

DIFFUSION WITH BREAKS*

PIOTR WEBER

Collegium Medicum, Nicolaus Copernicus University
Karłowicza 24, 85-092 Bydgoszcz, Poland

PIOTR PEPEŁOWSKI

Institute of Physics, Faculty of Physics, Astronomy and Informatics
Nicolaus Copernicus University
Grudziądzka 5, 87-100 Toruń, Poland

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In this paper, we present a stochastic model which is a normal diffusion interrupted by events lasting some period of time during which particle does not move. We assume, that waiting time is described by a one-sided Lévy α -stable distribution. For large times, we derive fractional differential equation (FDE) describing evolution of probability density. This asymptotic form is determined by parameters describing underlying stochastic motion. We also show density evolution according to fractional differential equation for asymptotic model and obtain a solution for various model parameters.

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1. Introduction

Simple deterministic dynamical models can exhibit very complex time evolution, whose extreme form is the deterministic chaos [1]. Trajectory of chaotic system is very sensitive on initial conditions *i.e.*, very small changes of initial conditions may lead to a completely different dynamics in a relatively short time. Although we are dealing with the deterministic system, its chaotic evolution very much resembles the stochastic process. It is one of the reasons why methods of classical statistical physics are successfully applied to nonlinear dynamical systems [2–4].

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As an illustration of the problem analysed in the present paper, one can consider the Chirikov standard map [5] for values of parameter K , where KAM barriers disappeared but there are relatively large areas corresponding to islands of stable periodic motion. Boundaries of such islands have very complicated structure resembling Cantor set (cantori) which is a result of destruction of successive KAM barriers. Dynamics of points lying outside these areas is well described by normal diffusion, but occasionally particle may be trapped by the cantori structure at the boundary of periodic islands and stay there for certain period of time. Depending on the form of waiting time distribution, this may lead to different effects and to subdiffusion among them.

Our work focuses on finding the suitable statistical model that can be associated with the observations of chaotic trajectories in the presence of cantori in the systems phase space. Here, we understand that probability density described in the phase space is averaged over the position variable, *i.e.*, we treat momentum as a random variable and want to find evolution of its probability density function.

2. Assumptions of the model

We assume that the particle moves in a diffusive way in some environment for some period of time t after which it sticks to some object. This may be a stationary element of environment or, like in the case of standard map, boundary of periodic island. The time at which the particle sticks to some object, which is the same as the duration of diffusive motion, is given by the Poissonian probability density function

$$w(t) = a \exp(-at). \quad (1)$$

Thus, the probability that particle does not stick longer than time t is given by the formula

$$\Omega(t) = \int_t^\infty w(\tau) d\tau. \quad (2)$$

For this phase of motion, we define density that in time t particle is in position x in diffusive phase by formula

$$\psi_G(x, t) = g(x|t)w(t), \quad (3)$$

where

$$g(x|t) = \frac{1}{\sqrt{4D\pi t}} \exp\left(-\frac{x^2}{4Dt}\right) \quad (4)$$

is a standard conditional probability formula. We further define function $\Psi_G(x, t)$ by

$$\Psi_G(x, t) = g(x|t) \int_t^\infty w(\tau) d\tau \quad (5)$$

which describes the probability density that the walker is in the position x in diffusive phase at time t . Calculating integral in (5) with density (1), one can easily find the following simple relation

$$\psi_G(x, t) = a\Psi_G(x, t). \quad (6)$$

After diffusive phase, the particle sticks to an object and waits for time t . In the present work, we assume that waiting time density $\gamma(t)$ is given by a Lévy α -stable process $g_\alpha(t)$ with $\alpha \in (0.5, 1)$. Last restriction on parameter α is explained in Section 4. We have also a function

$$\Gamma(t) = \int_t^\infty \gamma(\tau) d\tau \quad (7)$$

which describes the probability that the particle does not move up to time t .

Let us introduce a function $\eta(x, t)$ which describes probability density of arriving at position x at time t . This function obeys the following relation

$$\eta(x, t) = \int_{-\infty}^{\infty} \int_0^t \int_0^{t'} \eta(x', t'') \psi_G(x - x', t' - t'') \gamma(t - t') dx' dt'' dt' + \delta(x) \delta(t). \quad (8)$$

With the function η , the probability density $W(x, t)$ of particle being at position x at time t is then given by

$$\begin{aligned} W(x, t) = & \int_0^t \left[\int_{-\infty}^{+\infty} \eta(x', t') \Psi_G(x - x', t - t') dx' \right] dt' \\ & + \int_0^t \left[\int_{-\infty}^{+\infty} \left(\int_0^{t'} \eta(x', t'') \psi_G(x - x', t' - t'') dt'' \right) dx' \right] \Gamma(t - t') dt'. \end{aligned} \quad (9)$$

It means that the particle is at point x at time t if either it arrived at x' at time t' and stayed in the diffusive phase up to time t changing position to x , or arrived at x' at time t'' , stayed in the diffusive phase for time interval $t' - t''$ changing position to x and then did not move up to time t .

From the above description of this process, there are two types of time increments, which are alternating. This is a period of time when particle diffuse τ_d and waiting time τ_w . We assume that τ_d and τ_w are sequences of two independent random variables. We can see that the position variable is independent from τ_w but depends on τ_d .

3. Integral transforms

Applying standard techniques of Laplace and Fourier transforms to both sides of (8), we obtain the following formula

$$\eta(k, s) = \frac{1}{1 - \psi_G(k, s)\gamma(s)}. \quad (10)$$

It is easy to obtain the analytic formula on $\psi_G(k, s)$, which represents integral transforms of the density $\psi_G(x, t)$

$$\psi_G(k, s) = \frac{a}{a + s + Dk^2}. \quad (11)$$

Waiting time distribution $g_\alpha(t)$ chosen in the previous section has very simple Laplace transform

$$\gamma(s) = e^{-s^\alpha}. \quad (12)$$

Applying the same integral transforms to equation (9) and using formulas (10) and (11), we obtain the following formula for the propagator $W(k, s)$

$$W(k, s) = \frac{1}{a + s + Dk^2 - a\gamma(s)} \left(1 + a \frac{1 - \gamma(s)}{s} \right). \quad (13)$$

4. Differential equation

The formula for propagator contains the function $\gamma(s) = \exp(-s^\alpha)$, and it is next to impossible to obtain any useful results with this exact form. However, we can obtain analytic and numerical results for small values of s , *i.e.*, in the limit of large time, expanding γ into a power series of s and keeping only the lowest order terms. Such approximation is often used in continuous random time walk approach [18, 19] and leads to significant results. Inserting $\gamma(s) = 1 - s^\alpha$ into equation (13), one can write this equation in the following form

$$W(k, s) \approx \frac{1 + as^{\alpha-1}}{s + Dk^2 + as^\alpha} \quad (14)$$

or, after some simple algebra, in the equivalent form

$$sW(k, s) - 1 + a(s^\alpha W(k, s) - s^{\alpha-1}) + Dk^2 W(k, s) = 0. \quad (15)$$

Taking inverse Laplace and Fourier transforms of (15), we obtain following fractional differential equation

$$\frac{\partial W(x, t)}{\partial t} + a \left[{}_0^C D_t^\alpha W(x, t) \right] = D \frac{\partial^2 W(x, t)}{\partial x^2}, \quad (16)$$

where symbol ${}_0^C D_t^\alpha$ is a Caputo derivative of the order of α [9].

Let us notice that approximation used in derivation of (14) is valid only for $\alpha > 1/2$. In the case $\alpha < 1/2$, in the denominator in this formula, one has to consider the next term in the expansion of $\gamma(s)$, namely $-s^{2\alpha}/2$ instead (or in addition to) of the term s . The upper limit on parameter α comes from theorems which we used to obtain the differential equation (16) which imply that α should be between 0 and 1. Taking into account both these conditions, we get the interval $(1/2, 1)$ for parameter α .

5. Solution

In the present section, we demonstrate three methods of computing densities $W(x, t)$. The first method uses inverse transforms of propagator (14) and initial probability density in the form $W_0(x) = \delta(x)$. Formally, one can directly apply inverse Fourier transform to (14) and write density $W(x, t)$ as the formal inverse Laplace transform

$$W(x, t) = \mathcal{L}^{-1} \left[\frac{1 + as^{\alpha-1}}{2\sqrt{s + as^\alpha}} \sqrt{\frac{1}{D}} \exp \left(-\sqrt{\frac{s + as^\alpha}{D}} |x| \right) \right], \quad (17)$$

where $\text{Re}(\sqrt{(s + as^\alpha)/D}) > 0$ and $\mathcal{L}^{-1}[\cdot]$ denotes an inverse Laplace transform. Final results may be then obtained by numerical computations of this transform [11].

There is another way of obtaining solution in the integral form which uses explicitly density of one-sided Lévy process [10]. Let us write propagator (14) in the following integral form

$$W(k, s) = \int_0^\infty h(s, u) p(u, k) du, \quad (18)$$

where

$$h(s, u) = -\frac{\partial}{\partial u} g(s, u), \quad g(s, u) = \frac{1}{s} e^{-u(s + as^\alpha)} \quad (19)$$

and

$$p(u, k) = e^{-u D k^2}. \quad (20)$$

Let us first consider inverse Laplace transform of $g(s, u)$. It can be shown that it has the following integral form [10]

$$g(t, u) = \int_u^t \frac{1}{(au)^{\frac{1}{\alpha}}} g_{\alpha} \left(\frac{\tau - u}{(au)^{\frac{1}{\alpha}}} \right) d\tau, \quad (21)$$

where $g_{\alpha}(\cdot)$ represents density of one-sided Lévy process. For $\alpha = \frac{l}{k}$, where k and l are positive integer numbers with $k > l$, function $g_{\alpha}(t)$ may be represented in the form of Fox H -function [15, 16, 22]

$$g_{\frac{l}{k}}(t) = \frac{\sqrt{kl}}{(2\pi)^{(k-l)/2}} \frac{1}{t} H_{l,k}^{k,0} \left(\frac{l^l}{k^k t^l} \middle| \begin{matrix} (\frac{0}{k}, 1), (\frac{1}{k}, 1), (\frac{2}{k}, 1), \dots, (\frac{k-1}{k}, 1) \\ (\frac{0}{l}, 1), (\frac{1}{l}, 1), (\frac{2}{l}, 1), \dots, (\frac{l-1}{l}, 1) \end{matrix} \right), \quad t > 0. \quad (22)$$

We can now express inverse Laplace transform of function $h(s, u)$ in an explicit form

$$h(t, u) = \frac{1}{\alpha a^{\frac{1}{\alpha}}} \frac{t + (\alpha - 1)u}{u^{\frac{1}{\alpha} + 1}} g_{\alpha} \left(\frac{t - u}{(au)^{\frac{1}{\alpha}}} \right), \quad u \in (0, t). \quad (23)$$

Let us notice that function $h(t, u)$ is zero for all values of u not belonging to the interval $(0, t)$ since the function $g_{\alpha}(t) = 0$ for $t < 0$.

Equation (23) is very similar to formula (3.21) in [10] which describes the hitting time density of an extended stable subordinator with additional drift as a linear function of time (bt , where $b > 0$) [12–14]. Transforming density from [10] to the form

$$h(\bar{t}, u) = \frac{1}{\beta} \frac{\bar{t} + (\beta - 1)u}{\frac{1}{b} u^{1 + \frac{1}{\beta}}} g_{\beta} \left(\frac{\bar{t} - u}{\frac{1}{b} u^{\frac{1}{\beta}}} \right), \quad u \in \left(0, \frac{t}{b} \right), \quad (24)$$

where \bar{t} is a symbol of time, $b > 0$, $u > 0$ and $0 < \beta < 1$, one immediately notices the following correspondence

$$\bar{t} = bt \quad (25)$$

and

$$b = a^{-\frac{1}{\alpha}}. \quad (26)$$

Taking into account function $h(t, u)$ and inverse Fourier transform of $p(k, u)$, we obtain analytical integral form for solution of differential equation (16) with initial condition in a form $\delta(x)$ for $t = 0$

$$W(x, t) = \frac{1}{\alpha a^{\frac{1}{\alpha}} \sqrt{4\pi D}} \int_0^{\infty} \frac{t + (\alpha - 1)u}{u^{\frac{1}{\alpha} + \frac{3}{2}}} g_{\alpha} \left(\frac{(t - u)}{(au)^{\frac{1}{\alpha}}} \right) e^{\frac{-x^2}{4uD}} du. \quad (27)$$

We can conclude that process described in the work of Meerschaert and Scheffler [10] can be treated as a large time asymptotic for the process considered in the present work. This correspondence is related to the modification of inverse subordinator density according to the relations (25) and (26). From relation (26), we can see that this modification is defined directly by two characteristic parameters of our model a and α .

In figure 1, we present probability densities (27) (black lines) for three values of time. We also have drawn (grey lines) densities of normal Gaussian diffusion for the same moments of time. To calculate $W(x, t)$, we use relation between Fox H -function and Meijer G -function, compute the latter function and numerically evaluate the integral in the formula (27). We can see that process with density (27) disperses slower than normal diffusion. This effect will be described quantitatively by mean square displacement in the next section. Figure 2 presents density $W(x, t)$ for $t = 1000$ and two values of parameter $a = 0.5$ and $a = 16$.

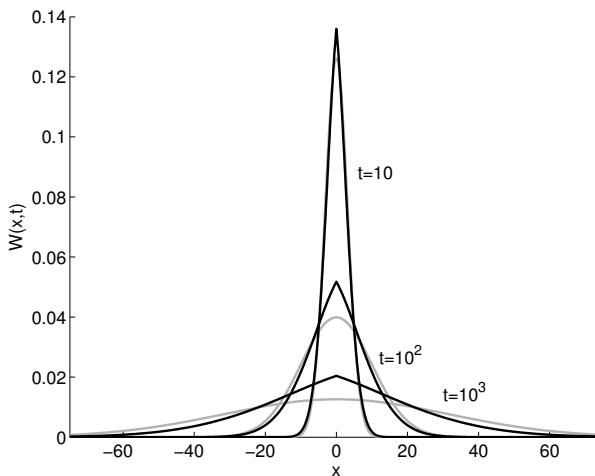


Fig. 1. Time evolution of $W(x, t)$, with parameters $\alpha = 0.75$, $a = 0.5$ and $D = 1$, obtained from (27) at three moments of time (black lines). They are compared to normal diffusion densities (grey lines) at the same times. In all cases, $W(x, 0) = \delta(x)$.

The third method of computing $W(x, t)$ uses numerical algorithm for solution of FDE due to Podlubny [20, 21]. We first use relation between Caputo and Riemann–Liouville derivative [17] and write (16) in a form

$$\frac{\partial W(x, t)}{\partial t} + a [{}_0^L D_t^\alpha W(x, t)] - D \frac{\partial^2 W(x, t)}{\partial x^2} = a W(x, 0) \frac{t^{-\beta}}{\Gamma(1 - \beta)}. \quad (28)$$

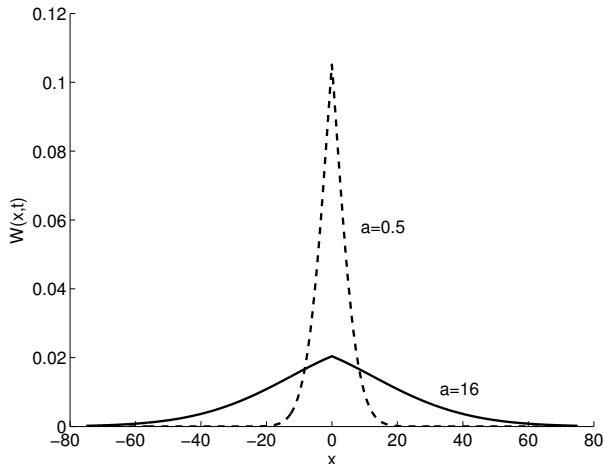


Fig. 2. Two densities $W(x, t)$ for parameter $a = 16$ (solid line) and $a = 0.5$ (dashed line) after time $t = 1000$. For both densities $D = 1$ and $\alpha = 0.75$.

It is convenient to introduce new function

$$\tilde{W}(x, t) = W(x, t) - W(x, 0), \quad (29)$$

and taking into account properties of Riemann–Liouville derivative the differential equation for $\tilde{W}(x, t)$ to write the corresponding FDE in a form

$$\frac{\partial \tilde{W}(x, t)}{\partial t} + a \left[{}_0^L D_t^\alpha \tilde{W}(x, t) \right] - D \frac{\partial^2 \tilde{W}(x, t)}{\partial x^2} = D \frac{\partial^2 W(x, t)}{\partial x^2} \Big|_{t=0}. \quad (30)$$

Our calculations are done on a grid in time and space. The interval of time $[0, t]$ is divided into equidistant time points with step Δt . Point number j is marked by t_j , where $j = 0, 1, \dots, N$ and $t_N = t$. The spatial variable is bounded to some interval $[-x_{\max}, x_{\max}]$ and next is divided into equidistant spatial points with step Δx . Spatial point number i is marked by x_i , where $i = 1, \dots, M$. We have $x_1 = -x_{\max}$ and $x_M = x_{\max}$. The pair (x_i, t_j) is called a node. Each has a value of function $\tilde{W}(x_i, t_j)$. This gets us the initial condition in a form $\tilde{W}(x_i, 0) = 0$. In this method, we also need to introduce boundary conditions in a form: $\tilde{W}(x_1, t_j) = 0$ and $\tilde{W}(x_M, t_j) = 0$, for all values j .

Following an idea of [20, 21], let us define a vector

$$\vec{W} = \left[\tilde{W}(x_1, 0) \tilde{W}(x_2, 0) \dots \tilde{W}(x_M, 0) \dots \tilde{W}(x_1, t_N) \dots \tilde{W}(x_M, t_N) \right]^T, \quad (31)$$

where ‘T’ means transposition. We also need another vector

$$\vec{P} = \left[W^{(2)}(x_1, 0) W^{(2)}(x_2, 0) \dots W^{(2)}(x_M, 0) \dots W^{(2)}(x_1, 0) \dots W^{(2)}(x_M, 0) \right]^T, \quad (32)$$

where $W^{(2)}(x_i, 0)$ is a second derivative of initial density at time $t = 0$ and point x_i . Vector $\vec{W}(x_i, t_j)$ consists of density values at all nodes defined by the space-time grid. With the above definitions, there is a possibility to discretize our problem in the following form of system of $(N + 1)M$ linear equations

$$[B_{N+1} \otimes I_M + aC_{N+1} \otimes I_M - DI_{N+1} \otimes S_M] \vec{W} = D\vec{P}, \quad (33)$$

where: \otimes is a symbol of Kronecker product, M is a number of spatial discretization points, $N + 1$ is a number of time points, symbols I_M and I_{N+1} represent identity matrixes of $M \times M$ and $(N + 1) \times (N + 1)$, respectively, $(N + 1) \times (N + 1)$ matrix B_{N+1} has a form

$$B_{N+1} = \frac{1}{\Delta t} \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ -1 & 1 & 0 & \dots & 0 \\ 0 & -1 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & 0 \\ 0 & 0 & \dots & -1 & 1 \end{pmatrix}, \quad (34)$$

$M \times M$ matrix S_M has a form

$$S_M = \frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & \dots & 0 \\ 0 & 1 & -2 & 1 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 & -2 \end{pmatrix}, \quad (35)$$

and $(N + 1) \times (N + 1)$ matrix C_{N+1} has a form

$$C_{N+1} = \frac{1}{\Delta t^\alpha} \begin{pmatrix} \omega_0^\alpha & 0 & \dots & 0 \\ \omega_1^\alpha & \omega_0^\alpha & \dots & 0 \\ \vdots & \vdots & \ddots & 0 \\ \omega_N^\alpha & \omega_{N-1}^\alpha & \dots & \omega_0^\alpha \end{pmatrix}, \quad (36)$$

where

$$\omega_j^\alpha = (-1)^j \binom{\alpha}{j} = (-1)^j \frac{\Gamma(1 + \alpha)}{\Gamma(1 + j)\Gamma(1 + \alpha - j)}. \quad (37)$$

The above formula represents general binomial coefficients, where in our case $\alpha \in (0.5, 1)$ and $j = 0, 1, \dots, N$. Representative results of numerical calculations are plotted in Fig. 3. We start from the same initial density for our model and standard diffusion. After time $t = 10$, we can observe similar difference as in the as for our first method.

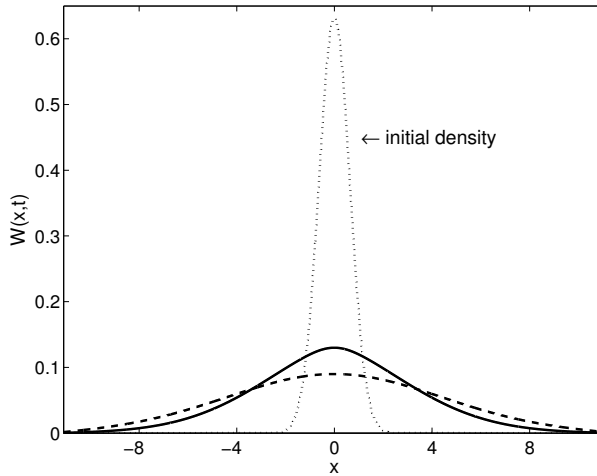


Fig. 3. Density $W(x, t)$ at time $t = 10$ obtained in numerical integration of fractional differential equation (solid black line) for Gaussian initial density (dotted line). Dashed line presents normal diffusion at time $t = 10$ started from the same initial density.

6. Mean square displacement

Taking into account above results, we can calculate the mean square displacement $\langle(\Delta x)^2\rangle$. We use the well known relation and represent it in Laplace space

$$\langle x^2(s) \rangle = -\frac{\partial^2}{\partial k^2} W(k, s) \Big|_{k=0}. \quad (38)$$

Calculating the second derivative of propagator (14), we obtain

$$\langle x^2(s) \rangle = \frac{2D}{s^2(1 + as^{\alpha-1})} \quad (39)$$

and the inverse Laplace transform of the right-hand side may be written in terms of Mittag-Leffler function $E_{1-\alpha, 2}$ [24]

$$\langle(\Delta x)^2\rangle = L^{-1} \left[\frac{2D}{s^2(1 + as^{\alpha-1})} \right] = 2Dt E_{1-\alpha, 2}(-at^{1-\alpha}). \quad (40)$$

As can be easily seen from (38) or from asymptotic behaviour of Mittag-Leffler function, for large t , one can write

$$\langle (\Delta x)^2 \rangle \sim \frac{D}{a\Gamma(a+1)} t^\alpha. \quad (41)$$

7. Conclusions

In this work, we have presented a model that can be used in describing processes characterized by non-linear relationship between the mean square displacement and time. Our motivation to build this model is related to the specific behaviour of chaotic trajectories near, in the presence of, periodic islands and cantori structures at their boundaries. We have analysed properties of this model for large times and it turned out that in this limit the process tends to the one known from the literature. But its important characteristics density of inverse subordinator is modified by the parameters characterizing our exact model. Using numerical methods and analytical results, we were able to follow the time evolution of the probability density of asymptotic model for various parameter values.

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