Anomalous diffusion, solutions, and first passage time: Influence of diffusion coefficient

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(Received 20 September 2004; published 20 January 2005)

We investigate the solutions and the first passage time for anomalous diffusion processes governed by the usual diffusion equation. We consider a space- and time-dependent diffusion coefficient and the presence of absorbing boundaries. We obtain analytical results for the probability distribution and the first passage time distribution for finite and semi-infinite intervals. In addition, we compare our results for the first passage time distribution with the one obtained by the usual diffusion equation with constant diffusion coefficient.

DOI: 10.1103/PhysRevE.71.012101 PACS number(s): 05.40.−a, 05.60.−k, 66.10.Cb

I. INTRODUCTION

Anomalous diffusion is a ubiquitous phenomenon in nature and it appears in several contexts related to physics, chemistry, and biology. The processes associated with anomalous diffusion are investigated, in general, by using the Langevin equation or differential equations for the probability density $\rho(x,t)$. Nowadays, there are several approaches at our disposal to describe these processes. For instance, the well-known cases are the Langevin equation and the corresponding Fokker-Planck equation, and the master equation. The other ones we could mention are the generalized Langevin equations [1], the generalized Fokker-Planck equation with memory effect [2], generalized thermostatistics [3], generalized master equations [4], continuous time random walk models [5], and fractional equations [6]. In connection to these approaches, the investigation of a stochastic process, such as anomalous diffusion, is also associated with the mean first passage time (MFPT). The MFPT is defined as the time $\mathcal{T}$ when a process, starting from a given point, reaches a predetermined level for the first time. Examples of the MFPT are the escape time from a random potential, intervals between neural spikes [7], and fatigue failure [8]. In this context, the knowledge of the first passage time (FPT) distribution $\mathcal{F}(t)$ is also essential. However, in only a few cases one has explicit analytical expressions for the FPT distribution, as was pointed out in Ref. 9. In this direction, our focus on this work is to analyze the MFPT, the FPT distribution, and the solutions related to the following diffusion equation:

$$\frac{\partial}{\partial t}\rho(x,t)=\frac{\partial}{\partial x}\left\{\mathcal{D}(t,x)\frac{\partial}{\partial x}\rho(x,t)\right\}, \tag{1}$$

where the diffusion coefficient is given by $\mathcal{D}(t,x)=\mathcal{D}(t)|x|^{-\theta}$. Note that Eq. (1) has as particular cases several situations present in the literature and it brings further aspects to explore, for example, physical systems whose dynamic aspects are governed by fractal-like structure and non-Markovian processes. The above equation has been applied to investigate turbulence [10,11], fast electrons in a hot plasma in the presence of a dc electric field [12], and diffusion on fractals [13].

The plan of this work is to investigate Eq. (1). In Sec. II, we present the solutions of Eq. (1) with natural boundary conditions and diffusion coefficient given by $\mathcal{D}(t,x)=\mathcal{D}(t)|x|^{-\theta}$. We analyze the mean squared displacement of these processes with different forms for $\mathcal{D}(t)$. In Sec. III, we investigate Eq. (1) subjected to the boundary condition $\rho(0,t)=\rho(L,t)=0$ and the initial condition $\rho(x,0)=\overline{\rho}(x)$. We also analyze this result by extending it to a semi-infinite interval, i.e., $L\to\infty$. Furthermore, we analyze the FPT distribution and the MFPT. Next in Sec. IV, we present our conclusion by giving a discussion about our results.

II. DIFFUSION EQUATION WITH NATURAL BOUNDARY CONDITIONS

The diffusion equation (1) with variable diffusion coefficient in space and/or in time has been considered by several authors. Richardson considered, by empirical argument, the spatial diffusion coefficient given by $\mathcal{D}(t,x)\sim|x|^{-\theta}$ (with $\theta=-4/3$) in order to study turbulent diffusivity [10], whereas Batchelor suggested $\mathcal{D}(t,x)\sim t^2$ for the same problem [14]. In a later step, Okubo [15] and Hentschel and Procaccia [16] (OHP) suggested mixed algebraic forms given by $\mathcal{D}(t,x)\sim t^a|x|^{-\theta}$, with the initial condition $\rho(0,x)=\delta(x)$. The solution of Eq. (1) for $\mathcal{D}(t,r)=K\mathcal{D}(t)r^{-\theta}$, in n dimensions with spherical symmetry, is given by

$$\rho(r,\overline{t})=\frac{(2+\theta)}{n\Gamma(n/(2+\theta))}\left[\frac{1}{K(2+\theta)^2\overline{t}}\right]^{n/(2+\theta)}e^{-r^{2+\theta}/k(2+\theta)^2\overline{t}}, \tag{2}$$

where $\overline{t}=\int\mathcal{D}(t)dt$. The corresponding mean squared displacement is $\langle r^2\rangle\sim\overline{t}^{2/(2+\theta)}$. Note that the non-Gaussian solution of Eq. (2) is due to the spatial diffusion coefficient. In particular, for the Batchelor model ($\theta=0$), the probability distribution has the Gaussian form. For $\mathcal{D}(t)=t^\alpha$ we recover the OHP solution which yields $\rho(r,t)\propto t^{-3(1+a)/(2+\theta)}e^{-C_2r^{2+\theta}/t^{1+a}}$. In particular, for $2\alpha-3\theta=4$ one has $\langle r^2\rangle\sim t^3$ which leads to the same behavior of the Richardson and Batchelor models. One can see that the above three models are linear in the logarithmic scale. To deviate from the linear behavior one can consider, for example, $\mathcal{D}(t)\sim d[(1+at^b)^c/(1+gt^q)^h]/dt$. For this last case, $\langle r^2\rangle$ is shown in Fig. 1. For t small $\langle r^2\rangle$ is dominated by the initial distance, and for large time the rate of $\langle r^2\rangle$ is less than that of the intermediate time. These behaviors seem to be verified in turbulent processes [11].

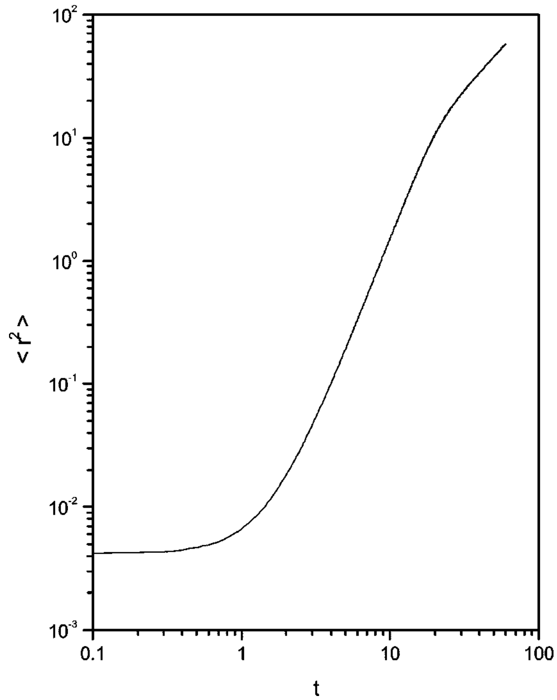

FIG. 1. Plot of $\langle r^2 \rangle$ as a function of t, in arbitrary units, with the diffusion coefficient $\mathcal{D}(r,t) \sim r^{-\theta} d[(1+at^b)^c/(1+gt^q)^h]/dt$. The parameters are $a=0.4$, $b=2.3$, $2c/(2+\theta)=1.36$, $g=7.7\times 10^{-8}$, $q=5.4$, and $2h/(2+\theta)=0.33$.

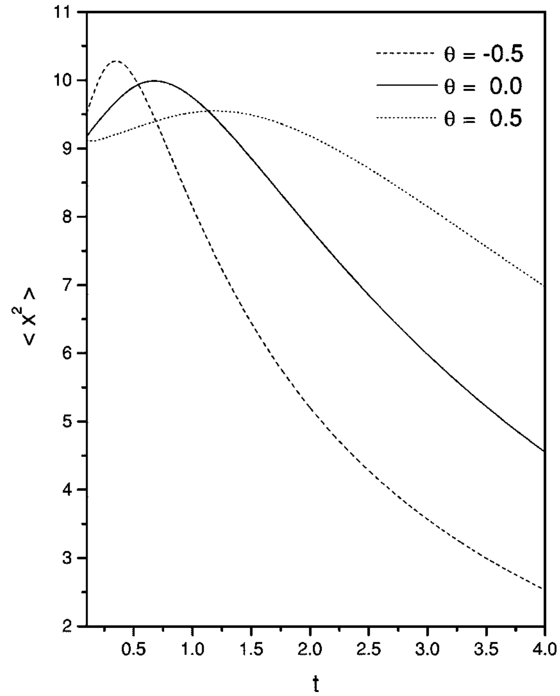

FIG. 2. We show the behavior of $\langle x^2 \rangle$ versus t, in arbitrary units, for typical values of θ by using, for simplicity, $x_0=3$, $L=6$, and $\mathcal{D}(t)=1$.

III. DIFFUSION EQUATION AND FPT DISTRIBUTION

We start this section by regarding a particle diffusing in an interval $[0,L]$, whose dynamics is governed by Eq. (1), subject to absorbing boundaries, i.e., $\rho(0,t)=\rho(L,t)=0$ and the initial condition given by $\rho(x,0)=\overline{\rho}(x)$. It is interesting to note that this kind of boundary condition may be useful to investigate stratified porous media [17] and to model photoconductivity in the amorphous semiconductor As_2Se_3 and the organic compound TNF-P [18]. In order to solve Eq. (1), subject to the conditions indicated above, the resolution method employed here is just the Green function method [19]. Thus, the solution obtained for Eq. (1) is given by

$$\rho(x,t) = \int_0^L dx_0 \mathcal{G}(x,x_0;t)\overline{\rho}(x_0),$$

$$\mathcal{G}(x,x_0;t) = \frac{\theta+2}{L^{\theta+2}} \sum_{n=1}^{\infty} \frac{(x_0 x)^{(1+\theta)/2} J_{(1+\theta)/(2+\theta)}\left(\dfrac{2\lambda_n}{2+\theta} x_0^{(2+\theta)/2}\right)}{\left\{J_{(3+2\theta)/(2+\theta)}\left(\dfrac{2\lambda_n}{2+\theta} L^{(2+\theta)/2}\right)\right\}^2} \times J_{(1+\theta)/(2+\theta)}\left(\frac{2\lambda_n}{2+\theta} x^{(2+\theta)/2}\right) \exp\left(-\lambda_n^2 \int_0^t dt' \mathcal{D}(t')\right) \tag{3}$$

for an arbitrary initial condition, where $\mathcal{G}$ is the Green function associated with the initial condition and λ_n are determined by the equation $J_{(1+\theta)/(2+\theta)}\{[2\lambda/(2+\theta)]L^{(2+\theta)/2}\}=0$, i.e., they correspond to the zeros of the Bessel function. Notice that the presence of the Bessel functions in Eq. (3) is due to the spatial dependence of the diffusion coefficient. In particular, this difference between Eq. (3) and the standard solution with constant diffusion coefficient is related to the changes obtained for the probability of a jump length due to the spatial time dependence of the diffusion coefficient. In order to show the differences between the standard case and this case we may analyze the second moment obtained from Eq. (3). It is given by

$$\langle x^2 \rangle = \frac{(2+\theta)^{1/(2+\theta)} L^2 x_0^{(1+\theta)/2}}{(4+\theta)\Gamma\left(\dfrac{3+2\theta}{2+\theta}\right)} \times \sum_{n=1}^{\infty} \frac{\lambda_n^{(1+\theta)/(2+\theta)} J_{(1+\theta)/(2+\theta)}\left(\dfrac{2\lambda_n}{2+\theta} x_0^{(2+\theta)/2}\right)}{\left\{J_{(3+2\theta)/(2+\theta)}\left(\dfrac{2\lambda_n}{2+\theta} L^{(2+\theta)/2}\right)\right\}^2} \times {}_1F_2\left(\frac{4+\theta}{2+\theta}; \frac{3+2\theta}{2+\theta}, \frac{6+2\theta}{2+\theta}; \frac{-L^{2+\theta}\lambda_n^2}{(2+\theta)^2}\right) \times \exp\left(-\lambda_n^2 \int_0^t dt\, \mathcal{D}(t)\right) \tag{4}$$

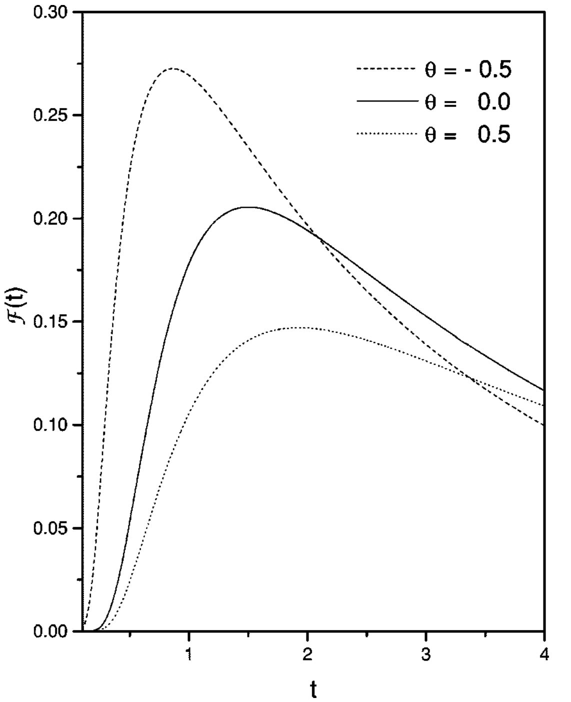

FIG. 3. We show the behavior of $\mathcal{F}(t)$ versus t, in arbitrary units, for typical values of θ by using, for simplicity, $x_0=3$, $L=6$, and $\mathcal{D}(t)=1$.

for the initial condition $\rho(x,0)=\delta(x-x_0)$, where ${}_1\mathrm{F}_2(\alpha_1;\beta_1,\beta_2;x)$ is a hypergeometric function [20]. Note that the above equation can exhibit several kinds of behaviors depending on the choices for $\mathcal{D}(t)$ and θ. In Fig. 2, we illustrate the behavior of Eq. (4) for typical values of θ by considering, for simplicity, $\mathcal{D}(t)=\text{const}$.

From the probability density $\rho(x,t)$, given in Eq. (3), we can obtain the FPT distribution with absorbing boundaries. For simplicity, we consider $\overline{\rho(x)}=\delta(x-x_0)$ and use the following expression [2,9]:

$$\mathcal{F}(t) = -\frac{d}{dt}\int_0^L dx\,\rho(x,t). \tag{5}$$

Substituting Eq. (3) into Eq. (5), we obtain the FPT distribution for the system governed by Eq. (1) as follows:

$$\mathcal{F}(t) = \frac{2\mathcal{D}(t)x_0^{(1+\theta)/2}}{L^{\theta+2}}\sum_{n=1}^{\infty}\frac{\lambda_n^2 J_{(1+\theta)/(2+\theta)}\left(\dfrac{2\lambda_n}{2+\theta}x_0^{(2+\theta)/2}\right)}{\left\{J_{(3+2\theta)/(2+\theta)}\left(\dfrac{2\lambda_n}{2+\theta}L^{(2+\theta)/2}\right)\right\}^2}$$
$$\times\exp\left(-\lambda_n^2\int_0^t dt'\mathcal{D}(t')\right)$$
$$\times\left[\frac{(2+\theta)^2}{2\lambda_n^2\Gamma\left(\dfrac{1+\theta}{2+\theta}\right)}\left(\frac{\lambda_n}{(2+\theta)}\right)^{(1+\theta)/(2+\theta)}\right.$$

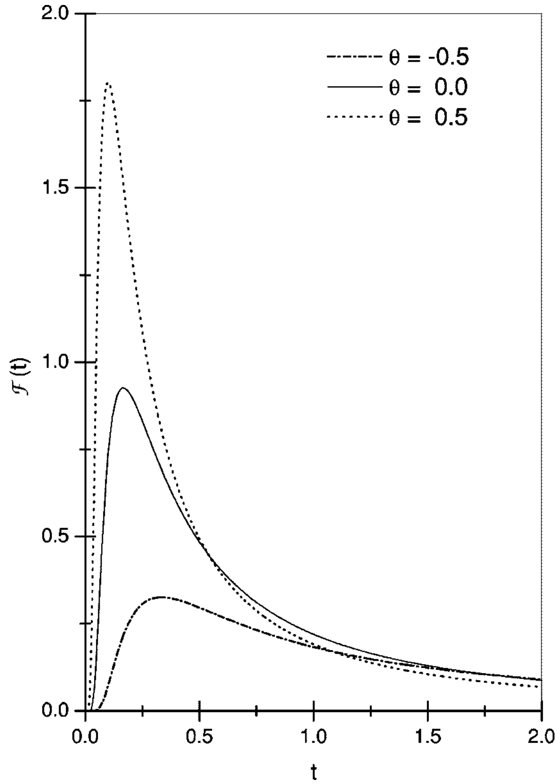

FIG. 4. We show the behavior of $\mathcal{F}(t)$ versus t, in arbitrary units, for typical values of θ by considering, for simplicity, $x_0=1$ and $\mathcal{D}=1$.

$$\left.-\frac{2+\theta}{2\lambda_n}L^{1/2}J_{-1/(2+\theta)}\left(\frac{2\lambda_n}{2+\theta}L^{(2+\theta)/2}\right)\right] \tag{6}$$

(see Fig. 3). From this expression, we can obtain the MFPT related to this process for $\mathcal{D}(t)=\text{const}$, as follows:

$$\mathcal{T} = \int_0^{\infty}dt\int_0^L dx\,\rho(x,t) = \frac{x_0^{1+\theta}(L-x_0)}{(2+\theta)\mathcal{D}}. \tag{7}$$

For the middle of the interval $[0,L]$, i.e., $x_0=L/2$, the above result yields $\mathcal{T}=[L^2/(8D)]^{(2+\theta)/2}[2(2\mathcal{D})^{\theta/2}/(2+\theta)]$. We note that the MFPT related to the system (1) is not invariant under translation of x (in statistical sense) due to the diffusion coefficient which depends on the position x. We now consider the MFPT on the intervals $[mL,(m+1)L]$, where m is an integer, with absorbing boundaries. The solution is given by

$$\mathcal{T}_m = \frac{L^{2+\theta}(2m+1)^{1+\theta}[(m+1)^{1+\theta}+m^{1+\theta}]}{\mathcal{D}2^{2+\theta}(2+\theta)[(m+1)^{1+\theta}-m^{1+\theta}]} - \frac{L^{2+\theta}[(m+1)m]^{1+\theta}}{\mathcal{D}(2+\theta)[(m+1)^{1+\theta}-m^{1+\theta}]}, \tag{8}$$

with $x_0=(2m+1)L/2$ put in the middle of the intervals. In fact, the above results give different results for different values of m. For $m=0$, we recover the result (7). For $\theta=0$, we recover the standard result $T=L^2/8\mathcal{D}$ which is independent of the value of m.

Now, let us extend the above results for $L\to\infty$, i.e., a semi-infinite interval. In this direction, the boundary condition is given by $\rho(0,t)=\rho(\infty,t)=0$. For the initial condition, we employ $\rho(x,0)=\tilde{\rho}(x)$. By using these considerations, we can show that the probability distribution is given by

$$\rho(x,t)\int_0^\infty dx'\tilde{\rho}(x')\mathcal{G}(x,x',t),$$

$$\mathcal{G}(x,x',t)=\frac{(xx')^{(1+\theta)/2}}{(2+\theta)\overline{t}}I_{(1+\theta)/(2+\theta)}\left(\frac{2(xx')^{(2+\theta)/2}}{(2+\theta)^2\overline{t}}\right)\times e^{-(x^{2+\theta}+x'^{2+\theta})/(2+\theta)^2\overline{t}}, \tag{9}$$

where $\overline{t}=\int_0^t dt'\mathcal{D}(t')$ and $I_\nu(x)$ is the modified Bessel function.

To obtain the FPT distribution from the above equation we apply Eq. (5) with, for simplicity, $\tilde{\rho}(x')=\delta(x'-x_0)$ and $\mathcal{D}(t)=\text{const}$. Thus, we have that

$$\mathcal{F}(t)=\frac{x_0^{1+\theta}}{t\Gamma\left(\frac{1+\theta}{2+\theta}\right)}\frac{e^{-x_0^{2+\theta}/\mathcal{D}(2+\theta)^2t}}{[(2+\theta)^2\mathcal{D}t]^{(1+\theta)/(2+\theta)}} \tag{10}$$

(see Fig. 4).

IV. SUMMARY AND CONCLUSIONS

In summary, we have investigated some solutions of Eq. (1) and the FPT for a system governed by the usual diffusion equation whose diffusion coefficient is space and/or time dependent. We have obtained an analytical solution for the probability density and for the FPT distribution in a finite interval $[0,L]$ and a semi-infinite interval with absorbing boundaries. Indeed, the determination of analytical solutions for a diffusion equation and, consequently, to the FPT distribution is important to the study of diffusion processes due to the fact that the systems can be analyzed concisely. In this direction, the study of diffusion processes with the diffusion coefficient $D(x,t)=\mathcal{D}(t)|x|^{-\theta}$ is significant to both theoretical and experimental physics due to the fact that it can be useful to describe diverse physical processes such as diffusion in systems with porous media [13,10,12,21]. We should mention that despite the singular nature of the diffusion coefficient at $x=0$, all the quantities obtained in this work are well behaved. Other aspects related to Eq. (1) have been considered in Ref. [22].

ACKNOWLEDGMENT

We thank Fundação Araucária (Brazilian agency) for partial financial support.

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