Negative superdiffusion due to inhomogeneous convection

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Fractional transport of particles on a comb structure in the presence of an inhomogeneous convection flow is studied [Baskin and Iomin, Phys. Rev. Lett. **93**, 120603 (2004)]. The large scale asymptotics is considered. It is shown that a contaminant spreads superdiffusively in the direction opposite to the convection flow. Conditions for the realization of this effect are discussed in detail.

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I. INTRODUCTION

Superdiffusion on a subdiffusive medium is an example of fractional transport due to inhomogeneous convection [1]. Investigation of a space-time evolution of an initial profile of particles in specific media due to the inhomogeneous convection flow has arisen in a variety of applications such as transport of external species (pollution) in water flows through porous geological formations [2,3], problems of diffusion and reactions in porous catalysts [4], and fractal physiology [5–7]. In this paper we consider fractional transport on a comb structure. The comb model (or structure) shown in Fig. 1 is an analog of subdiffusive one-dimensional (1D) media where subdiffusion has been already observed [8]. It is a particular example of a so-called continuous time random walk (CTRW) medium [8–10]. This model is known as a toy model for a porous medium used for exploration of low dimensional percolation clusters [11] and electrophoresis processes [12]. A special behavior of the diffusion on the comb structure is that 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 teeth) is a constant $D_{yy}=D$. The diffusion process in such media (modeled by the comb structure) is anomalously slow with a subdiffusive mean squared displacement of the order of $\langle x^2(t)\rangle \sim t^{\mu}$, $\mu<1$. There are external forces leading to convection. In the general case, the velocity of the convection flow is space dependent, i.e., convection is inhomogeneous. For instance, anomalous diffusion takes place in the presence of external potentials of special forms [13,14], where contrary to our consideration a convection flow takes place in superdiffusion media. The question under investigation is how the observable shape of the initial packet changes, when the space-time evolution of the packet is affected by the convection flow. Conditions on or changes in the Liouville equation that are necessary in order to observe superdiffusion in the comb model are important for understanding the nature of the fractional transport from the general point of view.

II. SUPERDIFFUSION ON A COMB

We study superdiffusion on the comb structure due to the inhomogeneous convection described by the 2D distribution function $G=G(t,x,y)$ and the current

$$\mathbf{j}=\left(v(x,y)G-\tilde{D}\delta(y)\frac{\partial G}{\partial x},-D\frac{\partial G}{\partial y}\right), \tag{1}$$

where $\tilde{D}\delta(y)$ and D are the diffusion coefficients for the x and y directions, respectively, while the inhomogeneous convection velocity is $v(x,y)=v(x)\delta(y)=v|x|^s \mathrm{sgn}(x)\delta(y)$. The function $\mathrm{sgn}(x)$ equals 1 for $x>0$ and -1 in the opposite case, while v is a dimension velocity constant such that $v|x|^s$ has the dimension of the diffusion coefficient D. The Liouville equation

$$\frac{\partial G}{\partial t}+\mathrm{div}\,\mathbf{j}=0 \tag{2}$$

corresponds to the following Fokker-Planck equation:

$$\frac{\partial G}{\partial t}+\hat{L}_{FP}(x)G\delta(y)-D\frac{\partial^2 G}{\partial y^2}=0, \tag{3}$$

where the Fokker-Planck operator in the x direction is

$$\hat{L}_{FP}(x)G=-\tilde{D}\frac{\partial^2 G}{\partial x^2}+v|x|^s\,\mathrm{sgn}(x)\frac{\partial G}{\partial x}+sv|x|^{s-1}G.$$

It is convenient to work with dimensionless variables. The dimensionless time and coordinates are obtained by rescaling with relevant combinations of the comb parameters D and $\tilde{D}$. One obtains the following new variables for time $D^3t/\tilde{D}^2\to t$ and coordinates $Dx/\tilde{D}\to x$, $Dy/\tilde{D}\to y$, while the dimensionless velocity parameter is $(\tilde{D}/D)^s vD^{-1}\to v$. Hence, we study the following dimensionless equation:

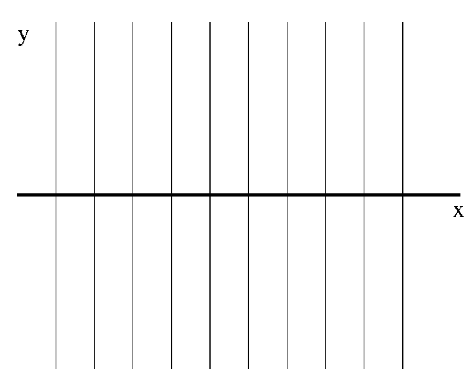

FIG. 1. The comb structure

$$\frac{\partial G}{\partial t} - \frac{\partial^2 G}{\partial x^2}\delta(y) - \frac{\partial v(x)G}{\partial x}\delta(y) - \frac{\partial^2 G}{\partial y^2} = 0, \tag{4}$$

where $v(x)$ is dimensionless as well. The initial condition is $G(0,x,y)=\delta(x)\delta(y)$, and the boundary conditions on the infinities have the form $G(t,\pm\infty,\pm\infty)=0$ and the same for the first derivatives with respect to x and y $G'_x(t,\pm\infty,\pm\infty)=G'_y(t,\pm\infty,\pm\infty)=0$. The transport of particles along the structure x axis is described by the function $G(t,x,y=0)=g(x,t)$. It is worth stressing that the tails of the distributions are the most interesting for applications. Therefore, we are studying here the large scale asymptotics when $|x|\gg 1$. In the Laplace-Fourier ($\mathcal{LF}$) space (p,k) Eq. (4) is transformed to the following fractional equation for the function $\tilde{g}=\tilde{g}(p,k)=\mathcal{LF}[g(t,x)]$:

$$k^2\tilde{g}(p,k) + ikv\frac{\partial^s}{\partial k^s}\hat{F}[\tilde{g}(p,k)] + 2\sqrt{p}\tilde{g}(p,k) = 1. \tag{5}$$

Here the fractional Reisz derivative is the result of the Fourier integration [10,15–17]

$$\int_0^\infty (ix)^s\tilde{g}(p,x)e^{ikx}dx = \frac{\partial^s}{\partial k^s}\int_0^\infty \tilde{g}(p,x)e^{ikx}dx.$$

The function $\hat{F}[\tilde{g}(p,k)]$ is a formal notation of the following integral:

$$\hat{F}[\tilde{g}(p,k)] = \int_0^\infty \sin(kx + s\pi/2)\tilde{g}(p,x)dx.$$

As one sees, Eq. (5) has unclosed form. Nevertheless, as will be seen from the following analysis, it does not lead to any deficiency, since we are looking for a solution in the (p,x) space. It should be stressed that the explicit form of Eq. (5) in the (p,x) space is important in order to justify the large scale asymptotics for $|x|\gg 1$.

The large scale asymptotics $|x|\gg 1$ corresponds to $|k|\ll 1$ in the Fourier space. Therefore, the first term in Eq. (5) can be omitted at the condition

$$\lim_{\substack{k\to 0\\ p\to 0}} \frac{k^2}{p^{1/2}} = 0. \tag{6}$$

This approximation depends on the form of singularity of the the convection velocity in the limit $x\to\infty$. It means that the asymptotic solution of the homogeneous part of Eq. (5) for $|k|\ll 1$ depends on the exponent s in the power law $|x|^s$ in Eq. (4) for $|x|\gg 1$ [18–20]. After performing the inverse Fourier transform, one obtains the asymptotic solution for $x\gg 1$ that corresponds to the homogeneous part of Eq. (5). It reads

$$\tilde{g}(p,x) = \frac{C}{v|x|^s}\exp\left[\frac{2\sqrt{p}|x|^{1-s}}{(s-1)v}\right], \tag{7}$$

where C is a constant. Since Eq. (7) is an asymptotic solution, one puts $C=1$ without losing generality. This solution describes asymptotic transport of any initial profile. To obtain the time-dependent solution one carries out the inverse Laplace transform $g(t,x)=\mathcal{L}^{-1}[\tilde{g}(p,x)]$. The necessary condition for the Laplace inversion needs the function in the exponential in Eq. (7) to be negative [21]. It depends only on s and the sign of v. When $s<1$, the initial profile of particles moves in the directions of the convection flow, namely, in the direction of $v=|v|>0$. It is enhanced superdiffusion due to the inhomogeneous convection. This case, together with $s=1$ and 0, has been considered in detail in [1]. The last two cases are specific. When $s=1$, Eq. (7) changes and corresponds to the log-normal distribution. Conversely, $s=0$ is the limit case of Eq. (7). The interplay between the homogeneous convection and traps leads to normal diffusion with the second moment $\langle x^2(t)\rangle=(v^2/D)t$, where the effective diffusion coefficient v^2/D is determined by the external forcing v.

III. NEGATIVE SUPERDIFFUSION

When $s>1$ the situation is more interesting and leads to different effect. Indeed, for $s>1$, the necessary condition to perform the inverse Laplace transform is negative $v<0$. Hence, the solution is

$$g(t,x) = \frac{|x|^{1-2s}}{v^2(s-1)\sqrt{\pi t^3}}\exp\left[-\frac{x^{2-2s}}{v^2(s-1)^2 t}\right]. \tag{8}$$

When $|x|\gg 1$ and t is large enough, the exponential is equal to unity. It results in a power law form for the distribution which corresponds to superdiffusion of particles,

$$g(t,x) \propto \frac{1}{|x|^{2s-1}\sqrt{\pi t^3}}. \tag{9}$$

All moments of x higher than $2s-2$ are equal to infinity. It means that on large scale asymptotics, when $x^{2(s-1)}t\gg 1$, there is superdiffusion, which is analogous to Lévy flights. It should be outlined that the flux on the infinities is vanishing. The important feature of this superdiffusion is that it occurs in the direction opposite to the inhomogeneous convection current.

This phenomenon is related to the relaxation process with diffusion, where the Kolmogorov conditions (see [15]) are necessary for the inferring of the Fokker-Plank equation (FPE). It means that in the absence of convection the solution of the FPE gives that at any moment $t>0$ the particles are spread over the whole x axis from minus infinity to plus infinity with exponentially small tails. Therefore, there is a finite concentration of the contaminant at any moment and in any point. It is correct not only for normal diffusion but also for subdiffusive relaxation on the comb structure with corresponding solution [11]

$$g(t,x) = \frac{1}{2\pi\sqrt{t^3}}\int_0^\infty \exp\left[-\frac{x^2}{4u} - \frac{u^2}{t}\right]u^{1/2}du. \tag{10}$$

This behavior described by Eq. (10) dominates for small x even in the presence of inhomogeneous convection. But for asymptotically large x the inhomogeneous convection in the direction opposite to the spreading of particles changes the shape of the tail of the packet from exponential to a power law according to Eq. (9). We call this solution the negative superdiffusion (NS) solution.

IV. FRACTIONAL FOKKER-PLANCK EQUATION

The total number of transporting particles on the structure axis decreases with time due to the comb structure [1,11]

$$\langle G\rangle = \int_{-\infty}^{\infty} g(t,x)dx = 1/2\sqrt{\pi t}. \qquad (11)$$

Therefore, the distribution function (8) describes the NS when the number of particles $\langle G\rangle$ is not conserved. The formulation of the NS problem with conservation of the total number of particles is equivalent to the case with a continuous distribution of the delay times [9], where the total number of particles is described by the function $G_1(t,x) = \int_{-\infty}^{\infty} G(t,x,y)dy$. It is the CTRW approach. It is straightforward to see from Eq. (4) that

$$G(t,x,y) = \mathcal{L}^{-1}[\tilde{g}(p,x)e^{-\sqrt{p}|y|}]. \qquad (12)$$

Taking this into account, one obtains the equation for G_1 by integrating Eq. (4) with respect to the variable y. It reads in the Laplace space for $\tilde{G}_1(p,x) = \mathcal{L}[G_1(t,x)]$

$$p\tilde{G}_1(p,x) + \hat{L}_{FP}(x)\tilde{g}(p,x) = \delta(x), \qquad (13)$$

where $\hat{L}_{FP}(x)$ is the same operator as in Eq. (3). It is straightforward to see by carrying out either the Laplace transform of Eq. (4) or the Fourier transform of Eq. (5) that

$$\hat{L}_{FP}\tilde{g}(p,x) = \delta(x) - 2\sqrt{p}\tilde{g}(p,x).$$

Substitution of this expression in Eq. (13) yields

$$\tilde{g}(p,x) = \frac{1}{2}\sqrt{p}\tilde{G}_1(p,x). \qquad (14)$$

Again, after substitution of this relation in Eq. (13), the CTRW equation in the Laplace space is

$$p\tilde{G}_1 + \frac{1}{2}p^{1/2}\hat{L}_{FP}(x)\tilde{G}_1 = \delta(x). \qquad (15)$$

We introduced here the Riemann-Liouville fractional derivatives (see, for example, [10,22]) $(\partial^{\alpha}/\partial t^{\alpha})f(t)$ by means of the Laplace transform $(0<\alpha<1)$

$$\mathcal{L}\left[\frac{\partial^{\alpha}}{\partial t^{\alpha}}f(t)\right] = p^{\alpha}\tilde{f}(p), \qquad (16)$$

where $\mathcal{L}[f(t)] = \tilde{f}(p)$, and it also implies $\partial^{\alpha}[1]/\partial t^{\alpha} = t^{-\alpha}/\Gamma(1-\alpha)$, $\Gamma(z)$ is a gamma function [22]. Using this definition, we write the CTRW equation, which corresponds to the comb model described by Eq. (4), in the following form:

$$\frac{\partial G_1}{\partial t} + \frac{1}{2}\frac{\partial^{1/2}}{\partial t^{1/2}}\hat{L}_{FP}(x)G_1 = 0. \qquad (17)$$

Here the initial condition is $G_1(0,x) = \delta(x)$. For the asymptotically large scale $x \gg 1$ (or $x \ll -1$), we neglect the inhomogeneous term together with the second derivatives with respect to x in Eq. (15) and obtain a solution determined by Eqs. (7) and (14). This is the NS related to the CTRW by the following result:

$$\tilde{G}_1(p,x) = \frac{2}{vx^s p^{1/2}}\exp\left[\frac{2p^{1/2}x^{1-s}}{v(s-1)}\right]. \qquad (18)$$

V. LIOUVILLE-GREEN APPROXIMATION

We infer here the NS in the framework of the Liouville-Green (LG) asymptotic solution for linear differential equations [19]. We show that the approximation performed above due to the condition (6) is sufficiently good and corresponds to the Liouville-Green approximation, also called the WKB approximation [23]. The CTRW equation (17) in the generalized form reads

$$\frac{\partial G_1}{\partial t} + \alpha\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\hat{L}_{FP}(x)G_1 = 0, \qquad (19)$$

where $0<\alpha<1$. Hence, for $x \gg 1$, we obtain the homogeneous part left-hand side of Eq. (15), where the item $p^{1/2}$ is substituted by $p^{1-\alpha}$. It reads

$$p\tilde{G}_1 + \alpha p^{1-\alpha}[-\tilde{G}_1'' + vx^s\tilde{G}_1' + svx^{s-1}\tilde{G}_1] = 0. \qquad (20)$$

The term in the first derivative is removed from the equation by the substitution

$$\tilde{G}_1 = p^{\alpha-1}\exp[vx^{s+1}/2(s+1)]w. \qquad (21)$$

Thus we have $w'' = R(x)w$, where

$$R(x) = \frac{v^2x^{2s}}{4}\left(1 + \frac{2s}{v}x^{-s-1} + \frac{4}{\alpha v^2}p^{\alpha}x^{-2s}\right).$$

The LG approximation for w, which satisfies the accepted boundary conditions [see Eq. (4)], is

$$w = BR^{-1/4}\exp\left[-\int R^{1/2}dx\right] = B\sqrt{\frac{v}{2}}\frac{1}{x^s}\exp\left[-\frac{vx^{s+1}}{2(s+1)} + \frac{p^{\alpha}x^{1-s}}{\alpha v(s-1)}\right], \qquad (22)$$

where B is a constant. Analogously, we obtain the LG solution for the negative $x \ll -1$. Therefore, taking $B=(2/v)^{3/2}$ and $\alpha=1/2$, we obtain that Eq. (21) coincides exactly with the solution (18). This means that removing the second derivatives from $\hat{L}_{FP}$ or the term k^2 in Fourier space in the limit $k \to 0$ corresponds to the Liouville-Green approximation for the Fokker-Planck equation with inhomogeneous (superdiffusive) convection. This asymptotic solution is superdiffusive transport of particles in the direction opposite to the convection current, namely, the NS.

VI. COUNTERINTUITIVE EXAMPLE

There are many possible values for the parameters s and v of the convection flow $v(x)$ in Eq. (1). But the Laplace transform chooses only that necessary range of parameters $v>0$, $s<1$ and $v<0$, $s>1$ which satisfies the physically meaningful realization. This is seen from the consideration of the dynamical flow of a tracer. By analogy with Sec. V we con-

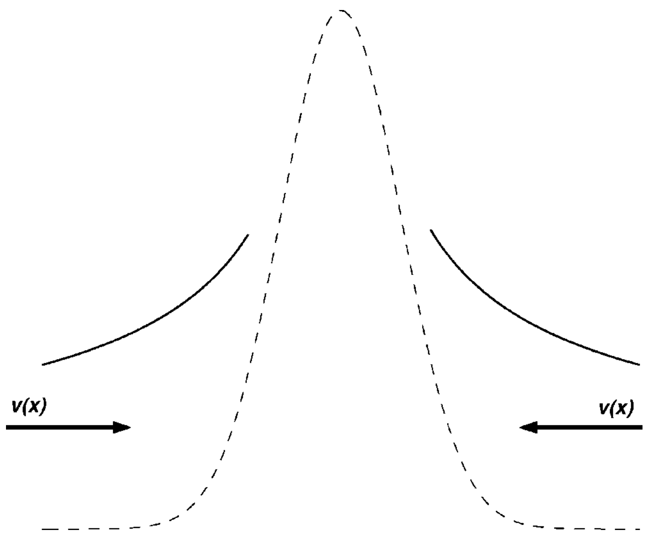

FIG. 2. A sketch of the NS, where $v(x)$ is the inhomogeneous convection in the direction opposite to the natural spreading of the contaminant. The dashed curve corresponds to the spreading due to the relaxation process, while the solid lines are the tails of the power law due to superdiffusion. The distributions are shown at the same moment t.

sider $x>0$ (for $x>0$ the consideration is the same). Hence, the equation of motion for the tracer reads

$$\dot{x} = vx^s \tag{23}$$

with the initial condition $x(t=0)=x_0$. The solution is

$$x(t) = x_0/[1-(s-1)x_0^{s-1}vt]^{1/(s-1)}. \tag{24}$$

When $s>1$ and $v>0$ this solution is singular, since during the finite $t=t_0\equiv 1/(s-1)vx_0^{s-1}$ the tracer reaches infinity with infinite velocity. Therefore, the only physical solution is when $v<0$. When $x_0=0$, the tracer does not move at all. Therefore, only particles with nonzero initial conditions move with the convection flow. A question is, how does a particle appear in the point $x_0\neq 0$ if the initial distribution is $\delta(x)$? The Kolmogorov mechanism, which is discussed in Sec. III and related to the second partial derivative $\tilde{D}\partial^2/\partial x^2$, distributes the initial packet of the contaminant over the entire x axis. The convection flow with $v<0$ brings these particles back to $x=0$. This process changes the distribution from a Gaussian one to the power law form, as shown in Fig. 2. It should be stressed again, in this connection, that there are many possibilities for v and s to realize the inhomogeneous convection flow, but the contaminant can be captured by convection only at physical conditions when $s>1$, $v<0$ or $s<1$, $v>0$. It is quite remarkable that the Laplace transform chooses just these physical solutions [24]. The solutions (7) and (18) describe other possibilities as well. For instance, when $v(x)=v|x|^s$ the NS solution exists for the conditions $s>1$, $v>0$, but $x<0$. In this case the convection flow is opposite to the natural spreading of the initial packet for $x<0$, while for $x>0$ there is no solution at all. When $s<1$ the solution with $v>0$ takes place for $x>0$ [1]. The case with $s=1$ stays separate, since the solutions are possible for both $v>0$ and $v<0$. This boundary case corresponds to the log-normal distribution and it was considered in [1] in detail. It also describes the fractional version of the Ornstein-Uhlenbeck process (see, e.g., [10]).

VII. CONCLUSION

We obtained superdiffusion due to inhomogeneous convection on a subdiffusive medium described by the comb model. A specific feature of this superdiffusion is the existence of Lévy flights in the direction opposite to the convection current. This effect is called here negative superdiffusion. This effect depends unambiguously on the system parameters $s>1$ and $\alpha=1/2$. These values are important both for the continuity condition of the contaminant and, at the same time, for the negative superdiffusion. Indeed, since we study the continuity equation (2), solutions (7) and (18) determine the continuity condition of the contaminant. Therefore, when $s>1$ this continuity ensures such a scenario when the inhomogeneous convection flows in the direction opposite to the natural spreading of the contaminant. This effect is sketched in Fig. 2, where the natural spreading is a process with increase of the width of the initial packet. Conversely, when $s<1$ the continuity condition ensures that the inhomogeneous convection moves in the same direction as the contaminant [1]. It should be stressed that this effect can be realized in a subdiffusive or CTRW medium only. In our case this is the comb structure, where $\alpha=1/2$. In this connection, the relation between s and α could be an important condition on continuity for a possible realization of negative superdiffusion in a CTRW medium, in the general case.

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[24] In this connection, it should be underlined that the observed solution reflects the theorem on the unique relation between the Laplace transform and the probability distribution function (PDF), which reads that distinct PDFs have distinct Laplace transforms; see W. Feller, *An Introduction to Probability Theory and Its Applications* (John Wiley and Sons, New York, 1971), Vol. 2, Chap. 13.