Influence of External Potentials on Heterogeneous Diffusion Processes

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***Abstract*—In this paper we consider heterogeneous diffusion processes with the power-law dependence of the diffusion coefficient on the position and investigate the influence of external forces on the resulting anomalous diffusion. We obtain analytic expressions for the transition probability as well as for the first and the second moments. By using these expression we demonstrate that the power-law exponent in the dependence of the mean square displacement on time does not depend on the external force. When the external force has a power-law exponent different than the power-law exponent of the noise induced drift, we can observe anomalous diffusion only in limited time interval. We expect that the results obtained in this paper may be useful for a more detailed understanding of anomalous diffusion processes in heterogeneous media.**

I. Introduction

In many systems we can observe processes exhibiting nonlinear dependence of the mean-square displacement (MSD) on time [1]. A family of such processes described by deviations from the linear time dependence of the MSD, typical for a classical Brownian motion, is called anomalous diffusion. Anomalous diffusion is characterized by the dependence of MSD on time in the form of a power-law $\langle \Delta x \rangle \sim t^{\theta}$. If θ varies between 1 and 2 we have so called super-diffusion. Super-diffusion has been experimentally observed in a study of tracer particles in a two-dimensional rotating flow [2]. If $\theta < 1$, we have another subclass of anomalous diffusion processes called the sub-diffusion. Theoretical models suggest that sub-diffusion can occur in polymer translocation through a nanopore [3].

Recently [4] it has been suggested that both cases of anomalous diffusion can be a result of a heterogeneous diffusion process (HDP), where the diffusion coefficient depends on the position. For example, heterogeneous diffusion processes has been used model subdiffusion in the study of thermal Markovian diffusion of tracer particles in a 2D medium with spatially varying diffusivity [5], mimicking recently measured, heterogeneous maps of the apparent diffusion coefficient in biological cells [6].

Here we consider HDPs with the power-law dependence of the diffusion coefficient on the particle position and analytically investigate the influence of external potentials on the resulting anomalous diffusion. The influence of the external forces on HDPs has not been methodically analyzed. We assume that introduction of the external potentials leads to drift terms in the from of power-law function of position. Such a drift terms appears in Langevin equation describing overdamped fluctuations of the position of a particle in nonhomogeneous medium [7]. As we demonstrate, the external force having a specific value of the power-law exponent does not restrict the region of diffusion. Such an external force does not change the scaling exponent θ, only the anomalous diffusion coefficient depends on the force. Other values of the power-law exponent in the deterministic force can cause the exponential cut-off in the probability density function (PDF) of the particle positions leading to the restriction of the time interval when the anomalous diffusion occurs.

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II. Influence of external potential on HDP

HDPs with the nonlinear dependence of the diffusion coefficient on the position is described by the Langevin equation

$$dx = \sigma |x|^{\eta} \circ dW_t \,. \tag{1}$$

Here x is the signal, η is the exponent of the power-law of multiplicative noise, parameter σ gives the intensity of the noise and W_t is a standard Wiener process. Eq. (1) is interpreted in Stratonovich sense. For mathematical convenience, in this paper we will use the Itô convention:

$$dx = \frac{1}{2}\sigma^2 \eta |x|^{2(\eta-1)} x dt + \sigma |x|^{\eta} dW_t \,. \tag{2}$$

First member of right hand side of Eq. (2) represents noise-induced drift. It has been shown that Eq. (1) leads to a nonlinear time dependence of the MSD [4]

$$\langle (x - \langle x \rangle)^2 \rangle \sim (\sigma^2 t)^{\frac{1}{1-\eta}} \,. \tag{3}$$

We will generalize the HDP by introducing an external force via the equation

$$dx = \sigma^2 \left(\eta - \frac{\nu}{2}\right) x^{2\eta-1} dt + \sigma x^{\eta} dW_t \,. \tag{4}$$

The new parameter ν defines the exponent of the steady-state PDF of the signal in interval $[x_{\min}, x_{\max}]$, $P_0(x) \sim x^{-\nu}$. Here $x_{\min}$, $x_{\max}$ are reflective boundaries at positive small and large x values, respectively.

Transformation of the variable x to a new variable $y = x^{1-\eta}$ (assuming that $\eta \neq 1$) leads to the stochastic differential equation (SDE)

$$dy = -\frac{1}{2}\sigma'^2 \nu' \frac{1}{y} dt + \sigma' dW_t \,, \tag{5}$$

where

$$\nu' = \frac{\eta - \nu}{\eta - 1} \,, \qquad \sigma' = |\eta - 1| \sigma \,. \tag{6}$$

Equation (5) has the form of a Bessel process [8]. The known analytic form of the solution of the Fokker-Planck equation

$$\frac{\partial}{\partial t}P_y = \frac{1}{2}\sigma'^2\nu'\frac{\partial}{\partial y}y^{-1}P_y + \frac{1}{2}\sigma'^2\frac{\partial^2}{\partial y^2}P_y \tag{7}$$

corresponding to SDE (5) is [8]

$$P(y,t|y_0,0) = \frac{y^{\frac{1-\nu'}{2}}y_0^{\frac{1+\nu'}{2}}}{\sigma'^2 t}\exp\left(-\frac{y^2+y_0^2}{2\sigma'^2 t}\right)I_{-\frac{\nu'+1}{2}}\left(\frac{yy_0}{\sigma'^2 t}\right). \tag{8}$$

Here $I_n(z)$ is the modified Bessel function of the first kind. This PDF satisfies the initial condition $P(y,t=0|y_0,0) = \delta(y-y_0)$. The PDF (8) can be normalized if $\nu' < 1$.

Transforming back to x we obtain the time-dependent PDF

$$P(x,t|x_0,0) = \frac{x^{\frac{1-2\eta-\nu}{2}}x_0^{\frac{1-2\eta+\nu}{2}}}{|\eta-1|\sigma^2 t}\exp\left(-\frac{x^{2(1-\eta)}+x_0^{2(1-\eta)}}{2(\eta-1)^2\sigma^2 t}\right) \times I_{\frac{\nu+1-2\eta}{2(\eta-1)}}\left(\frac{x^{(1-\eta)}x_0^{(1-\eta)}}{(\eta-1)^2\sigma^2 t}\right). \tag{9}$$

This PDF satisfies the initial condition $P(x,t=0|x_0,0) = \delta(x-x_0)$. Using the PDF (9) the time-dependent average of a power of x can be calculated:

$$\begin{aligned}\langle x^a\rangle_{x_0} =& \int_0^\infty x^a P(x,t|x_0,0)dx \\ =& \frac{\Gamma\left(\frac{\nu-1-a}{2(\eta-1)}\right)}{\Gamma\left(\frac{\nu-1}{2(\eta-1)}\right)}\left(2(\eta-1)^2\sigma^2 t\right)^{\frac{a}{2(1-\eta)}} \\ &\times {}_1F_1\left(\frac{a}{2(\eta-1)};\frac{\nu-1}{2(\eta-1)};-\frac{x_0^{2(1-\eta)}}{2(\eta-1)^2\sigma^2 t}\right)\end{aligned} \tag{10}$$

Here ${}_1F_1(a;b;z)$ is the Kummer confluent hypergeometric function. For large time the hypergeometric function is approximately equal to 1, thus

$$\langle x^a\rangle_{x_0} \approx \frac{\Gamma\left(\frac{\nu-1-a}{2(\eta-1)}\right)}{\Gamma\left(\frac{\nu-1}{2(\eta-1)}\right)}\left(2(\eta-1)^2\sigma^2 t\right)^{\frac{a}{2(1-\eta)}}. \tag{11}$$

From Eq. (11) we can see that the average of the square of x depends on time as $\langle x^2\rangle_{x_0} \sim t^{1/(1-\eta)}$ for large time t, that is when

$$\frac{x_0^{2(1-\eta)}}{2(\eta-1)^2\sigma^2 t} \ll 1. \tag{12}$$

The average of the x depends on time as $t^{1/2(1-\eta)}$. Therefore the MSD $\langle(x-\langle x\rangle)^2\rangle = \langle x^2\rangle - \langle x\rangle^2$ has the same dependence on time

$$\langle(x-\langle x\rangle)^2\rangle \sim t^{1/(1-\eta)} \tag{13}$$

as the original HDP equation (1).

III. Exponential restriction of diffusion

Here we introduce an external deterministic force that is no longer proportional to the noise induced drift, but has a power-law dependence on x with the power-law exponent different than $2\eta-1$. In particular, the external force can linearly dependence on x,

$$dx = \left(\mu x + \sigma^2\left(\eta-\frac{\nu}{2}\right)x^{2\eta-1}\right)dt + \sigma x^\eta dW_t. \tag{14}$$

Analytical expression of time-dependent PDF for SDE (14) can also be obtained by performing the same steps as in previous section. If μ has the same sign as $\eta-1$ and $t\to\infty$ then the time-dependent PDF reaches the steady-state

$$P_0(x) = \frac{2|\eta-1|x_{\mathrm{m}}^{\nu-1}}{\Gamma\left(\frac{\nu-1}{2(\eta-1)}\right)}x^{-\nu}\exp\left(-\left(\frac{x_{\mathrm{m}}}{x}\right)^{2(\eta-1)}\right), \tag{15}$$

where x_{m} is defined via the equation

$$\mu = \sigma^2(\eta-1)x_{\mathrm{m}}^{2(\eta-1)}. \tag{16}$$

The time-dependent average of a power of x reads

$$\begin{aligned}\langle x^a\rangle_{x_0} =& \frac{\Gamma\left(\frac{\nu-1-a}{2(\eta-1)}\right)}{\Gamma\left(\frac{\nu-1}{2(\eta-1)}\right)}\frac{x_{\mathrm{m}}^a}{(1-e^{-2(\eta-1)\mu t})^{\frac{a}{2(\eta-1)}}} \\ &\times {}_1F_1\left(\frac{a}{2(\eta-1)};\frac{\nu-1}{2(\eta-1)};-\frac{x_{\mathrm{m}}^{2(\eta-1)}x_0^{2(1-\eta)}}{e^{2(\eta-1)\mu t}-1}\right)\end{aligned} \tag{17}$$

The growth of the second moment $\langle x^2\rangle_{x_0}$ can be separated into three parts. For small times

$$t \ll \frac{x_0^{2(1-\eta)}}{2(\eta-1)^2\sigma^2}$$

the diffusion is approximately normal, $\langle x^2\rangle_{x_0}$ depends linearly on time t. For the intermediate times

$$\frac{x_0^{2(1-\eta)}}{2(\eta-1)^2\sigma^2} \ll t \ll \frac{1}{2(\eta-1)\mu} = \frac{x_{\mathrm{m}}^{2(1-\eta)}}{2(\eta-1)^2\sigma^2}$$

$\langle x^2\rangle_{x_0}$ remains power-law function on time $\langle x^2\rangle_{x_0} \sim t^{1/(1-\eta)}$ For large times we cannot observe anomalous diffusion, because the cut-off position x_{m} starts to influence the diffusion and $\langle x^2\rangle_{x_0}$ relax to the steady-state value

IV. Conclusion

We found that the power-law exponent in the dependence of the mean square displacement on time does not depend on the external force; this force changes only the anomalous diffusion coefficient (see Fig. 1 (d) and (e)). Anomalous diffusion occur only for specific parameters values if $\nu < 3$ and $\eta < 1$ (or $\nu < 1$ and $\eta < 1$). As we can see in Fig. 1 (c) and (f), in other cases anomalous diffusion does not occur due to the localization of particles. We obtained analytic expressions for the transition probability and moments in two cases: when external force is proportional to noise induced drift and when additional external force (besides the noise induced drift) has a linear dependence on the position. Introduction of such a

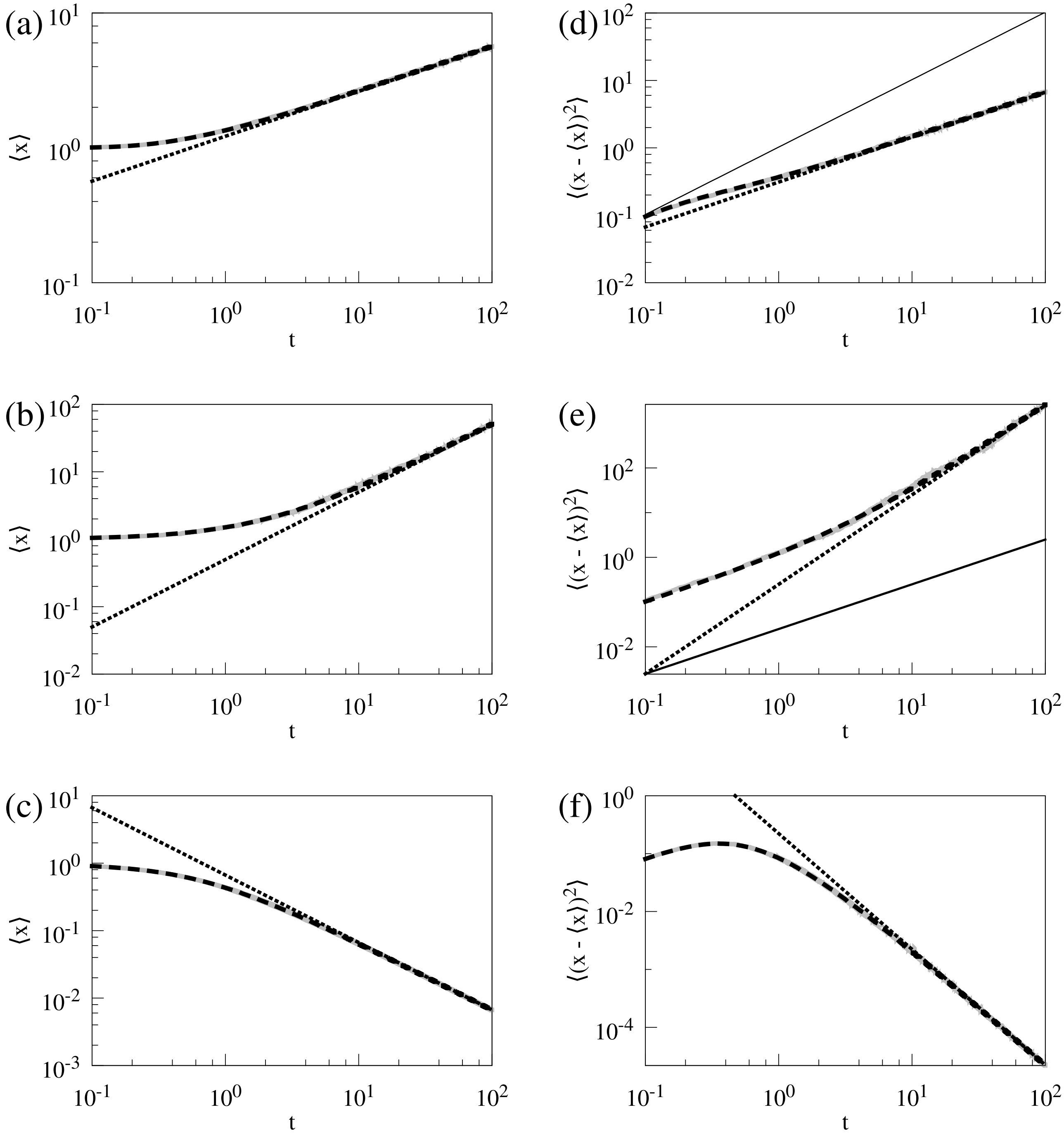

Fig. 1. Dependence of the mean (a,b,c) and variance (d,e,f) on time for various values of the parameters η and ν when the position of the diffusing particle changes according to Eq. (4). Solid gray lines show numerical result, dashed black lines are calculated using Eq. (10), black dotted lines show the power-law dependence on time $\sim t^{1/[2(1-\eta)]}$ for (a,b,c) and $\sim t^{1/(1-\eta)}$ for (d,e,f). The solid black line in (e,d) shows mean squared displacement (MSD) linear dependence on time. In (d) we see subdiffusion and supper diffusion in (e). The parameters are $\sigma = 1$ and $\eta = -\frac{1}{2}$, $\nu = -1$ for (a,d); $\eta = \frac{1}{2}$, $\nu = 0$ for (b,c); $\eta = \frac{3}{2}$, $\nu = 5$ for (c,f). The initial position is $x_0 = 1$.

force leads to the restriction of the time interval when the anomalous diffusion occurs. (see Fig. 2 (d) and (e)).

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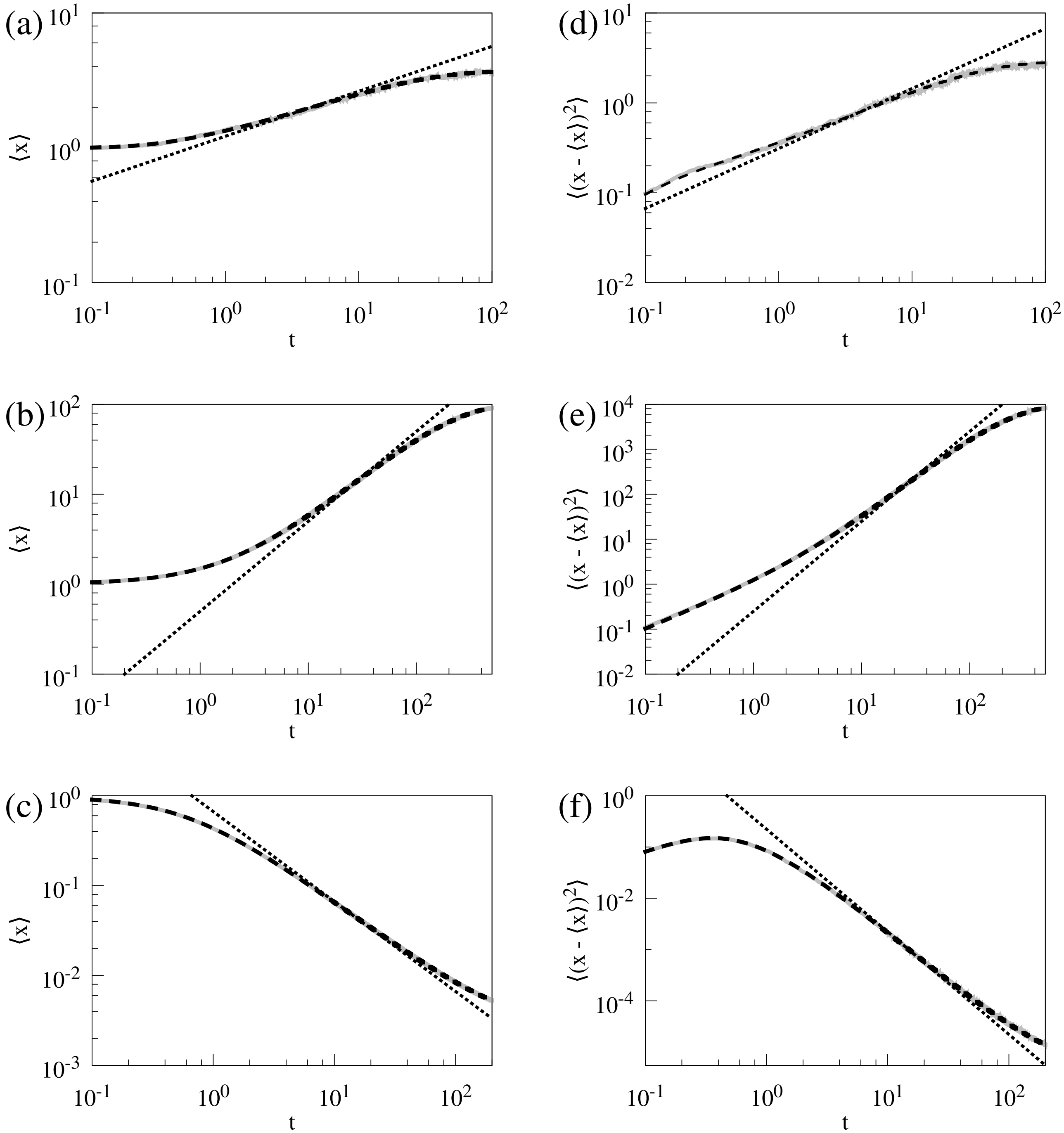

Fig. 2. Dependence of the mean (a,b,c) and variance (d,e,f) on time for various values of the parameters η and ν when the position of the diffusing particle changes according to Eq. (14). Solid gray lines show numerical result, dashed black lines are calculated using (17), dotted lines show the power-law dependence on time $\sim t^{1/[2(1-\eta)]}$ for (a,b,c) and $\sim t^{1/(1-\eta)}$ for (d,e,f). The parameters are $\sigma = 1$ and $\eta = -\frac{1}{2}$, $\nu = -1$, $x_{\mathrm{m}} = 5$ for (a,d); $\eta = \frac{1}{2}$, $\nu = 0$, $x_{\mathrm{m}} = 100$ for (b,c); $\eta = \frac{3}{2}$, $\nu = 5$ $x_{\mathrm{m}} = 0.01$ for (c,f). The initial position is $x_0 = 1$.

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