PHYSICAL REVIEW E **83**, 052106 (2011)

Subdiffusion on a fractal comb

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(Received 14 December 2010; revised manuscript received 13 March 2011; published 31 May 2011)

Subdiffusion on a fractal comb is considered. A mechanism of subdiffusion with a transport exponent different from 1/2 is suggested. It is shown that the transport exponent is determined by the fractal geometry of the comb.

DOI: 10.1103/PhysRevE.83.052106 PACS number(s): 05.40.Fb, 05.45.Df

A comb model was introduced for understanding anomalous transport in percolating clusters [1,2] and it was considered as a toy model for a porous medium used for exploration of low-dimensional percolation clusters [1,3], as well. It is a particular example of a non-Markovian phenomenon, which was explained in the framework of continuous time random walks [2,4–7]. In the last decade the comb model has been extensively studied for understanding of different realizations of non-Markovian random walks, both continuous [8–10] and discrete [11].

Anomalous diffusion on the comb is usually described by the 2D distribution function $P = P(x,y,t)$, and a special behavior is that the displacement in the x direction is possible only along the structure axis (x axis at $y = 0$). Therefore, diffusion in the x direction is highly inhomogeneous; namely the diffusion coefficient is $D_{xx} = \tilde{D}\delta(y)$, while the diffusion coefficient in the y direction (along fingers) is a constant $D_{yy} = D$. Therefore, this inhomogeneous diffusion is described by the Fokker-Planck equation in the dimensionless time and coordinates

$$\hat{L}_{\mathrm{FP}}P(x,y,t) \equiv \partial_t P - \delta(y)\partial_x^2 P - \partial_y^2 P = 0\,. \tag{1}$$

It is obtained by the rescaling with relevant combinations of the comb parameters D and $\tilde{D}$, such that the dimensionless time and coordinates are $D^3t/\tilde{D}^2 \to t$ $Dx/\tilde{D} \to x$, $Dy/\tilde{D} \to y$, correspondingly [12].

The fractional transport along the structure x axis is described by the transporting contaminant distribution $p(x,t) = \int_{-\infty}^{\infty} P(x,y,t)dy$. It was shown [12] that Eq. (1) is equivalent to the fractional Fokker-Planck equation

$$\partial_t^{\frac{1}{2}} p(x,t) - \frac{1}{2}\partial_x^2 p(x,t) = 0, \tag{2}$$

from where subdiffusion can be immediately obtained: $\int x^2 p(x,t)dx \sim \sqrt{t}$. Here $\partial_t^{\frac{1}{2}}$ is a fractional time derivative, which is a formal notation of an integral with a power law memory kernel. For $0 < \alpha < 1$ it reads

$$\partial_t^{\alpha} f(t) = \int_0^t \frac{(t-\tau)^{-\alpha-1}}{\Gamma(1-\alpha)}\partial_\tau f(\tau)d\tau. \tag{3}$$

Subdiffusive mechanism with an arbitrary transport exponent was also suggested by either changing the boundary conditions for diffusion in the fingers [13–16] or introducing a dependence of the diffusion coefficient on time and space [17]. In this paper we consider a fractal comb (see Fig. 1), when diffusion is highly inhomogeneous along the y fingers, as well; namely, it takes place for those coordinates of the x axis, which belong to a fractal set $S_\nu(x)$ and is defined by a characteristic function $\chi(x)$, such that $D_{yy} = D\chi(x)$, where $\chi(x) = 1$, if $x \in S_\nu(x)$ and $\chi(x) = 0$, if $x \notin S_\nu(x)$. The fractal set $S_\nu(x)$ is a random fractal with a fractal dimension $0 < \nu < 1$ embedded in the 1D Euclidian space (of the x axis). Such generalization of the comb model to a discrete (fractal) comb model for consideration of fractional transport in discrete systems is more realistic situation for theoretical studies of transport properties in discrete systems with complicated topology including fractal ones like porous discrete media [18], electronic transport in semiconductors with a discrete distribution of traps, cancer development with definitely fractal structure of the spreading front (see, e.g., Refs. [7,19]), and infiltration of diffusing particles from one material to another [20].

Hence, we study the following dimensionless equation:

$$\partial_t \mathcal{P} - \delta(y)\partial_x^2 \mathcal{P} - \chi(x)\partial_y^2 \mathcal{P} = 0. \tag{4}$$

The initial condition is $\mathcal{P}(x,y,0) = \delta(x)\delta(y)$, and the boundary conditions on infinities have the form $\mathcal{P}(\pm\infty, \pm\infty, t) = 0$ and the same for the first derivatives with respect to x and y $\mathcal{P}_x'(\pm\infty, \pm\infty, t) = \mathcal{P}_y'(\pm\infty, \pm\infty, t) = 0$.

Our main purpose is to evaluate the second moment

$$\langle x^2\rangle(t) = \int x^2 \mathcal{P}(x,y,t)dxdy \tag{5}$$

as a function of time. Therefore, the forthcoming analysis of Eq. (4) is supposed to be carried out under the integration sign. Using properties of the characteristic function

$$\chi^2(x) = \chi(x) \text{ and } \partial_x\chi(x) = 0, \tag{6}$$

a solution of Eq. (4) can be presented in the form

$$\mathcal{P}(x,y,t) = \chi(x)P(x,y,t), \tag{7}$$

where $P(x,y,t)$ is a solution of the continuous comb model and we shall show that an equation for this function coincides with Eq. (1). But first, one should understand a physical meaning of the distribution $\mathcal{P}(x,y,t)$ based on properties of the characteristic function $\chi(x)$. While the first property in Eq. (6) is obvious and follows from the definition of $\chi(x)$, the second expression deserves an explanation. To show this, let us consider the Nth step of the fractal set S_ν construction. It is a union of disjoint intervals Δx_N. In general case of a random fractal, these are random intervals. In the limiting case one obtains $S_\nu = \lim_{N\to\infty} \bigcup \Delta x_N$. Therefore, the characteristic function on every interval $\Delta x_j = [x_j, x_j + \Delta x_N]$ is $\chi(\Delta x_N) = \Theta(x - x_j) - \Theta(x - x_j - \Delta x_N)$. Differentiation of the characteristic function on every interval yields $\frac{\partial}{\partial x}\chi(\Delta x_N) = \delta(x - x_j) - \delta(x - x_j - \Delta x_N)$. In the limit $N \to \infty$ it tends to

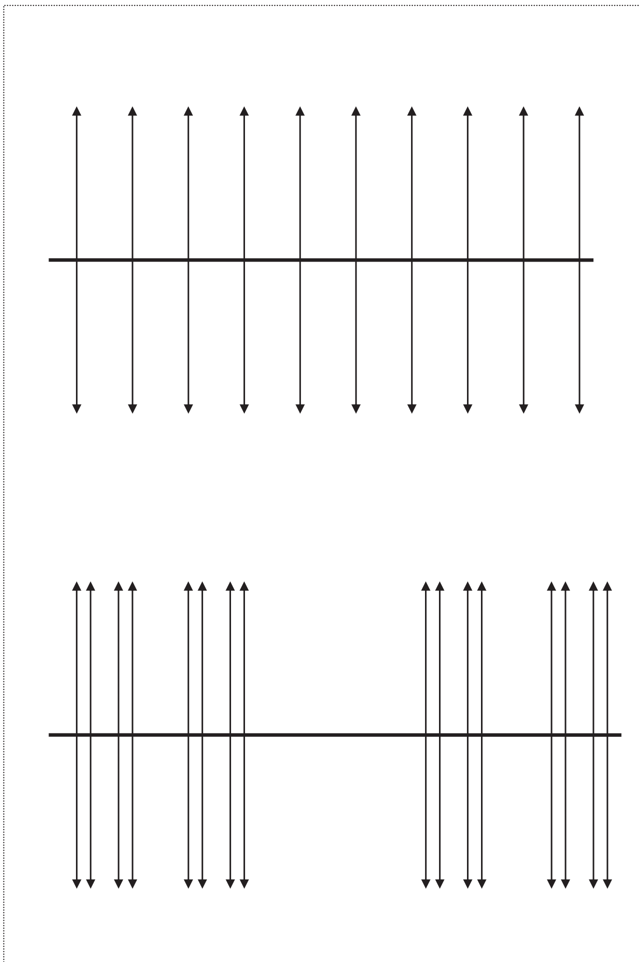

FIG. 1. Comb structures. The upper strip corresponds to the continuous comb model. The lower strip is a sketch of the fractal comb with a specific distribution of fingers, which corresponds to the one-third Cantor set (at the forth step of the construction). Notably, one should recognize that this construction is not representative. Therefore, the fractal set F_ν can be considered as a random fractal distribution of the fingers without any specifically defined construction algorithm. It is worth admitting that the fractal distribution of teeth, in general case, is multifractal, and the uncertainty of this construction should be stressed as well.

zero (under the integration), since $P(x,y,t)$ and its derivatives are continuous functions.

Now we can return to the continuity property of $\mathcal{P}(x,y,t)$ that can be understood from the calculation of the second moment $\langle x^2\rangle(t)$ in Eq. (5). The presence of the characteristic function in this expression means that the integration is performed over the fractal volume [21]. It means that $\int\chi(x)dx \to \frac{1}{\Gamma(\nu)}\int|x|^{\nu-1}dx \sim \frac{1}{\Gamma(\nu+1)}|x|^\nu$, where $\Gamma(\nu)$ is the Γ function. This yields the expression for $\langle x^2\rangle(t)$

$$\langle x^2\rangle(t) = \frac{1}{\Gamma(\nu)}\int_{-\infty}^{\infty} x^2|x|^{\nu-1}P(x,y,t)dxdy. \tag{8}$$

Using this smoothing procedure, we can show that an equation for the distribution function $P(x,y,t)$ is Eq. (1). We have from Eqs. (4) and properties (6) of the characteristic function $\chi(x)$ that for any arbitrary function $f(x)$

$$\int_{-\infty}^{\infty}|x|^{\nu-1}f(x)\hat{L}_{\rm FP}P(x,y,t)dx = 0. \tag{9}$$

Therefore, we have equation $\hat{L}_{\rm FP}P(x,y,t)=0$, which exactly coincides with Eq. (1) and is valid for all x.

Now we at a position to determine $\langle x^2\rangle(t)$. Taking into account Eq. (8), one obtains the following from the integration of Eq. (9) over y with $f(x)=x^2$:

$$\partial_t\langle x^2\rangle(t) = \frac{1}{\Gamma(\nu)}\int_{-\infty}^{\infty}|x|^{\nu-1}x^2\partial_x^2 P(x,0,t)dx. \tag{10}$$

Here we take into account that $\int_{-\infty}^{\infty}\partial_y^2 P(x,y,t)=0$ due to the boundary conditions. A relation between $P(x,0,t)$ and $P(x,y,t)$ can be established in the Laplace domain. Performing the Laplace transform $\hat{\mathcal{L}}P(x,y,t)=\tilde{P}(x,y,s)$ in Eq. (1), it is readily seen that $\tilde{P}(x,y,s)=\tilde{P}(x,0,s)e^{-\sqrt{s}|y|}$ satisfies the equation. After integrating over y, it yields

$$\tilde{P}(x,0,s) = \frac{1}{2}\sqrt{s}\int_{-\infty}^{\infty}\tilde{P}(x,y,s)dy = \frac{1}{2}\sqrt{s}\,\tilde{p}(x,s). \tag{11}$$

This result can be taken into account after the Laplace transform in Eq. (10), which yields an expression for the second moment in the Laplace domain $\hat{\mathcal{L}}[\langle x^2\rangle(t)] = \widetilde{\langle x^2\rangle}(s)$. It reads

$$s\widetilde{\langle x^2\rangle}(s) = \frac{1}{\Gamma(\nu)}\int_{-\infty}^{\infty}|x|^{1+\nu}\partial_x^2\tilde{p}(x,s)dx, \tag{12}$$

where $\tilde{p}(x,s)=\frac{1}{\sqrt{2s^{3/2}}}\exp(-\sqrt{2s^{1/2}}|x|)$ can be obtained from Eq. (2). After the Laplace inversion one obtains the second moment

$$\langle x^2\rangle(t) = K_\nu t^{\frac{1+\nu}{4}}, \tag{13}$$

where $K_\nu=\Gamma(2+\nu)/\Gamma(\frac{5}{4}+\frac{\nu}{4})\Gamma(\nu)\sqrt{2^{1+\nu}}$ is a generalized diffusion coefficient. Finally, we obtain subdiffusion on the comb $\langle x^2\rangle(t)\sim t^\mu$ with the transport exponent $\frac{1}{4}<\mu<\frac{1}{2}$. When $\nu=1$, one observes subdiffusion with $\mu=1/2$. To obtain subdiffusion with $\frac{1}{2}<\mu<1$, one considers advection along the structure x axis instead of diffusion. This yields $\mu=\frac{1+\nu}{2}$ for the transport exponent.

The main deficiency of the obtained result in Eq. (13) is that it is based on the presentation of the probability distribution function as a product of a continuous function and the characteristic function in Eq. (7). Although the inferring of Eq. (13) is correct, this presentation can leads to wrong result, because the probability distribution function $\mathcal{P}(x,y,t)$ must be continuous at every point. To overcome this deficiency, we refuse the locality property. To this end, the following procedure of coarse graining of the Fokker-Planck equation (4) is suggested. First, we apply the Fourier transform to Eq. (4) with respect to the x coordinate. To apply this transformation to the last term in Eq. (4), we use the following auxiliary identity

$$\chi(x)f(x) = \partial_x\int_0^x\chi(y)f(y)dy.$$

Here for brevity we define $f(x) \equiv \mathcal{P}(x,y,t)$. This integration with the characteristic function can be carried out by means of a convolution [22]. Note that

$$\int_0^x \chi(y)f(y)dy = \sum_{x_j\in S_\nu[0,x]} \int_{-\infty}^{\infty} f(y)\delta(y-x_j)dy, \quad (14)$$

where we use that

$$\sum_{x_j\in S_\nu} \delta(y-x_j) = \mu'(x) \sim x^{\nu-1}$$

is a fractal density, such that on the finite interval $(0,x)$, the integral $\int_0^x d\mu(y) \sim x^\nu$ corresponds to the fractal volume. Therefore, Eq. (14) reads

$$\int_0^x \chi(y)f(y)dy = \int_0^x f(y)d\mu(y).$$

The last expression can be rewritten as a convolution integral. Due to Theorem 3.1 in Ref. [23], we have

$$\int_0^x f(y)d\mu(y) \simeq \frac{A_\nu}{\Gamma(\nu)} \int_0^x (x-y)^{\nu-1} f(y)dy, \quad (15)$$

where A_ν is a constant, defined by the conditions of the theorem. In sequel we disregard this parameter, putting $A_\nu = 1$. This integration is a Riemann-Liouville integral (see, e.g., Refs. [5,24])

$$\partial_{x\,0}I_x^\nu f(x) \equiv \frac{1}{\Gamma(\nu)}\partial_x \int_0^x (x-y)^{\nu-1} f(y)dy.$$

Here we use a standard notation ${}_0I_x^\nu f(x)$ to define integration with a power law kernel; see Eq. (3). The integration can be presented in the form of the inverse Laplace transform $\hat{\mathcal{L}}f(x) = \tilde{f}(s)$, which reads

$${}_0I_x^\nu f(x) = \hat{\mathcal{L}}^{-1}\hat{\mathcal{L}}[{}_0I_x^\nu f(x)] = \hat{\mathcal{L}}^{-1} s^{-\nu}\tilde{f}(s).$$

Therefore, after the variable change $s = iz$, the Fourier transform of the last term in Eq. (4) yields

$$\hat{\mathcal{F}}_x[\chi(x)\mathcal{P}(x,y,t)] = (ik)^{1-\nu}\hat{\mathcal{P}}(k,y,t), \quad (16)$$

where $\hat{\mathcal{F}}_x f(x) = \hat{\mathcal{P}}(k,y,t) = \tilde{f}(ik)$. One takes into account that the result should be symmetrical with respect to the negative $x < 0$. Therefore, the Fourier transform of Eq. (4) yields

$$\partial_t\hat{\mathcal{P}}(k,y,t) = -\delta(y)k^2\hat{\mathcal{P}}(k,y,t) + |k|^{1-\nu}\partial_y^2\hat{\mathcal{P}}(k,y,t)\,. \quad (17)$$

Now we perform the Laplace transform with respect to time $\hat{\mathcal{L}}\hat{\mathcal{P}}(k,y,t) = \hat{\tilde{\mathcal{P}}}(k,y,s) \equiv G(k,y,s)$. This yields

$$sG = -\delta(y)k^2G + |k|^{1-\nu}\partial_y^2G + \delta(y) \quad (18)$$

with the solution

$$G(k,y,s) = \exp(-|y|\sqrt{s|k|^{\nu-1}})g(k,s), \quad (19)$$

where $g(k,s) = G(k,0,s)$ is the Fourier-Laplace image on the structure axis at $y = 0$. Again, we are interesting in dynamics along the structure axis by studying the probability distribution function $\mathcal{P}_1$ [see Eq. (11)]:

$$\mathcal{P}_1(x,t) = \int_{-\infty}^{\infty} \mathcal{P}(x,y,t)dy. \quad (20)$$

Integrating Eq. (19) over y one obtains

$$G(k,0,s) = \frac{\sqrt{s|k|^{\nu-1}}}{2}\int_{-\infty}^{\infty} G(k,y,s)dy. \quad (21)$$

Therefore, integrating Eq. (18) over y yields the Montrall-Weiss equation that, after the Fourier and the Laplace inversions, reduces to the fractional Fokker-Planck equation. It is a particular case of a general equation

$$\partial_t^\alpha\mathcal{P}_1(x,t) = \frac{1}{2}\nabla_x^\beta\mathcal{P}_1(x,t)\,, \quad 0 \leqslant \alpha \leqslant 1, \quad (22)$$

where $\beta = \frac{3}{2} + \frac{\nu}{2}$. It describes a competition between long rests and long flights. We stress that when $\alpha = 1/2$, it corresponds to the comb model; see Eq. (2). Here we use the formal definition for the Riesz-Weyl fractional space derivative in form of the Fourier inversion (see, e.g., Refs. [5,25]):

$$\nabla_x^\nu f(x) = \hat{\mathcal{F}}^{-1}[|k|^\nu\hat{f}(k)]. \quad (23)$$

This equation was studied in Refs. [26,27] (see also Ref. [5]). The correct form of the mean-squared displacement, which estimates the competition of "laminar motion events" (flights) and "localization" (waiting) events in the Lévy walk picture, was obtained through the relation [26] valid for Eq. (22)

$$\langle x^2(t)\rangle \sim t^\mu = t^{1-\frac{\nu}{2}}. \quad (24)$$

One easily checks that this result with $\mu = 1 - \nu/2$ has a correct limit for $\nu = 1$, when it corresponds to the continuous comb model with $\mu = 1/2$.

In conclusion, we presented two approaches to study subdiffusion on the fractal comb, when the fractal trap distribution is determined by the characteristic function $\chi(x)$. In this case, it is tempting to look for a solution in the multiplicative form of Eq. (7). Thus the forthcoming analysis, based on this presentation of the probability distribution function is rigorous. The main deficiency of this approach is that it violates the continuity property of the probability distribution function. To overcome this deficiency, a coarse graining procedure of the Fokker-Planck equation (4) is suggested. It is based on the possibility of performing the Fourier transform for Eq. (4) exactly. We obtained that inhomogeneous, fractal distribution of traps in the comb model leads to Lévy jumps that complicates fractal diffusion and leads to the competition between long jumps and localization inside traps. This phenomenon is described by the fractional Fokker-Planck equation (22). As a result of this competition, subdiffusion, which is the dominant process, is realized.

We admit that the results of the either approach of Eqs. (13) or (24) have correct limits for $\nu = 1$. A specific property of Eq. (24) is that for $\nu = 0$, it corresponds to normal diffusion with $\mu = 1$. While the first limit with $\nu = 1$ is well understood, the second one is not so obvious. Indeed, when the Hausdorff dimension is $\nu = 0$, there are no traps, and normal diffusion is anticipated. Nevertheless, this behavior results from the fractional Fokker-Planck equation (22) with $3/2$ fractional space derivative and $1/2$ fractional time derivative. This is a special point of a transition from subdiffusion to superdiffusion

[5,26]. For the comb model subdiffusion is the dominant process, there is no superdiffusion, and $\mu = 1$ is the boundary point.

This research was supported in part by the Israel Science Foundation (ISF) and by the US-Israel Binational Science Foundation (BSF).

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