Fractional diffusion on a fractal grid comb

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A grid comb model is a generalization of the well known comb model, and it consists of \(N\) backbones. For \(N = 1\) the system reduces to the comb model where subdiffusion takes place with the transport exponent \(1/2\). We present an exact analytical evaluation of the transport exponent of anomalous diffusion for finite and infinite number of backbones. We show that for an arbitrarily large but finite number of backbones the transport exponent does not change. Contrary to that, for an infinite number of backbones, the transport exponent depends on the fractal dimension of the backbone structure.

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I. INTRODUCTION

The comb-like models have been introduced to investigate anomalous diffusion in low-dimensional percolation clusters \([1,4]\). It means that the mean square displacement (MSD) has power-law dependence on time \(\langle x^2(t) \rangle \sim t^\alpha \) \([2]\). An elegant form of equation which describes the diffusion on a comb-like structure was introduced by \([2]\)

\[
\frac{\partial}{\partial t} P(x,y,t) = D_x \delta(y) \frac{\partial^2}{\partial x^2} P(x,y,t) + D_y \frac{\partial^2}{\partial y^2} P(x,y,t),
\]

where \(P(x,y,t)\) is the probability distribution function (PDF), \(D_x \delta(y)\) is the diffusion coefficient in \(x\) direction, and \(D_y\) is the diffusion coefficient in \(y\) direction. The \(\delta\)-function in the diffusion coefficient in \(x\) direction implies that the diffusion along the \(x\) direction occurs only at \(y = 0\). Thus, this equation can be used to describe diffusion in the backbone (at \(y = 0\)) where the teeth play the role of traps.

Nowadays, comb models have many applications. They have been used for the understandings of continuous \([4,8]\) and discrete \([4]\) non-Markovian random walks. There are generalizations of this equation by introducing time fractional derivatives and integrals in \([10,11]\).

Such generalized comb-like models have been used to describe anomalous diffusion in spiny dendrites, where the MSD along the \(x\) direction has a power-law dependence on time \([10,11]\), or for describing subdiffusion on a fractal comb \([12]\), the mechanism of superdiffusion of ultra-cold atoms in a one dimensional polarization optical lattice \([13]\) as a phenomenology of experimental study \([14]\), and to describe diffusion processes on a backbone structure \([15]\). Different generalizations of the comb model have been shown to represent more realistic models for describing transport properties in discrete systems, such as porous discrete media \([16]\), electronic transport in semiconductors with a discrete distribution of traps, cancer development with definitely fractal structure of the spreading front \([17,18]\), infiltration of diffusing particles from one material to another \([19]\), description of diffusion of active species in porous media \([20]\), etc. Furthermore, in \([21]\) it is shown that in a comb-like model a negative superdiffusion occurs due to the presence of an inhomogeneous convection flow.

In this paper we consider a generalization of equation \((\text{1})\) where we allow that diffusion along \(x\)-direction may occur on many backbones, located at \(y = l_j, j = 1,2,\ldots,N, 0 \leq l_1 < l_2 < \ldots < l_N\). This means that we have a comb grid where \(N\) can be arbitrarily large, even infinity. The governing equation for such a structure is given by

\[
\frac{\partial}{\partial t} P(x,y,t) = D_x \sum_{j=1}^{N} w_j \delta(y - l_j) \frac{\partial^2}{\partial y^2} P(x,y,t) + D_y \frac{\partial^2}{\partial y^2} P(x,y,t),
\]

\[\text{(2)}\]
where \( w_j \) are structural constants such that \( \sum_{j=1}^{N} w_j = 1 \). The initial condition is given by

\[
P(x, y, t = 0) = \delta(x)\delta(y),
\]

and the boundary conditions for \( P(x, y, t) \) and \( \frac{\partial}{\partial y} P(x, y, t) \), \( q = \{x, y\} \) are set to zero at infinity, \( x = \pm \infty, y = \pm \infty \). One can easily verify that for \( l_1 = 0 \), \( w_1 = 1 \), and \( w_2 = w_3 = ... = w_N = 0 \) equation (2) becomes (1). The case of a fractal structure of backbones will be described by an appropriate generalization of equation (2).

The paper is organized as follows. In Section II we analyze the PDF and the MSD in both directions for the force free case. Anomalous diffusive behavior appears in \( x \)-direction due to the comb structure of the system. General results for the MSD in case of finite number of backbones \( N \) are presented. We also investigate the effects of an external constant force, applied along the backbones, on the particle behavior. In Section III we consider an infinite number of backbones. It is shown that an infinite number of backbones, different from the case of a finite number of backbones, changes the transport exponent. The summary is given in Section IV.

II. FINITE NUMBER OF BACKBONES. MSD

We apply a Laplace transform \( (\mathcal{L}[f(t)] = \hat{f}(s)) \) to equation (2), and then a Fourier transform with respect to the \( x \) \((\mathcal{F}_x[f(x)] = \hat{f}(\kappa_x)) \) and \( y \) \((\mathcal{F}_y[f(y)] = \hat{f}(\kappa_y)) \) variables. Thus, we obtain

\[
\tilde{P}(\kappa_x, \kappa_y, s) = \frac{\hat{P}(\kappa_x, \kappa_y, t = 0)}{s + D_y \kappa_y^2} - \sum_{j=1}^{N} w_j \hat{P}(\kappa_x, \kappa_y = l_j, s) \exp(\kappa_y l_j) \frac{D_x \kappa_x^2}{s + D_y \kappa_y^2},
\]

(4)

where \( \hat{P}(\kappa_x, \kappa_y, t = 0) = 1 \). From relation (4), the inverse Fourier transform with respect to \( \kappa_y \) yields

\[
\hat{P}(\kappa_x, \kappa_y, s) = \exp\left(-\sqrt{\frac{\kappa_x^2}{\kappa_y^2}}|y|\right) \frac{D_x \kappa_x^2}{2\sqrt{D_y} s^{1/2}} \sum_{j=1}^{N} w_j \hat{P}(\kappa_x, \kappa_y = l_j, s) \exp\left(-\sqrt{\frac{\kappa_x^2}{\kappa_y^2}}|y - l_j|\right) \frac{1}{2\sqrt{D_y} s^{1/2}}.
\]

(5)

In the setting of a comb model, the nontrivial and interesting motion is along the backbones, i.e., along the \( x \)-direction, while the \( y \)-direction is an auxiliary subspace. Therefore, integrating the motion in the \( y \)-direction, we analyze the PDF \( P_1(x, t) = \int_{-\infty}^{\infty} dy P(x, y, t) \). By integration of equation (2) with respect to \( y \) and performing the Laplace transform with respect to time \( t \), and the Fourier transform with respect to \( x \), one obtains

\[
\tilde{p}_1(\kappa_x, s) = \frac{1}{s} \left[ 1 - D_x \kappa_x^2 \sum_{j=1}^{N} w_j \hat{P}(\kappa_x, \kappa_y = l_j, s) \right].
\]

(6)

From the PDF (6) we calculate the MSD along the \( x \)-direction by the following formula

\[
\langle x^2(t) \rangle = \mathcal{L}^{-1} \left[ -\frac{\partial^2}{\partial \kappa_x^2} \tilde{p}_1(\kappa_x, s) \right]_{\kappa_x = 0}.
\]

(7)

From relations (5), (6) and (7) for the MSD we derive

\[
\langle x^2(t) \rangle = \frac{D_x}{\sqrt{D_y}} \mathcal{L}^{-1} \left[ s^{-3/2} \sum_{j=1}^{N} w_j e^{-\sqrt{\frac{\kappa_x^2}{\kappa_y^2}} l_j} \right] = \frac{D_x}{\sqrt{D_y}} \sum_{j=1}^{N} w_j \left[ \frac{2}{\sqrt{\pi}} l_j^{1/2} e^{-\frac{|l_j|^2}{4D_x s}} - \frac{|l_j|}{\sqrt{4D_y}} \text{erfc}\left(\frac{|l_j|}{\sqrt{4D_y s}}\right) \right].
\]

(8)

where \( \text{erfc}(x) \) is the complementary error function \( \text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_{x}^{\infty} e^{-u^2} du \).

For \( l_1 = 0 \) it follows

\[
\langle x^2(t) \rangle = \frac{2w_1 D_x}{\sqrt{D_y}} t^{1/2} + \frac{D_x}{\sqrt{D_y}} \times \sum_{j=2}^{N} w_j \left[ \frac{2}{\sqrt{\pi}} l_j^{1/2} e^{-\frac{|l_j|^2}{4D_x s}} - \frac{|l_j|}{\sqrt{4D_y}} \text{erfc}\left(\frac{|l_j|}{\sqrt{4D_y s}}\right) \right].
\]

(9)

For the long time scale when \( \frac{|l_j|}{\sqrt{D_y s}} \ll 1, j = 2, 3, ..., N, \) the MSD reads

\[
\langle x^2(t) \rangle = \frac{2 \sum_{j=1}^{N} w_j D_x}{\sqrt{D_y}} t^{1/2},
\]

(10)

which means that all backbones contribute in the MSD. In contrast to this, on a short time scale, when \( \frac{|l_1|}{\sqrt{D_x t}} \gg 1, j = 2, 3, ..., N, \) one finds that the main contribution in the MSD is due to the first backbone, i.e.

\[
\langle x^2(t) \rangle \simeq \frac{2w_1 D_x}{\sqrt{D_y}} \frac{t^{1/2}}{\Gamma\left(\frac{1}{2}\right)}.
\]

(11)

This result is expected since for short times the particles move mainly in the first backbone because they had not enough time to reach the other ones by diffusion in the \( y \)-direction. This can be easily verified by considering diffusion along \( y \)-direction. We analyze the PDF \( p_2(y, t) = \int_{-\infty}^{\infty} dx P(x, y, t) \), for which we find that

\[
\tilde{p}_2(\kappa_y, s) = \frac{1}{s + D_y \kappa_y^2}.
\]

(12)
i.e., $p_2(y,t) = \frac{1}{\sqrt{4\pi D_y t}} \exp\left(-\frac{y^2}{4D_y t}\right)$. For the MSD along $y$-direction one finds a linear dependence on time

$$\langle y^2(t) \rangle = \mathcal{L}^{-1}\left[-\frac{\partial^2}{\partial y^2} \tilde{p}_2(k_y, s)\right]_{k_y=0} = 2D_y t,$$ (13)

i.e., normal diffusion along the $y$-direction. Therefore, the probability to find the particle at the first backbone is $p_{2,1}(y, t) = \frac{1}{\sqrt{4\pi D_y t}}$ ($l_1 = 0$), while at the second backbone it is $p_{2,2}(y, t) = \frac{1}{\sqrt{4\pi D_y t}} \exp\left(-\frac{l_2^2}{4D_y t}\right)$, and so on.

Since for the short time scales, $p_{2,1}(y, t) \gg p_{2,2}(y, t) \gg ...$, we conclude that the main contribution in the MSD for short times is due to the displacements in the first backbone.

From relation (10) for $w_1 = 1$, $w_2 = w_3 = ... = w_N = 0$, and $l_1 = 0$ (which means one backbone) we obtain the MSD for the comb-like model (11)

$$\langle x^2(t) \rangle = 2D_x t^{\frac{1}{\nu}} \sqrt{\frac{D_y}{\Gamma(\frac{1}{\nu})}}.$$ (14)

These results are supported by graphical representation in Fig. 1 of the MSD in case of two backbones and five backbones. It is assumed that the first backbone is at $y = 0$ and all the other backbones are at distances equal to $L, 2L, 3L, 4L$.

From relations (10) and (11) we conclude that any finite number of backbones does not change the transport exponent in the short and long time limit. In the intermediate times there is more complicated behavior of the MSD given by relation (9).

In the presence of a constant external force $F$ along the backbones we arrive at the following Fokker-Planck equation

$$\frac{\partial}{\partial t} P(x,y,t) = \sum_{j=1}^{N} w_j \delta(y - l_j)$$

$$\times \left[ -\frac{F}{m\eta_x} \frac{\partial}{\partial x} + D_x \frac{\partial^2}{\partial x^2} \right] P(x,y,t) + D_y \frac{\partial^2}{\partial y^2} P(x,y,t),$$ (15)

where $m$ is the mass and $\eta_x$ is the friction coefficient.

One can compute the first moment as a function of time

$$\langle x(t) \rangle_F = \frac{F}{2m\eta_x \sqrt{D_y}} \mathcal{L}^{-1}\left[ s^{-3/2} \sum_{j=1}^{N} w_j e^{-\sqrt{s} \frac{l_j}{D_y}} \right],$$ (16)

from where by comparing it with relation (8) we conclude that the generalized Einstein relation is fulfilled (5)

$$\langle x(t) \rangle_F = \frac{F}{2k_BT} \langle x^2(t) \rangle_{F=0},$$ (17)

where $k_B T = m\eta_x D_x$.

### III. FRACTAL STRUCTURE OF BACKBONES

To introduce a fractal structure of the backbones we go back to equation (2) and replace the summation $\sum_{j=1}^{N} w_j \delta(y - l_j)$ with summation over a fractal set $S_v$, i.e., $\sum_{l_j \in S_v} \delta(y - l_j)$, which means that the backbones are at positions $y$ which belong to the fractal set $S_v$ with fractal dimension $0 < \nu < 1$.

A simple toy example, which corresponds to an infinite fractal set, can be treated as follows. In relation (8) we calculate $\sum_{j=1}^{N} w_j e^{-\sqrt{s} \frac{l_j}{D_y}} = \sum_{l_j \in S_v} e^{-\sqrt{s} \frac{l_j}{D_y}}$. One should recognize that fractal set (like a Cantor set) are uncountable. Therefore, the last expression is pure formal and its mathematical realization corresponds to integration to fractal measure $\mu_{\nu} \sim \nu^{\nu}$ such that $\sum_{l_j \in S_v} \delta(l - l_j) = \frac{1}{\nu^{\nu-1}} \nu^{\nu}$ is the fractal density (23,24), and $d\mu_{\nu} = \frac{1}{\nu^{\nu-1}} \nu^{\nu-1}dl$. That finally yields the following integration

$$\frac{1}{\Gamma(\nu)} \int_{l_0}^{\infty} dl \nu^{-1} e^{-\sqrt{s} \frac{l}{D_y}} = \left(\frac{D_y}{s}\right)^{\nu/2}.$$ (18)

For the MSD, we obtain from (8)

$$\langle x^2(t) \rangle = \frac{D_x}{D_y^{1/\nu}} \frac{t^{\frac{1}{\nu} + \frac{1}{2}}}{\Gamma\left(1 + \frac{1}{\nu} + \frac{1}{2}\right)}.$$ (19)
i.e. anomalous diffusive behavior with the transport exponent equal to \( \nu < \frac{1 + \nu}{2} < 1 \). Thus, the fractal set \( S_\nu \) of the infinite number of backbones changes the transport exponent, from \( 1/2 \) to \( \frac{1 + \nu}{2} \). For \( \nu = 1 \) the MSD becomes \( \langle x^2(t) \rangle \approx t \), which is consistent with expectations, and for \( \nu = 0 \), we are back to the finite-\( N \) case. Indeed, the fractal dimension of any number of discrete points is \( \nu = 0 \).

We further consider a random fractal set \( S_\nu \in [a, b] \), with finite limits. From relation (3), in a same way as in [15], for a finite integration in \([0, L] \), one finds a result in the form of an incomplete gamma function \( \gamma(a, x) = \int_0^x dt t^{a-1}e^{-t} \) [22]

\[
\frac{1}{\Gamma(\nu)} \int_0^L d\nu^{\nu-1}e^{-\nu^2} = \left(\frac{D_y}{s}\right)^{\nu/2} \frac{\Gamma(\nu, L)}{\Gamma(\nu)}. \tag{20}
\]

Thus, the MSD becomes

\[
\langle x^2(t) \rangle = \frac{D_x}{D_y^{\nu/2}} \frac{\Gamma(\nu, L)}{\Gamma(1 + \nu/2)}. \tag{21}
\]

Again, for \( \nu = 1 \) the normal diffusive behavior along the \( x \)-direction appears, i.e. \( \langle x^2(t) \rangle \approx t \).

Here we note that the result for the MSD [19] can be obtained in the framework of fractional integration as well. By integration of equation (2) over \( y \) and using the summation on the fractal set as above in this section, for the PDF \( p_1(x, t) \) one obtains

\[
\frac{\partial}{\partial t} p_1(x, t) = D_x \sum_{l_j \in S_\nu} \frac{\partial^2}{\partial x^2} p(x, y = l_j, t). \tag{22}
\]

The Laplace transform to (22) yields

\[
s \hat{p}_1(x, s) - p_1(x, t = 0) = D_x \sum_{l_j \in S_\nu} \frac{\partial^2}{\partial x^2} \hat{p}(x, y = l_j, s). \tag{23}
\]

By representing the solution \( p(x, y, s) \) in the following way \( \hat{p}(x, y, s) = \hat{g}(x, s)e^{-\frac{n_y}{s}y} \), i.e. \( \hat{p}(x, y = l_j, s) = \hat{g}(x, s)e^{-\frac{n_y}{s}\sum_{j=1}^l y_j} \), for the \( p_1(x, s) \) we find

\[
\hat{p}_1(x, s) = \int_{-\infty}^\infty dp(x, y, s) = 2\hat{g}(x, s)\sqrt{\frac{D_y}{s}}. \tag{24}
\]

From the other side, by using the previous approach of summation, we have

\[
\sum_{l_j \in S_\nu} \hat{p}(x, y = l_j, s) = \hat{g}(x, s) \frac{1}{\Gamma(\nu)} \int_0^\infty d\nu^{\nu-1}e^{-\nu^2} \frac{D_y}{s}^{\nu/2} = \hat{g}(x, s) \left(\frac{D_y}{s}\right)^{\nu/2} = \frac{1}{2D_y^{\nu/2}} \nu^{1-\nu/2} p_1(x, s). \tag{25}
\]

By substituting relation (25) in (26), we obtain

\[
s^{1+\nu} p_1(x, s) - s^{1+\nu-1} p_1(x, t = 0) = \frac{D_x}{2D_y^{\nu/2}} \frac{\partial^2}{\partial x^2} \hat{p}_1(x, s). \tag{26}
\]

From this, the inverse Laplace transform yields the following time fractional diffusion equation

\[
\frac{\partial^{1+\nu}}{\partial t^{1+\nu}} p_1(x, t) = \frac{D_x}{2D_y^{\nu/2}} \frac{\partial^2}{\partial x^2} p_1(x, t), \tag{27}
\]

where \( \frac{\partial^{1+\nu}}{\partial t^{1+\nu}} \) is the Caputo time fractional derivative of order \( \frac{1}{2} < \frac{1 + \nu}{2} < 1 \) [23, 24]. From here we easily obtain the MSD \( \langle x^2(t) \rangle = \int_0^\infty dxx^2 p_1(x, t) \) that is of form (19). The solution for the PDF \( p_1(x, t) \) can be represented in terms of the Fox H-function \( H^{p, q}_{m, n}(z) \) [24, 30]

\[
p_1(x, t) = \frac{1}{2|x|} H^{1, 1}_{1, 1} \left[ \left(\frac{|x|}{\sqrt{D_v t^{(1+\nu)/2}}} \right) \frac{(1, 1 + \nu)/4}{(1, 1)} \right], \tag{28}
\]

where \( D_v = D_x/2D_y^{\nu/2} \) is the diffusion coefficient. Therefore, as shown, the infinite number of backbones changes the transport exponent.

IV. SUMMARY

In this paper, we introduce a diffusion equation for a comb structure where the displacements in the \( x \)-direction are possible along many backbones, even an infinite number of backbones, and we call this system by grid comb. We analyze the MSD and we show that by adding a finite number of backbones, the transport exponent in the long time limit does not change. Differently from that, an infinite number of backbones changes the transport exponent. Considering a fractal structure of backbones with fractal dimension \( \nu \) we obtained the dependence of the transport exponent on \( \nu \). We stress that the performed analysis is exact, more precisely, that the evaluation of the contribution of the fractal structure \( S_\nu \) to anomalous diffusion is exact. Finally, we show how the fractal structure \( S_\nu \) relates to the fractional Riesz derivative [23]. Let us consider the fractal structure of backbones in equation (22) separately. In the Fourier-Fourier \((\kappa_x, \kappa_y)\) space it reads

\[
-D_x \kappa_x^2 \sum_{j=1}^\infty w_j e^{i\kappa_y l_j} \tilde{P}(\kappa_x, y = l_j, t)
\]

\[
= -D_x \kappa_x^2 \sum_{j=1}^\infty \frac{w_j e^{i\kappa_y l_j}}{2\pi} \int_{-\infty}^\infty dk_y \tilde{P}(\kappa_x, \kappa_y, t) e^{-i\kappa_y l_j},
\]

\[
= -D_x \kappa_x^2 \kappa_y \int_{-\infty}^\infty dk_y \Psi(\kappa_y - \kappa_y') \tilde{P}(\kappa_x, \kappa_y', t), \tag{29}
\]

where \( \Psi(\kappa_y - \kappa_y') \) is the Weierstrass function [27]. It can be obtained by the following procedure [28]. Let us use \( w_j = \frac{1}{\sqrt{l}} \left(\frac{\chi}{l}\right)^j \), where \( l, b > 1 \), \( l - b \ll b \). Thus

\[
\sum_{j=1}^\infty w_j = \frac{l - b}{l} \sum_{j=0}^\infty \left(\frac{b}{l}\right)^j = 1, \tag{30}
\]
means that $\Psi(z) \sim \frac{1}{l^\nu}$, where $\nu = \log \frac{1}{l} / \log l$ is the fractal dimension. Thus, for relation (29) we have

$$-\mathcal{D}_x \kappa^2 \frac{L^{1-\nu}}{2\pi} \int_{-\infty}^{\infty} dk_y |\kappa_y - \kappa_y'|^{-1-\nu} \hat{P}(k_x, \kappa_y', t).$$

(34)

This integration is the Riesz fractional derivative. Note that the first attempt to take into account a fractal structure of traps was performed in [12] in the framework of a coarse graining procedure of the Fokker-Planck equation that leads to the fractional differentiation in the real space. In contrast to that, in the present analysis we are able to perform an exact analysis for the fractal structure $S_\nu$. This also relates to exact fractional differentiation in the reciprocal Fourier space.

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