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FIRST PASSAGE TIME IN A SYSTEM WITH SUBDIFFUSIVE MEMBRANE*

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We study the first passage time (FPT) of a particle passing through a subdiffusive membrane; the membrane separates the media where normal diffusion occurs. The transport inside the membrane is described by the subdiffusion equation with fractional time derivative. Outside the membrane the normal diffusion equation is used. Starting with the solutions of the equations, we find the probability density of FPT and discuss its properties.

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1. Introduction

The First Passage Time (FPT) was used to characterize a diffusive transport in various systems [1], for example, in population genetics (FPT is identified with the time of fixation of gene in population) [2], in the transport of DNA in subdiffusive media [3], in spreading of viruses [4], and in the transport of polymers through membranes [5, 6]. FPT is defined as the time t, which is needed to a particle, starting from x_0, to reach arbitrary chosen point x for the first time. Till now, the FPT probability density function $F(x,t;x_0)$ was usually derived for homogeneous systems

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where normal diffusion or subdiffusion occurs [3, 7–11]. In this paper we study the one-dimensional unbounded system containing a medium, where the normal diffusion occurs, and a subdiffusive membrane. To describe the transport process in the system we use the normal diffusion equation outside the membrane and the subdiffusion one with fractional time derivative. We find the probability density of FPT of a particle passing through the membrane in the long time limit. We also briefly discuss its properties.

2. Model

We consider the system schematically presented in Fig. 1. In the region $(-\infty, x_1) \cup (x_2, \infty)$ the normal diffusion occurs, which is described by the equation

$$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2 C(x,t)}{\partial x^2}\,. \tag{1}$$

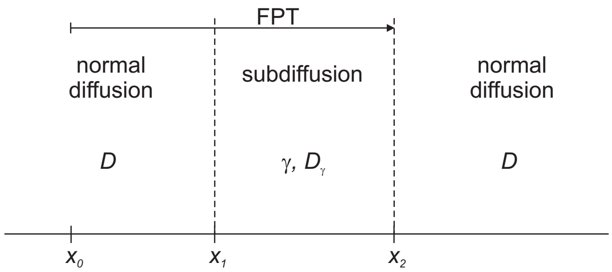

Fig. 1. The system under considerations, the membrane surfaces are located at x_1 and x_2, D is the normal diffusion coefficient, γ and D_γ are the subdiffusion parameters.

In the region (x_1, x_2), occupied by the membrane, there is a subdiffusion described by the following equation

$$\frac{\partial C(x,t)}{\partial t} = D_\gamma \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \frac{\partial^2 C(x,t)}{\partial x^2}\,, \tag{2}$$

where $\partial^{1-\gamma}/\partial t^{1-\gamma}$ denotes the fractional Riemann–Liouville time derivative, γ is the subdiffusion parameter ($\gamma < 1$) and D_γ denotes subdiffusion coefficient. These parameters occur in the relation defining subdiffusion $\left\langle \Delta x^2 \right\rangle = 2D_\gamma t^\gamma / \Gamma(1+\gamma)$, where $\left\langle \Delta x^2 \right\rangle$ is the mean square displacement of the particle. We assume that the fluxes and concentrations are continuous at the membrane surfaces

$$J_1(x_1,t) = J_{M\gamma}(x_1,t)\,, \qquad C_1(x_1,t) = C_M(x_1,t)\,, \tag{3}$$

$$J_{M\gamma}(x_2,t) = J_2(x_2,t)\,, \qquad C_M(x_2,t) = C_2(x_2,t)\,, \tag{4}$$

where indexes 1, M and 2 corresponds to the regions $x < x_1$, $x_1 < x < x_2$ and $x > x_2$, respectively and $J_{1,2} = -D\frac{\partial C_{1,2}}{\partial x}$ are the normal diffusion fluxes and $J_{M\gamma} = -D_\gamma \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \frac{\partial C_M}{\partial x}$ is the subdiffusion one. The probability density function of finding the particle at the point x and at the time t under the condition that it started from x_0, which is known as the Green function $G(x,t;x_0)$, is given by the solution of Eqs. (1) and (2) with the boundary conditions (3), (4) and $G(\pm\infty,t;x_0) = 0$, and with the initial condition

$$G(x,0;x_0) = \delta(x - x_0)\,. \tag{5}$$

Knowing the Greens function, one finds the concentration of transported substances $C(x,t)$ using the integral formula

$$C(x,t) = \int G(x,t;x_0)C(x_0,t)dx_0\,.$$

3. Results

We are interested in finding the probability density function of FPT $F(x_2,t;x_0)$ for the process where a particle reaches the point x_2 for the first time starting from the point x_0 localized in the region $(-\infty, x_1)$. This function fulfills the equation

$$F(x_2,t;x_0) = -\frac{dP(x_2,t;x_0)}{dt}\,, \tag{6}$$

where $P(x_2,t;x_0)$ denotes the probability of finding a random walker in the region $(-\infty, x_2)$ at the time t under the condition that the particle did not reach the point x_2 at earlier moments. This probability reads

$$P(x_2,t;x_0) = \int_{-\infty}^{x_1} G_{1\mathrm{abs}}(x,t;x_0)dx + \int_{x_1}^{x_2} G_{2\mathrm{abs}}(x,t;x_0)dx\,, \tag{7}$$

where $G_{1\mathrm{abs}}$ (for $x < x_1$) and $G_{2\mathrm{abs}}$ (for $x_1 < x < x_2$) denote the Green's functions for the system with fully absorbing wall located at x_2. These functions fulfill the boundary conditions (3), $G_{1\mathrm{abs}}(-\infty,t;x_0) = 0$ and

$$G_{2\mathrm{abs}}(x_2,t;x_0) = 0\,. \tag{8}$$

In terms of the Laplace transform $L[f(t)] \equiv \hat{f}(s) \equiv \int_0^\infty e^{-st}f(t)dt$ the Green's functions read

$$
\begin{aligned}
\hat{G}_{1\mathrm{abs}}(x,s;x_0) &= \frac{1}{2\sqrt{Ds}}\left[\exp\left(-\frac{s^{1/2}|x-x_0|}{\sqrt{D}}\right)\right. \\
&\quad \left. -\exp\left(-\frac{s^{1/2}(2x_1-x-x_0)}{\sqrt{D}}\right)\right] \\
&\quad + \frac{1-\exp\left(-2s^{\gamma/2}d/\sqrt{D_\gamma}\right)}{\sqrt{D_\gamma}s^{1-\gamma/2}\left[1+k+(1-k)\exp\left(-2s^{\gamma/2}d/\sqrt{D_\gamma}\right)\right]} \\
&\quad \times \exp\left(-\frac{s^{1/2}(2x_1-x-x_0)}{\sqrt{D}}\right), \qquad (9)
\end{aligned}
$$

$$
\begin{aligned}
\hat{G}_{2\mathrm{abs}}(x,s;x_0) &= \frac{\exp\left(-s^{1/2}(x_1-x_0)/\sqrt{D}\right)}{\sqrt{D_\gamma}s^{1-\gamma/2}\left[1+k+(1-k)\exp\left(-2s^{\gamma/2}d/\sqrt{D_\gamma}\right)\right]} \\
&\quad \times\left[\exp\left(-\frac{s^{\gamma/2}(x-x_1)}{\sqrt{D_\gamma}}\right)-\exp\left(-\frac{s^{\gamma/2}(2x_2-x_1-x)}{\sqrt{D_\gamma}}\right)\right], \qquad (10)
\end{aligned}
$$

where $k=\sqrt{D/D_\gamma}s^{(\gamma-1)/2}$ and $d=x_2-x_1$. The Laplace transform of Eq. (6) is

$$\hat{F}(x_2,s;x_0)=1-s\hat{P}(x_2,s;x_0)\,. \qquad (11)$$

Combining Eqs. (7) and (9)–(11) we get

$$\hat{F}(x_2,s;x_0)=\exp\left(-\frac{s^{1/2}(x_1-x_0)}{\sqrt{D}}\right)\frac{2\exp\left(-2s^{\gamma/2}d/\sqrt{D_\gamma}\right)}{1+k+(1-k)\exp\left(-2s^{\gamma/2}d/\sqrt{D_\gamma}\right)}\,. \qquad (12)$$

We find the function F for long times, which corresponds to the limit of small s in Eq. (12). Expanding $\hat{F}(x_2,s;x_0)$ into the power series with respect to s, taking into account the leading terms and using the following formula [12] (we assume that $\gamma>1/2$)

$$L^{-1}\left(s^\nu e^{-as^\rho}\right)\equiv f_{\nu,\rho}(t;a)=\frac{1}{t^{1+\nu}}\sum_{n=0}^{\infty}\frac{1}{n!\,\Gamma(-n\rho-\nu)}\left(-\frac{a}{t^\rho}\right)^n, \qquad (13)$$

where $a>0$, $0<\rho\le 1/2$ and the parameter ν is not limited, we get

$$F(x_2,t;x_0) = \frac{u}{2\sqrt{\pi t^3}}\exp\left(-\frac{u^2}{4t}\right)+\frac{d}{\sqrt{D}}f_{\gamma/2,1/2}\left(t,u\right)$$

$$-\frac{\sqrt{D}d^2}{D_\gamma} f_{\gamma-1/2,1/2}\left(t,u\right) - \frac{\sqrt{D}d^2}{D_\gamma^{3/2}} f_{3\gamma/2-1/2,1/2}\left(t,u\right)$$
$$+\frac{Dd^2}{D_\gamma^2} f_{2\gamma-1,1/2}\left(t,u\right) + \frac{2\sqrt{D}d^3}{D_\gamma} f_{2\gamma-1/2,1/2}\left(t,u\right)$$
$$-\frac{2Dd^3}{D_\gamma^{5/2}} f_{5\gamma/2-1/2,1/2}\left(t,u\right) + \frac{Dd^4}{D_\gamma^3} f_{3\gamma-1,1/2}\left(t,u\right) , \quad (14)$$

where $u = (x_1 - x_0)/\sqrt{D}$. The term 'leading terms' means that adding any term of neglected ones to the r.h.s. of Eq. (14), the plots of the function (14) do not noticeable differ from these in Figs. 2–5. We note that putting $\gamma = 1$, $D_\gamma = D$ in Eq. (12) and using the formula $L^{-1}[\exp(-a\sqrt{s/D})] = (1/2\sqrt{\pi D t^3})\exp(-a/4Dt)$, $a > 0$, we get the well-known FPT probability density for the normal diffusion

$$F(x,t;x_0) = \frac{1}{2\sqrt{\pi D t^3}} \exp\left(-\frac{(x-x_0)^2}{4Dt}\right) . \quad (15)$$

The probability that the particle, which starts form x_0, passes the point x_2 at least one time in the time interval $(0,t)$, is defined by the integral formula $S(x_2,t;x_0) = \int_0^t F(x_2,t';x_0)dt'$ and its Laplace transform reads

$$\hat{S}(x_2,s;x_0) = s^{-1}\hat{F}(x_2,s;x_0) . \quad (16)$$

From Eqs. (12), (13), (14) and (16), after simple calculation, we obtain

$$S(x_2,t;x_0) = \mathrm{erfc}\left(\frac{u}{2\sqrt{t}}\right) + \frac{d}{\sqrt{D}} f_{\gamma/2-1,1/2}\left(t,u\right)$$
$$-\frac{\sqrt{D}d^2}{D_\gamma} f_{\gamma-3/2,1/2}\left(t,u\right) - \frac{\sqrt{D}d^2}{D_\gamma^{3/2}} f_{3\gamma/2-3/2,1/2}\left(t,u\right)$$
$$+\frac{Dd^2}{D_\gamma^2} f_{2\gamma-2,1/2}\left(t,u\right) + \frac{2\sqrt{D}d^3}{D_\gamma} f_{2\gamma-3/2,1/2}\left(t,u\right)$$
$$-\frac{2Dd^3}{D_\gamma^{5/2}} f_{5\gamma/2-3/2,1/2}\left(t,u\right) + \frac{Dd^4}{D_\gamma^3} f_{3\gamma-2,1/2}\left(t,u\right) . \quad (17)$$

The plots of $F(x_2,t;x_0)$ are given in Fig. 2 (in the linear scale) and in Figs. 3 and 4 (in the log–log scale); in all cases we take $D = D_\gamma = 1$, $x_0 = 1$, $x_1 = 5$, and $x_2 = 6$ (all quantities are given in arbitrary units), the parameter γ is presented in the legends of the plots. In Figs. 2 and 3 we compare the plots of F calculated for different values of the subdiffusion membrane

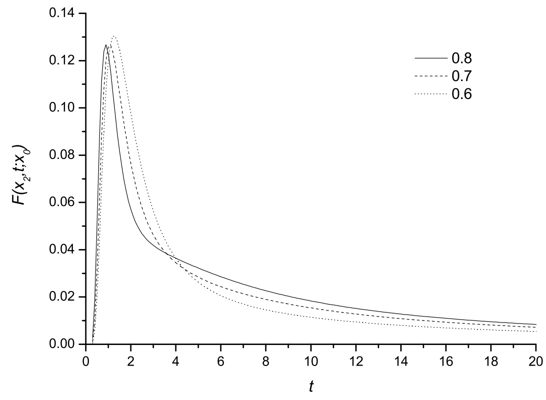

Fig. 2. The first passage time density $F(x_2, t; x_0)$ for different values of γ given in the legend, here $D = D_\gamma = 1$. The values of the other parameters are mentioned in the text.

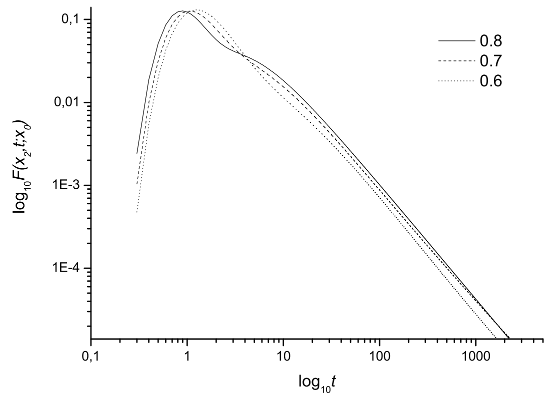

Fig. 3. The double-logarithmic plot of the functions presented in Fig. 2.

parameter γ. For each plot we observe two time domains where $F \sim t^{-\beta}$ with different values of β (this function can be represented by a linear function in the log–log plot with slope $-\beta$, see Fig. 4). The domains are separated by the time t_S. The more detailed analysis of the linear approximations of F is presented in Fig. 4. In the relatively small time domain, which is approximately defined by the inequality $0.3 < \log_{10} t < 0.9$, the slope of linear approximation is equal -0.54, whereas in the time domain $\log_{10} t > 1.1$ the slope is equal -1.38. More precisely, the linear approximations are expressed by the functions $\log_{10} F(x_2, t, x_0) = -0.54 \log_{10} t - 1.12$ in the first time interval and by $\log_{10} F(x_2, t, x_0) = -1.38 \log_{10} t - 0.23$ in the second one. These intervals are separated by the point t_S which we define as the time of crossing the linear approximations in log–log plot (for the case presented in Fig. 4 we get $\log_{10} t_S \approx 1$). The plots of the probability $S(x_2, t; x_0)$ for different γ are presented in Fig. 5.

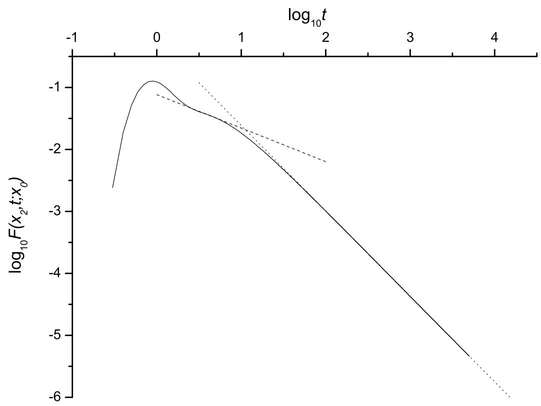

Fig. 4. The double-logarithmic plot of the function $F(x_2, t; x_0)$ for $\gamma = 0.8$. The slope of the dashed line is -0.54 and the dotted one is -1.38.

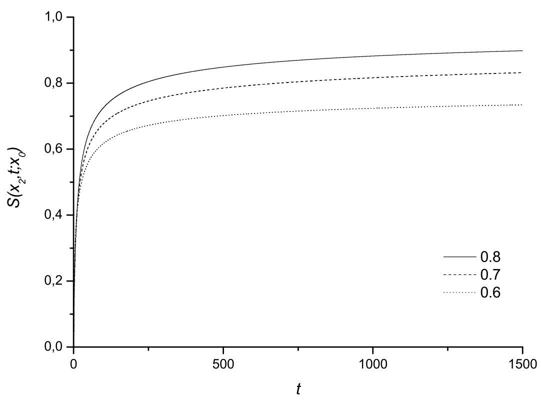

Fig. 5. The probability $S(x_2, t; x_0)$ calculated for different values of the parameter γ given in the legend.

4. Final remarks

Based on the Laplace transform of the probability density of the first passage time through the subdiffusive membrane (Eq. (12)), we derive the long-time approximation of this function (Eq. (14)). We find that there exist two time domains for sufficiently long times (which are separated from each other by the point t_S), where F can be approximated by the power functions of time with different exponents $F \sim t^{-\nu}$ for $t < t_S$ and $F \sim t^{-\theta}$ for $t > t_S$, where $\theta > \nu$. We note that the FPT in the homogeneous unbounded system with subdiffusion parameter γ has not such a property, as for long times there is $F \sim t^{-(1+\gamma/2)}$ [10]. However, in some subdiffusive systems the functions characterizing transport have the form of the power function $1/t^{\beta}$ for long times, where β takes different values in different time domains. A typical example is the time dependence of the transient photocurrent $I(t)$ in amorphous materials, where the transition from $I(t) \sim t^{-(1-\gamma)}$ to $I(t) \sim t^{-(1+\gamma)}$ for larger times was experimentally observed [13]. In such a system similar behavior of FPT density is also expected. Let us note that the results presented in this paper reveal the following features: the power approximation obtained for the first time interval (for $t < t_S$) are closed to the function $t^{-(1-\gamma/2)}$, whereas for $t > t_S$ the function can be approximated by $t^{-(1+\gamma/2)}$. Let us also note that the function F cannot be approximated by the function characteristic for the normal diffusion (15). Thus, we conclude, that the FPT is determined by the properties of the subdiffusive membrane. This suggestion is confirmed by Fig. 5, where the probability S of passing through the membrane at least one time in the time interval $(0,t)$ strongly depends on the subdiffusion parameter of the membrane. However, the medium where normal diffusion occurs influences the function F in such a manner that it creates the relatively small time domain (for $t < t_S$), where the function F can be approximated by the power function with the exponent approximately equal to $-(1-\gamma/2)$.

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