infinite number of backbones which positions belong to a fractal set $\mathcal{S}_\nu$ with fractal dimension $0<\nu<1$. In this case anomalous diffusion is observed and the transport exponent depends on the fractal dimension ν. In this paper we consider heterogeneous diffusion on such comb and fractal grid structures, where the diffusivity is position dependent with power-law diffusion coefficient of Eq. (3).

The investigation of anomalous diffusion processes in complex systems leads to appearance of fractional differintegration in the corresponding stochastic and kinetic equation representing the memory effect in the system. Therefore, the mathematical background of the theory of fractional differential and integral equations [20–22], and associated Mittag–Leffler and Fox H-functions [23,24] for analysis of such processes are of the primary importance. From the other side, diffusion on fractal structures, and the connection between the fractal dimension and fractional differintegration, as well as description of fractal processes by fractional calculus have been discussed in the scientific community [25].

The paper is organized as follows. In Section 2 we consider a two-dimensional diffusion equation for a comb with the position dependent (power-law) diffusion coefficient along the backbone. Exact results for the PDF and MSD are obtained and various diffusion regimes are observed, such as anomalous subdiffusion, superdiffusion and hyperdiffusion. The case of heterogeneous diffusion on a fractal grid structure is considered in Section 3, and exact results for the PDF and MSD are derived. The summary is given in Section 4.

2. Heterogeneous diffusion on a comb

We consider the two dimensional diffusion equation on a heterogeneous comb for the PDF $P(x, y, t)$

$$\frac{\partial}{\partial t}P(x,y,t)=\delta(y)\frac{\partial}{\partial x}\left[\sqrt{\mathcal{D}(x)}\frac{\partial}{\partial x}\left(\sqrt{\mathcal{D}(x)}P(x,y,t)\right)\right]+\mathcal{D}_y\frac{\partial^2}{\partial y^2}P(x,y,t), \quad (7)$$

where $\mathcal{D}(x)$ is the position dependent diffusion coefficient along the backbone, $\mathcal{D}_y$ is the diffusion coefficient along the fingers. This equation is a generalization of the one-dimensional heterogeneous diffusion Eq. (2) to a two-dimensional comb structure. The initial condition is

$$P(x,y,t=0)=\delta(x)\delta(y), \quad (8)$$

and the boundary conditions for $P(x, y, t)$ and $\frac{\partial}{\partial q}P(x,y,t)$, $q=\{x,y\}$ are set to zero at infinities, $x=\pm\infty$, $y=\pm\infty$. The position dependent diffusion coefficient has power-law form (3) with $\alpha<2$, therefore the physical dimension of the diffusion coefficient along the backbone $\mathcal{D}_x\delta(y)$ is $[\mathcal{D}_x\delta(y)]=\mathrm{m}^{2-\alpha}\mathrm{s}^{-1}$, and the physical dimension of $\mathcal{D}_y$ is $[\mathcal{D}_y]=\mathrm{m}^2\mathrm{s}^{-1}$.

Inserting the diffusion coefficient (3) in Eq. (7) one obtains

$$\frac{\partial}{\partial t}P(x,y,t)=\mathcal{D}_x\delta(y)\frac{\partial}{\partial x}\left[|x|^{\alpha/2}\frac{\partial}{\partial x}\left(|x|^{\alpha/2}P(x,y,t)\right)\right]+\mathcal{D}_y\frac{\partial^2}{\partial y^2}P(x,y,t). \quad (9)$$

From the Laplace transform,[2] it follows

$$sP(x,y,s)-P(x,y,t=0)=\mathcal{D}_x\delta(y)\frac{\partial}{\partial x}\left[|x|^{\alpha/2}\frac{\partial}{\partial x}\left(|x|^{\alpha/2}P(x,y,s)\right)\right]+\mathcal{D}_y\frac{\partial^2}{\partial y^2}P(x,y,s). \quad (10)$$

We present the solution of the Eq. (10) in the form of the ansatz

$$P(x,y,s)=g(x,s)\exp\left(-\sqrt{\frac{s}{\mathcal{D}_y}}|y|\right), \quad (11)$$

from where it follows that

$$P(x,y=0,s)=g(x,s)\,. \quad (12)$$

We also introduce the reduced PDF, which describes the transport along the backbones only

$$p_1(x,t)=\int_{-\infty}^{\infty}dy\,P(x,y,t),$$

and yields

$$p_1(x,s)=2g(x,s)\sqrt{\frac{\mathcal{D}_y}{s}}. \quad (13)$$

Integrating Eq. (9) over y, one finds

$$sp_1(x,s)-p_1(x,t=0)=\mathcal{D}_x\frac{\partial}{\partial x}\left[|x|^{\alpha/2}\frac{\partial}{\partial x}\left(|x|^{\alpha/2}g(x,s)\right)\right], \quad (14)$$

where the initial condition $p_1(x,t=0)=\delta(x)$. Therefore, from Eqs. (14) and (13) we obtain the differential equation

$$2\sqrt{\mathcal{D}_y}s^{1/2}g(x,s)-\mathcal{D}_x\frac{\partial}{\partial x}\left[|x|^{\alpha/2}\frac{\partial}{\partial x}\left(|x|^{\alpha/2}g(x,s)\right)\right]=\delta(x). \quad (15)$$

After the substitution $f(x,s)=|x|^{\alpha/2}g(x,s)$, from Eq. (15) we obtain

$$2\sqrt{\mathcal{D}_y}s^{1/2}|x|^{-\alpha/2}f(x,s)-\mathcal{D}_x\frac{\partial}{\partial x}\left[|x|^{\alpha/2}\frac{\partial}{\partial x}f(x,s)\right]=\delta(x). \quad (16)$$

We take into account symmetrical property of the equation, which is invariant with respect to inversion $x\to-x$. Therefore, in order to solve this equation, we use $z=|x|$, from where by partial differentiation with respect to x we find[3]

$$2\sqrt{\mathcal{D}_y}s^{1/2}z^{-\alpha/2}f(z,s)-\mathcal{D}_x(\alpha/2)z^{\alpha/2-1}\frac{\partial}{\partial z}f(z,s)-\mathcal{D}_xz^{\alpha/2}\frac{\partial^2}{\partial z^2}f(z,s)-2\mathcal{D}_xz^{\alpha/2}\frac{\partial}{\partial z}f(z,s)\delta(x)=\delta(x). \quad (17)$$

This equation splits into the system of equations

[1] In Ref. [7], where inhomogeneous advection in a comb was considered, this regime has been named by negative superdiffusion.

[2] The Laplace transform of a given function $f(t)$ is defined by $f(s)=\mathcal{L}[f(t)]=\int_0^\infty dt\,e^{-st}f(t)$.

[3] We also use here the following property $x=|x|\mathrm{sign}(x)$, and $\mathrm{sign}(x)\partial_z=\partial_x$.