

Subdiffusion in random compressible flows

Konstantin Chukbar¹ and Vasily Zaburdaev^{1,2,*}

¹RRC "Kurchatov Institute," Pl.Kurchatova, 1, 123182 Moscow, Russia

²Max-Planck-Institute for Dynamics and Self-Organization, Bunsenstr.10, 37073 Goettingen, Germany

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In this work, we study the diffusion of admixture particles in a one-dimensional velocity field given by a gradient of a random potential. This refers us to the case of random compressible flows, where previously only scaling estimates were available. We develop a general approach which allows to solve this problem analytically. With its help we derive the macroscopic transport equation and rigorously show in which cases transport can be subdiffusive. We find the Fourier-Laplace transform of the Green's function of this equation and prove that for some potential distributions it satisfies the subdiffusive equation with fractional derivative with respect to time.

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I. INTRODUCTION

Diffusion of particles in a random environment is a general physical problem which continuously receives attention in the context of a wide range of phenomena. Various anomalous (compared to the classical diffusion) types of behavior were discovered and investigated [1–4]. Of course, one tries to find a universal language for the description of such kinds of processes. One of the possibilities is a language of fractional derivatives which have already proved to be a useful and flexible tool for the description of a number of stochastic processes. In this paper we employ this language to address the question of anomalous diffusion in static random compressible flows. The influence of convection on molecular diffusion has been studied in many theoretical works (see cited reviews and Refs. [5,6]). As a rule, incompressible velocity fields are considered. We should especially mention the work of Vergassola and Avellaneda [7] on the scalar transport in compressible flows, which is closely related to the subject being considered here. Their work showed that static potential one-dimensional flow can deplete the diffusion due to the trapping of particles, while in the majority of cases, convection leads to enhanced diffusion. The case of random potential, which is particularly interesting, was only mentioned. By their analogy with Sinai's problem [8] (see also Ref. [3]) the authors of Ref. [7] anticipated the scaling of the subdiffusion regime.

In our work, we show rigorously that, under some conditions on the velocity potential, transport is subdiffusive. The analytical expression for the Fourier-Laplace transform of the Green's function of the macroscopic transport equation is the central result of this paper. Moreover, for some particular classes of velocity distributions, transport is governed by the subdiffusion equation with fractional derivative with respect to time, which means that the exact analytical solution of the problem in usual time and space coordinates can be found. It is remarkable, that the general method used for this derivation is also applicable to the problem of the diffusion on

comblike structures, and, in simplified form, to the periodic potential case. The contents of this paper is organized in the following way. First, we consider the case of a periodic velocity field and recover the result of Ref. [7] on the depletion of the transport. In Sec. III, we solve analytically the problem of subdiffusion of a passive scalar in a one-dimensional compressible random velocity field. The averaging procedure and fractional derivative equations are also briefly considered there. In the last section, we conclude and discuss open problems.

II. PERIODIC POTENTIAL

We will consider the advection-diffusion equation and first restrict ourselves to the one-dimensional case,

$$\frac{\partial n}{\partial t} + \nabla(nv) = D\Delta n,$$

$$n = n(x, t), \quad v = v(x), \quad D = \text{const.} \quad (1)$$

The velocity field is static and its characteristic scale is much smaller than the scale of the gradients of the macroscopic density of particles. Nontrivial influence of advection on the particle diffusion could be found even for the simplest case of the periodic velocity field $v = -\nabla\varphi$, where $\varphi(x)$ is a periodic potential with period l , $\varphi(x+l) = \varphi(x)$. One can bear in mind the following example, $\varphi(x) = b[\sin(2\pi x/l) - 1]$, where b is the well depth. Equation (1) can be rewritten in terms of flow q ,

$$\frac{\partial n}{\partial t} = -\nabla q,$$

$$q = nv - D\frac{\partial n}{\partial x}.$$

One can find the stationary solution of (1),

$$\frac{\partial n}{\partial t} = 0, \quad q = q_0 = \text{const},$$

*Electronic address: vasily.zaburdaev@mpi-sf.mpg.de

$$n_{st}(x) = \left(\int_{x_0}^x \frac{q_0}{D} e^{\varphi(y)/D} dy \right) e^{-\varphi(x)/D} \quad (2)$$

from which it is easy to see that wells collect an exponential number of particles leaving rarefied regions in between.

Now we will look for small perturbation of the stationary solution and substitute q_0 by slow varying (see below) $q(x, t)$,

$$\frac{\partial n}{\partial t} = -\nabla q(x, t).$$

We will look for the time-dependent solution in the form

$$n(x, t) = \left(\int_{x_0}^x \frac{q(y, t)}{D} e^{\varphi(y)/D} dy \right) e^{-\varphi(x)/D}.$$

We are interested in the macroscopic concentration of particles, which corresponds to the average over several characteristic lengths (periods) of the potential $\langle n \rangle = (1/L) \int_{x-L/2}^{x+L/2} n(y, t) dy$, $L \gg l$. Now it is desirable to connect the gradient of macroscopic density distribution with the flow q ,

$$\frac{\partial \langle n \rangle}{\partial x} = \frac{\partial}{\partial x} \frac{1}{L} \int_{x-L/2}^{x+L/2} \left(\int_{z_0}^z \frac{q(y, t)}{D} e^{\varphi(y)/D} dy \right) e^{-\varphi(z)/D} dz.$$

Taking in account the slow variation of $q(x, t)$ on the averaging scale L and the periodic property of the potential we arrive at

$$\frac{\partial \langle n \rangle}{\partial x} = \frac{q(x, t)}{D} \left(\text{const} + \frac{\alpha}{L} \int_0^L e^{-\varphi(z)/D} dz \right), \quad (3)$$

where α defined as

$$\int_{z_0+x}^{z_0+x} e^{\varphi(y)} dy \approx \alpha(z - z_0).$$

The first term in the parentheses in (3) is of the order of unity, whereas the second one is of the order of $\exp(b/D)$ (where b is the depth of the potential well) and is therefore dominant. Finally we can write

$$q(x, t) = D^* \frac{\partial \langle n \rangle}{\partial x},$$

$$\frac{\partial \langle n \rangle}{\partial t} = D^* \frac{\partial^2 \langle n \rangle}{\partial x^2}, \quad D^* \propto e^{-b/D}.$$

The macroscopic transport would still be diffusive but with an exponentially small (depending on the potential well depth) effective diffusion coefficient. This result was recovered in several previous works (see Refs. [3,7]) and it could be anticipated based on the very simple physical picture of the process. Each potential well is a trap which attracts an exponentially large number of particles, but the macroscopic transport is only due to the diffusion of particles between these wells, whose population, respectively, is exponentially

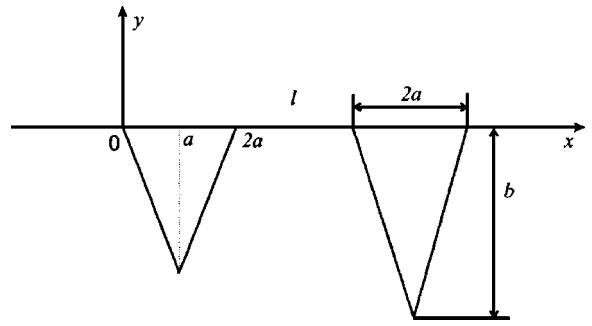


FIG. 1. Random potential of the velocity field $\varphi(x)$.

small, compared to the total amount of admixture being transported. This leads to the exponential decrease in the diffusion constant.

III. DIFFUSION IN A RANDOM VELOCITY FIELD

Now consider the case of the random velocity field, given by a random potential. We notice from the previous example, that the basic property of the potential, which is important for transport, is the capacity of wells and the distance between them, which gives one of the characteristic space scales of the problem. For the simplicity of the intermediate calculations, we choose a model potential with symmetric triangular wells of equal width $2a$, separated by equal distances l but with random distribution of depths b (see Fig. 1).

First, we reformulate the approach, which we have already implicitly applied for the periodic potential, for the case of the random velocity field. The essential point here is the separation of the particles $n(x, t)$ into two groups, diffusing between the wells $n_x(x, t)$ and wondering inside them $n_w(x, t)$. The concentration of particles, as well as their total number inside each well $N_w(t)$, depends on the $n_x(t)$, taken on its boundaries, and on the well depth. The idea now is to connect the two concentrations and write the macroscopic transport equation for the total concentration of particles taking into account that only a part of them is actually responsible for the transport.

We are in a typical situation of the quenched disorder [3,4] when the motion of particles in a fixed but random environment is considered. That is why inevitably we are faced with an averaging procedure, which helps us to pass to the macroscopic transport equation.

We have a fixed realization $b(x) = b(x_n) = b_n$ of a random process (well depths) with the probability distribution $P(b)$. There are several ways how to simplify this problem. The first and the most common is the ensemble averaging, or averaging over the realizations of the random potential. This does not fit our purposes, as we are trying to predict the macroscopic dynamics in a fixed sample, but not its statistical properties. This is why we use another approach which incorporates the “self-averaging” feature of our random variable. There are discussions on the different ways of averaging [9,10], some of which lead to paradoxical and nonphysical results. The method suggested below seems to be natural from the physical point of view and correctly recovers all

limiting cases. We are looking for the macroscopic dynamics on scales reasonably exceeding characteristic potential scale l . Quantities which are physically important or measured values would characterize an area of the size \hat{L} around point X containing a large number of wells N ,

$$\overline{f(X)} = (1/N) \sum_{n=0}^N f(b_n),$$

where b_n is a subset of the realization of the random process, b_m and b_k are independent if $m \neq k$. If N is sufficiently large, for the typical realization b_n we can write

$$\bar{f} = \int_0^\infty f(b) P(b) db. \quad (4)$$

Here we used the law of large numbers. This transition can also be called self-averaging. Now we can finally state the hierarchy of scales in our problem,

$$l \ll \hat{L} \ll X, \quad (5)$$

where \hat{L} is the averaging window, and X is the scale of the macroscopic change of the concentration of particles.

Thus the total concentration can be written as

$$n(x, t) = n_x(x, t) + \frac{\bar{N}_w(n_x(x, t))}{l}.$$

But the macroscopic transport is only due to the free particles n_x , that is why in principle it can be slower than classical diffusion,

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n_x}{\partial x^2}. \quad (6)$$

For the periodic potential we know (2) that N_w is simply proportional to the n_x , but the coefficient of the proportionality is exponentially big, then from (6) it follows directly that transport is diffusive but depleted. The situation becomes entirely different when allowance for the deep wells changes the time behavior of N_w . We will now consider this case.

We must find the capacity of the well $N_w(t)$ as a function of time and boundary conditions. To do this analytically, we have chosen the simplest form of the potential well—triangular and symmetric. Then the velocity of particles is equal to $v = b/a = \text{const}$ on the left slope and $-v$ on the right slope of the well, where b and $2a$ are the depth and width of the well, respectively (see Fig. 1). We choose the left boundary of the well as an origin for the frame of reference. At the left ($x=0$) and right ($x=2a$) boundary, the concentration of particles in the well n_w is equal to $n_x(t)$ (variation of the macroscopic concentration on the size of the well is negligible), in the center of the well ($x=a$) we set the zero flow condition because of the symmetry of the problem,

$$n_w|_{x=0} = n_x(t), \quad q = q(x=a-) + q(x=a+) = 0,$$

$$q(x = \pm a) = \mp n_w v + D \frac{\partial n_w}{\partial x} \Big|_{x=a\pm}.$$

Other physically reasonable boundary conditions could be set up as well, but in the calculation of the total number of trapped particles they give the same asymptotic result. The transport equation in the well itself is

$$\frac{\partial n_w}{\partial t} \pm n_w v = D \frac{\partial^2 n_w}{\partial x^2}. \quad (7)$$

We use the Laplace transform method to solve it. Starting from initially empty wells $n_w(x)|_{t=0}=0$ we can get the answer for the Laplace component of the concentration (e.g., in the left part of the well)

$$n_{w,p} = c_1 e^{(v+q)/2D} + c_2 e^{(v-q)/2D}, \quad q = \sqrt{4Dp + v^2}.$$

One can subtract the stationary solution of (7) and consider only the perturbation to it. In any case what one needs to know is how fast the well reacts on the change of boundary conditions and how many particles it is able to swallow. The coefficients c_1 and c_2 are found from the boundary conditions,

$$c_1 = \frac{-(q+v)n_{x,p}}{e^{qa/D}(v-q)-v-q}, \quad c_2 = \frac{e^{qa/D}(v-q)n_{x,p}}{e^{qa/D}(v-q)-v-q}.$$

Then the total number of particles in the well, $N_{w,p}$, is

$$N_{w,p} = 2 \int_0^a n_{w,p}(x) dx = 2 \frac{n_{x,p} 2D (1 - e^{aq/D})}{-q - v + e^{aq/D}(v - q)}.$$

As we are interested in the asymptotic behavior for large time scales corresponding to small p we can make the expansion,

$$N_{w,p} = 2 \frac{n_{x,p} D (1 - e^{av/D})}{-v - \frac{D}{v} (e^{av/D} + 1)p} = n_{x,p} g_p(v). \quad (8)$$

In ordinary time, the expression for $g(t)$ is

$$g(t) = 2 \frac{(e^{av/D} - 1) v e^{-v^2 t / D (e^{av/D} + 1)}}{e^{av/D} + 1}.$$

To follow the rate of the filling and the capacity of the well we impose the constant condition on its boundaries $n_x(x=0)=n_x(2a)=n_0$,

$$N_w(t) = \frac{n_0 D}{v} (e^{av/D} - 1) (1 - e^{-v^2 t / D (1 + e^{av/D})}).$$

From the above expression we can see that the filling process is exponentially slow and the capacity is exponentially big. This is the crucial feature of the system. Each well represents a trap which swallows almost all particles approaching it. In principle, it can terminate all transport. This is the specific side of the quenched disorder (compared to the annealed one). Once a realization of the potential with one extremely deep well is given, it would collect all of the particles and no

transport would be possible. This property is hidden in Eq. (4), when we pass from the sum to the integral we use the notion of typical realization of the random process and convergence in the probabilistic sense. The question of convergence for exponential fluctuations is particularly delicate and requires additional mathematical treatment in the context of quenched disorder phenomena. Meanwhile we leave this problem for future investigations.

Nevertheless if one assumes that the distribution of depths is decaying fast enough to prevent the appearance of extremely deep wells, one can proceed with calculating macroscopic transport equations according to the suggested approach.

Moving onto the macroscopic description we perform the averaging of (8) [scaling relations (5) should be kept in mind] with a distribution function of depths of wells $f(b)[f(v)]$ and find its asymptotic at small p or large t . We choose $f(b)$ in the form

$$\frac{A}{D^2} \frac{be^{-ab/D}}{(1+b/D)^\beta}, \quad (9)$$

where $A(\alpha, \beta)$ is a normalizing factor. The averaging integral reads

$$2a \int_0^\infty \frac{(e^x - 1)e^{-\alpha x}}{x^2 + \frac{a^2 p}{D}(e^x + 1)} \frac{x^2}{(1+x)^\beta} dx. \quad (10)$$

In case $\alpha > 1$ deep wells are suppressed and the transport, as we showed before, is purely diffusive. But for $\alpha < 1$ the above integral diverges as p tends to zero due to the exponential growth of the integrand at large x . The accurate calculation of the p asymptotic of this integral is quite a delicate problem and we do it in a detailed manner in the Appendix, which gives us the following result:

$$g_p = O\left(\frac{p^{(\alpha-1)}}{\ln^{\beta+2(\alpha-1)} p}\right). \quad (11)$$

Choosing $\beta=2(1-\alpha)$ one can have purely fractional power law divergence at small p .

Now it is the right time to remember Eq. (6). After Laplace and Fourier transformation with respect to time and coordinate x , respectively, (6) reads

$$pn_{p,k} - n_0 = -k^2 Dn_{w,k,p}. \quad (12)$$

From (8) we know the connection between total number of particles and the concentration on its boundaries, thus

$$n_{k,p} = n_{x,k,p} + \bar{N}_{w,p}/l = n_{x,k,p}(1 + g_p/l), \quad (13)$$

where g_p is given by (11). Combining (12) and (13) we obtain the answer for the Fourier-Laplace transform of the concentration of particles,

$$n_{p,k} = \frac{n_{0k} \lambda p^{\alpha-1}}{(\lambda p^\alpha + Dk^2)},$$

$$\alpha < 1, \quad \lambda = \frac{2a}{l} \pi \csc[\pi(1-\alpha)] \left(\frac{a^2}{D}\right)^{\alpha-1}. \quad (14)$$

This formula gives the analytical solution of the problem. It is remarkable that (14) represents a standard form of writing an anomalous diffusion equation with fractional derivatives in Fourier-Laplace space [11–13]. Transforming it back to normal space and time coordinates we obtain

$$\frac{\partial^\alpha n}{\partial t^\alpha} = \frac{D}{\lambda} \frac{\partial^2 n}{\partial x^2} + \frac{n_0(x)}{t^\alpha}. \quad (15)$$

Complete information about anomalous diffusion equations in fractional derivatives, their properties, solutions and applications can be found in a number of excellent reviews [2,11,14,15]. Subdiffusion equations are of particular interest because in fewer cases they can be rigorously derived from the underlying physical problem. In addition to those being discussed in the current paper, Refs. [6,16–18] should also be noted in this connection. We will mention here only the basic features of (15) [12,13]. The solution of (15) has self-similar form

$$G(r,t) = \frac{1}{t^{\alpha/2}} \Phi\left(\frac{x}{t^{\alpha/2}}\right). \quad (16)$$

This self-similarity, which in general drastically simplifies the problem, here is self-attracting. It means that for any initial distribution after some time the profile of the Green's function of the equation would be formed. The spreading of the cloud is governed by slower than classical diffusion scaling law $\bar{x} \propto t^{\alpha/2}$. Here the question of memory effects arises [19]. Besides obvious memory included in the nonlocal time derivative operator (which is a convolution type integral with a power law function), there exists a strong dependence on the initial condition. One can easily check that (15) does not possess the semigroup property or, in other words, breaks the continuity of the evolution. It was shown in Ref. [19] that only by taking into account microscopic details of the transport, one can have a complete and exact description of the problem. Moreover, by special choice of the initial microscopic distribution evolution can differ from (15) on microscopic times. In the case of the diffusion in a random compressible flow, it is the initial filling of wells which plays the role of microdistribution. That is why setting them to be empty in the beginning is a quite critical assumption.

For the general case [other possible values of β in (9) and (11)], evolution is still subdiffusive and its Green's function can be found in the spirit of (14) with a more complicated (usually logarithmic) dependence on p , although it cannot be represented in the language of fractional derivatives,

$$n_{p,k} = \frac{n_{0k}(1 + g_p/l)}{[p(1 + g_p/l) + Dk^2]}, \quad (17)$$

where g_p is given by the average of (8). Thus for any given velocity distribution the problem reduces to the calculation of the average (8) and inverse Fourier-Laplace transform of

(17) which, with a power of modern numerical techniques, is not at all difficult.

It should be noted, that the approach developed and used in this paper can be successfully applied to the problem of the diffusion on comblike structures [9,10,16,20–23]. It allows to derive macroscopic equations in a natural way as well as to establish a connection to the continuous time random walk model [15]. The results perfectly reproduce recent theoretical works [9,22] and numerical simulations [10], but the more detailed description of this topic is beyond the scope of this paper.

IV. CONCLUSIONS

We have proposed a simple approach, which is based on the separation of particles into two classes, resting and wandering in traps (wells of the potential of the velocity field) and working as carriers in between resting points, which drive the transport of the whole population of both classes. Capability of traps to accept and accommodate particles plays the essential role in the overall transport. The analytical solution for this problem was found in terms of the Fourier Laplace transform of the Green's function of the effective transport equation. It was shown that random potential field of velocities can lead not only to the depletion of the diffusion, but also to the slower subdiffusion behavior with different self-similarity $\bar{x} \propto t^\gamma$, $0 < \gamma < 1/2$. In these cases, the transport can be described in terms of fractional derivative equations. We believe that using the language of fractional derivatives, which naturally appear in various physical problems, significantly simplifies them and visualizes their solutions and properties. It was also noted that the averaging procedure and results obtained with its help, should be referred to the real experimental conditions carefully. To the best of our knowledge, the mathematical side of this procedure in the context of the quenched disorder was scarcely investigated and remains an open problem.

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APPENDIX

To estimate (10) we note that x^2 in the nominator allows us to replace $e^x - 1 \rightarrow e^x$ without creating discontinuity in 0 [this convenience is the reason for the choice of the distribution function (9)]. We also substitute $e^x + 1 \rightarrow e^x$,

$$\int_0^\infty \frac{e^x e^{-\alpha x}}{x^2 + p' e^x (1+x)^\beta} dx = \int_0^\infty \frac{e^{-\alpha x}}{x^2 e^{-x} + p' (1+x)^\beta} \frac{x^2}{dx},$$

where $p' = (a^2 p / D) \rightarrow 0$. By the change of variables $y = e^{-x} / p'$ it is converted to

$$p'^{(\alpha-1)} \int_0^{1/p'} \frac{y^{(\alpha-1)}}{y \ln^2(p'y) + 1} \frac{\ln^2(p'y)}{[1 - \ln(p'y)]^\beta} dy.$$

The asymptotic of this integral at small p is determined by a small region in the vicinity of 0. Let us split it into two parts

$$I = \int_0^{1/p'} = \int_0^{p'} + \int_{p'}^{1/p'} = I_1 + I_2.$$

Then, in the first integral, we can neglect $\ln p'$ compared to $\ln y$ and vice versa in the second,

$$\int_0^{p'} \frac{y^{(\alpha-1)}}{y \ln^2 y + 1} \frac{\ln^2 y dy}{(1 - \ln y)^\beta} + \int_{p'}^{1/p'} \frac{y^{(\alpha-1)}}{y \ln^2 p' + 1} \frac{\ln^2 p' dy}{(1 - \ln p')^\beta}.$$

The first integral is obviously small as $O(p)$. Introducing a variable $z = y \ln^2 p'$ we can rewrite I_2 in the following way:

$$\begin{aligned} \int_{p' \ln^2 p'}^{\ln^2 p' / p'} \frac{z^{(\alpha-1)}}{z+1} \frac{\ln^{2(1-\alpha)} p'}{(1 - \ln p')^\beta} dz &\approx \frac{1}{\ln^{\beta+2(\alpha-1)} p'} \int_0^\infty \frac{z^{(\alpha-1)}}{z+1} dz \\ &= \frac{-\pi \csc[\pi(\alpha-1)]}{\ln^{\beta+2(\alpha-1)} p'}, \end{aligned}$$

which is the leading term and gives the asymptotic of g_p ,

$$g_p = O\left(\frac{p^{(\alpha-1)}}{\ln^{\beta+2(\alpha-1)} p}\right).$$

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