

TRANSPORT IN DIFFUSIVE–SUBDIFFUSIVE SYSTEM*

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Dedicated to Professor Andrzej Fuliński on the occasion of his 70th birthday

We study a transport in composite system where the subdiffusive solvent (as for example gel) is separated by a thin membrane from the region where normal diffusion occurs. The solutions of the diffusion equation with fractional derivative are found in the system of interest. We also discuss the dependence of mean square displacement σ^2 on time in long-time approximation.

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1. Introduction

The normal diffusion reflects the Brownian motion of the particles where each particle walks randomly with finite mean square displacement of the jump length σ^2 and mean waiting time for a step τ . Then, the diffusion is characterised by linear dependence of σ^2 on time. However, there are systems where the jumps occur with “extremely low frequency” (which gives infinite values of τ), as for example in porous media or gel solvent [1, 2]. In such a system, the transport is subdiffusive and it is characterised by the relation [2]

$$\sigma^2(t) = \frac{2D_\alpha}{\Gamma(1+\alpha)} t^\alpha, \quad (1)$$

where D_α is the subdiffusion coefficient measured in the units $[\text{m}^2/\text{s}^\alpha]$, α is the subdiffusion parameter ($0 < \alpha < 1$). The case of $\alpha = 1$ corresponds to the normal diffusion.

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In this paper we study a composite system where the subdiffusive solvent is separated from the one where normal diffusion occurs by a thin membrane. Using the Green's functions obtained from subdiffusion and diffusion equations we find the dependence of mean square displacement σ^2 on time.

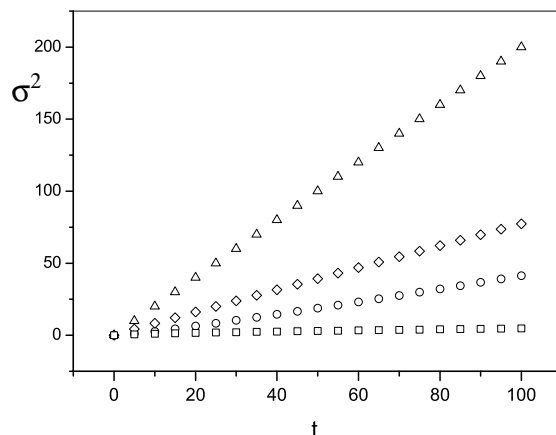


Fig. 1. The mean square displacement σ^2 as a function of time: σ_+^2 ($\diamond$), σ_-^2 ($\circ$), σ^2 for homogeneous system of normal diffusion ($\triangle$) and for homogeneous system of subdiffusion ($\square$). The parameters equal $D = 1$, $D_\alpha = 0.1$ (in arbitrary units), $\alpha = 2/3$.

To obtain the concentration profiles C of transported substance in subdiffusive systems one uses the subdiffusion equation with fractional time derivative of the Riemann–Liouville form [2]

$$\frac{\partial C(x, t)}{\partial t} = D_\alpha \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \frac{\partial^2 C(x, t)}{\partial x^2}. \quad (2)$$

For $\alpha = 1$ above equation appears to be the Fick equation for the normal diffusion. The Green's function $G(x, t; x_0)$ is defined as a solution of the equation (2) with the initial condition $G(x, 0; x_0) = \delta(x - x_0)$ and appropriate boundary conditions. This function gives the probability density to find a random walker at the position x in time t ; the walker starts from x_0 at $t = 0$.

2. Green's functions for diffusive–subdiffusive system

Let us assume that the normal diffusion occurs in the region $x < 0$ and subdiffusion is present for $x > 0$. In the following the index α is assigned to the function defined in the region with subdiffusion. Since the diffusion equation is of the second order, with respect to the space variable, one needs

two boundary conditions at the discontinuity of the system. Here we adopt the following boundary conditions at the membrane located at $x = 0$ [3]

$$J(0^-, t) = J_\alpha(0^+, t), \quad (3)$$

$$C(0^-, t) = \lambda C_\alpha(0^+, t), \quad (4)$$

where J denotes the flux of transported substance, the dimensionless parameter λ controls the membrane permeability. To obtain the Green's functions for considered system we use the procedure described in the paper [4], which is particularly useful for the multi-part systems. The starting point of the procedure is the solution corresponding to the analogous multi-part system where only normal diffusion is present but with different diffusion coefficients. So, at first we consider the two-part system where normal diffusion occurs with diffusion coefficients D and D_1 in the regions $x < 0$ and $x > 0$, respectively. Next, we get the Laplace transform (which is defined by the relation $\hat{f}(s) = L(f(t)) = \int_0^\infty e^{-st} f(t) dt$) of the solutions of normal diffusion and we obtain the ones for the subdiffusive system by means of the substitution $D_1 = D_\alpha s^{1-\alpha}$, which is done in the part of the system where subdiffusion occurs. To obtain the inverse Laplace transform we find the series expansion of the considered function in terms of $s^\nu e^{-as^\beta}$, and use the following formula

$$\begin{aligned} L^{-1}(s^\nu e^{-as^\beta}) &= f_{\nu,\beta}(t; a) \\ &= -\frac{1}{\pi t^{1+\nu}} \sum_{k=0}^{\infty} \frac{\sin[\pi(k\beta + \nu)] \Gamma(1 + k\beta + \nu)}{k!} \left(-\frac{a}{t^\beta}\right)^k, \end{aligned}$$

where $a > 0$, $\beta > 0$ and the parameter ν is not limited.

Solving the normal diffusion and subdiffusion equations with boundary conditions (3) and (4), we obtain the following Green's functions

$$\begin{aligned} G_{--}(x, t; x_0) &= \frac{1}{2\sqrt{\pi Dt}} \left[e^{-(x-x_0)^2/4Dt} + e^{-(x+x_0)^2/4Dt} \right] \\ &+ \frac{1}{\sqrt{D}} \sum_{n=0}^{\infty} (-\gamma)^{n+1} f_{((1-\alpha)n-\alpha)/2, \alpha/2} \left(t; \frac{-x-x_0}{\sqrt{D}} \right), \quad (5) \end{aligned}$$

$$G_{+-}(x, s; x_0) = \frac{1}{\sqrt{D}} \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} (-\gamma)^n \frac{1}{k!} \left(\frac{x_0}{\sqrt{D}} \right)^k f_{((1-\alpha)n+k-1)/2, \alpha/2} \left(t; \frac{x}{\sqrt{D}} \right), \quad (6)$$

$$G_{-+}(x, s; x_0) = \frac{1}{\sqrt{D}} \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} (-\gamma)^n \frac{1}{k!} \left(-\frac{x_0}{\sqrt{D}}\right)^k f_{((1-\alpha)n+\alpha k-1)/2, \alpha/2} \left(t; \frac{-x}{\sqrt{D}}\right), \quad (7)$$

$$G_{++}(x, t; x_0) = \frac{1}{2\sqrt{D_\alpha t}} \left[f_{\alpha/2-1, \alpha/2} \left(t; \frac{|x-x_0|}{\sqrt{D_\alpha}}\right) + f_{\alpha/2-1, \alpha/2} \left(t; \frac{x+x_0}{\sqrt{D}}\right) \right] - \frac{1}{\sqrt{D_\alpha}} \sum_{n=0}^{\infty} (-\gamma)^n f_{((1-\alpha)n+\alpha-1)/2, \alpha/2} \left(t; \frac{x+x_0}{\sqrt{D}}\right), \quad (8)$$

where $\gamma = \sqrt{\frac{D_\alpha}{D}} \frac{1}{\lambda}$. Here the indexes $-$ and $+$ of the Green's functions are assigned to the regions $x < 0$ and $x > 0$, respectively. The first index corresponds to the location of the point x , the latter, to the location of the point x_0 .

3. Time evolution of mean square displacement

The mean square displacement (MSD) σ^2 is calculated from the formula $\sigma_j^2 = \langle x_j^2 \rangle - \langle x_j \rangle^2$, where

$$\langle x_j^k(t) \rangle = \int_{-\infty}^0 x^k G_{-,j}(x, t; x_0) dx + \int_0^{\infty} x^k G_{+,j}(x, t; x_0) dx, \quad (9)$$

$k = 1, 2$. The dispersion is calculated separately for $x_0 < 0$ (where $j = -$) and for $x_0 > 0$ ($j = +$). The relations (5)–(9) provide to rather complicated functions of MSD, therefore, we perform the calculations in the limit of large time. From numerical calculations we can deduce that for typical values of the parameters ($D_\alpha \sim 10^{-10} \text{ m}^2/\text{s}^\alpha$, $D \sim 10^{-9} \text{ m}^2/\text{s}$, $x_0 \sim 10^{-3} \text{ m}$) the limit of “large time” is of the order of seconds. After calculations, we obtain for $x_0 < 0$

$$\langle x_-(t) \rangle \approx x_0 - 2\sqrt{\frac{Dt}{\pi}}, \quad \sigma_-^2 \approx 2DA t - B_1 t^{(1+\alpha)/2},$$

and for $x_0 > 0$

$$\langle x_+(t) \rangle \approx x_0 - 2\sqrt{\frac{Dt}{\pi}}, \quad \sigma_+^2 \approx 2DA t + B_2 t^\alpha,$$

where $A = 1 - \frac{1}{2\Gamma^2(3/2)} \approx 0.363$, $B_1 = \frac{2\sqrt{DD_\alpha}}{\Gamma((3+\alpha)/2)}$ and $B_2 = \frac{2D_\alpha}{\Gamma(1+\alpha)}$.

4. Final remarks

Character of the transport in the considered system differs from pure diffusive as well as from pure subdiffusive one. The mean square displacement σ^2 , which for long times is independent of membrane permeability, is a combination of linear function and a power function of time with the exponent smaller the unity. The dominant term in both parts of the system is very similar to the one for the pure diffusion system, but it is reduced by the factor A with respect to the normal diffusion case. The “subdiffusive corrections” are appreciable except the cases when $\alpha \rightarrow 1$ or $\alpha \rightarrow 0$. In the first case the system transforms to the one where the normal diffusion occurs. In the latter limit we deal with the system of normal diffusion with fully absorbing wall placed at $x = 0$. Let us note that the mean position of the random walker changes with time. Such an effect is observed in non-homogeneous systems of normal diffusion and it is not only determined by the “subdiffusive part” of the considered system.

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