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From the solutions of diffusion equation to the solutions of subdiffusive one

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Abstract

Starting with Green's functions found for normal diffusion, we construct exact time-dependent Green's functions for a subdiffusive equation with fractional time derivatives. Green's functions satisfy the boundary conditions involving a linear combination of fluxes and concentrations. The method is particularly useful to calculate the concentration profiles in a multi-part system where different kinds of transport occur in each part of it. As an example, we find the solution of the subdiffusive equation for the system composed of two parts with normal diffusion and subdiffusion.

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1. Introduction

Subdiffusion occurs in many physical systems such as amorphous semiconductors, porous media [1–3] or gel solvents [4, 5]. The subdiffusion is defined by the relation

$$\langle \Delta x^2 \rangle \sim t^\alpha \quad (1)$$

with $0 < \alpha < 1$, where $\langle \Delta x^2 \rangle$ denotes the mean square displacement of the transported particle and t is the time. The case of $\alpha = 1$ corresponds to normal diffusion. To obtain the concentration profiles (C_α) of a transported substance in subdiffusive systems, one uses the subdiffusion equation with fractional time derivative [2, 3, 6]

$$EQ_\alpha(C_\alpha) \equiv \left(\frac{\partial}{\partial t} - D_\alpha \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \frac{\partial^2}{\partial x^2} \right) C_\alpha(x, t) = 0, \quad (2)$$

with the Riemann–Liouville fractional derivative defined as (for $\alpha > 0$)

$$\frac{\partial^\alpha f(t)}{\partial t^\alpha} = \frac{1}{\Gamma(n-\alpha)} \frac{\partial^n}{\partial t^n} \int_0^t dt' \frac{f(t')}{(t-t')^{1+\alpha-n}},$$

where n is the smallest integer larger than α and D_α is the subdiffusion coefficient measured in the units $(\frac{m^2}{s^\alpha})$. While there is a huge literature about normal diffusion in a variety of systems (see e.g. [7] and references therein), subdiffusion is satisfactorily described in a few cases only. The procedure of solving equation (2) appears to be rather complicated. Below, we present a practical method to calculate the solutions of the equations describing in a multi-part system where diffusion and subdiffusion occur. The starting point is the solution corresponding to the analogous multi-part system where only normal diffusion is present.

Until now mostly homogeneous systems have been studied. However, the multi-part systems discussed here, in particular the membrane systems, are important for several fields of technology and biophysics. We mention here as examples the membranes used as micro filters and the (sub-)diffusion processes in living cells which are crucial for cell physiology. There are a few attempts described in the literature to obtain solutions of equation (2) from the ones corresponding to normal diffusion. A powerful method seems to be mapping of the solutions of diffusion equation $C_1(x, t)$ into the subdiffusive ones $C_\alpha(x, t)$ by means of the relation [8–11]

$$C_\alpha(x, t) = \int_0^\infty n(u, t) C_1(x, u) du, \quad (3)$$

where the Laplace transform of the function n is

$$\hat{n}(u, s) = \frac{D_1}{D_\alpha s^{1-\alpha}} e^{-\frac{D_1 s^\alpha}{D_\alpha} u}, \quad (4)$$

(throughout this paper the index α is assigned to the functions corresponding to subdiffusion; index 1 refers to normal diffusion). Another method is to ‘rescale’ the time as $t \rightarrow t^\alpha$ [12]. Using the substitution, one obtains solutions of the normal diffusion equation with diffusion coefficient depending on time. However, both procedures have been used for the homogeneous system only and it is unclear how to apply these approaches to a multi-part system, where various kinds of diffusion occur (e.g. a porous material, where subdiffusion proceeds, is adjoined to a normal diffusive medium). Thus, a more general procedure is needed.

In this paper, we discuss a method of constructing solutions of the one-dimensional subdiffusive equation with given boundary conditions starting with those of normal diffusion, which can be obtained rather easily. Our method gives the Green’s functions (GF) for subdiffusive equation in the form of series of the Fox functions which is convenient for numerical calculations. The method splits into two steps. In the first one, the Laplace transform of the subdiffusive Green’s function is obtained from the normal diffusion counterpart, and in the second one the Laplace transform is inverted. In contrast to the previous papers [8–12], we include boundary conditions into considerations. As an illustration of our method, we find the solutions of equation (2) for the system consisting of two parts where normal diffusion and subdiffusion occur, respectively.

We restrict our considerations to the case of boundary conditions which are given in the form of a linear combination of concentrations and fluxes. We note that this is not a serious restriction as linear boundary conditions often occur in normal diffusion problems (and can be adapted for the subdiffusion cases). For example, for the system with fully reflecting, fully absorbing [7] and partially absorbing walls [13], respectively, the boundary conditions read: $J(x_M^-, t) = 0$, $C(x_M^-, t) = 0$, and $J(x_M^-, t) = \gamma C(x_M^-, t)$, where x_M denotes a position of the wall. For the partially permeable wall two different boundary conditions have been used: $C(x_M^-, t) = \gamma C(x_M^+, t)$ [14, 15] or $J(x_M^-, t) = \lambda(C(x_M^-, t) - C(x_M^+, t))$ [16], both of which should be supplemented by the continuity of the flux $J(x_M^-, t) = J(x_M^+, t)$.

2. The method

Since Green's function for normal diffusion is mapped onto the subdiffusion within the method presented below, we first discuss the connection between the equation of normal diffusion and the subdiffusive equation.

2.1. Normal diffusion

We start with the normal diffusion equation

$$EQ_1(C_1) \equiv \left(\frac{\partial}{\partial t} - D_1 \frac{\partial^2}{\partial x^2} \right) C_1(x, t) = 0, \quad (5)$$

and assume that each of the boundary conditions involves a linear combination of fluxes and concentrations. When the system under consideration is divided into two parts by the membrane located at $x = x_M$, the boundary condition (BC) at x_M is assumed to be of the form

$$L_1(C_1) \equiv \delta_1 C_1(x_M^-, t) + \delta_2 C_1(x_M^+, t) + \delta_3 J_1(x_M^-, t) + \delta_4 J_1(x_M^+, t) = 0, \quad (6)$$

where the flux J_1 is given as

$$J_1(x, t) = -D_1 \frac{\partial C_1(x, t)}{\partial x}, \quad (7)$$

and δ_i ($i = 1, 2, 3, 4$) are parameters independent of t . The solution of equation (5) can be found due to the following integral formula:

$$C_1(x, t) = \int G_1(x, t; x_0) C_1(x_0, 0) dx_0,$$

where $C_1(x_0, 0)$ is the initial concentration, and Green's function G_1 is defined as a solution of equation (5) with the initial concentration

$$G_1(x, 0; x_0) = \delta(x - x_0), \quad (8)$$

with the appropriate boundary conditions. Since the diffusion equation is of second order with respect to the space variable, one needs two boundary conditions at the discontinuity of the system. When the system is infinite, the additional BC are needed at $x \rightarrow \pm\infty$ and they are usually of the form $G_\alpha(x, t; x_0)|_{x \rightarrow \infty} = 0$ and $G_\alpha(x, t; x_0)|_{x \rightarrow -\infty} = 0$, which can be treated as special cases of equation (6) ($\delta_1 = 1, \delta_2 = \delta_3 = \delta_4 = 0$ for $x \rightarrow -\infty$, and $\delta_2 = 1, \delta_1 = \delta_3 = \delta_4 = 0$ for $x \rightarrow \infty$, respectively).

One usually solves the normal diffusion equation by means of the Laplace transform (LT) [7, 17]

$$\hat{C}(x, s) = \int_0^\infty e^{-st} C(x, t) dt.$$

LT of equation (5), boundary conditions (6) and flux (7) are, respectively,

$$EQ_1(\hat{C}_1) \equiv s\hat{C}_1(x, s) - D_1 \frac{d^2 \hat{C}_1(x, s)}{dx^2} - C_1(x, 0) = 0, \quad (9)$$

$$L_1(\hat{C}_1) \equiv \delta_1 \hat{C}_1(x_M^-, s) + \delta_2 \hat{C}_1(x_M^+, s) + \delta_3 \hat{J}_1(x_M^-, s) + \delta_4 \hat{J}_1(x_M^+, s) = 0, \quad (10)$$

and

$$\hat{J}(x, s) = -D_1 \frac{d\hat{C}_1(x, s)}{dx}. \quad (11)$$

The general solution of equation (9) with the initial condition (8) is [17]

$$\begin{aligned} \hat{G}_1(x, s; x_0) &= A_1(s) \exp(x\sqrt{s/D_1}) + B_1(s) \exp(-x\sqrt{s/D_1}) \\ &+ \frac{1}{2\sqrt{D_1 s}} \exp(-|x - x_0|\sqrt{s/D_1}), \end{aligned} \quad (12)$$

where $A_1(s)$ and $B_1(s)$ are determined by the boundary conditions.

2.2. Subdiffusion

The subdiffusive flux generated by the gradient of the concentration C_α is given by the formula

$$J_\alpha(x, t) = -D_\alpha \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \frac{\partial C_\alpha(x, t)}{\partial x},$$

which combined with the continuity condition

$$\frac{\partial C_\alpha(x, t)}{\partial t} + \frac{\partial J_\alpha(x, t)}{\partial x} = 0,$$

provides the subdiffusion equation (2). The boundary condition at $x = x_M$ is assumed to be of a form fully analogous to that of normal diffusion (6) i.e.

$$L_\alpha(C_\alpha) \equiv \delta_1 C_\alpha(x_M^-, t) + \delta_2 C_\alpha(x_M^+, t) + \delta_3 J_\alpha(x_M^-, t) + \delta_4 J_\alpha(x_M^+, t) = 0. \quad (13)$$

The Laplace transform of the subdiffusion equation, subdiffusive flux [18] and boundary conditions are, respectively,

$$EQ_\alpha(\hat{C}_\alpha) \equiv s\hat{C}_\alpha(x, s) - s^{1-\alpha} D_\alpha \frac{d^2 \hat{C}_\alpha(x, s)}{dx^2} - C_\alpha(x, 0) = 0, \quad (14)$$

$$\hat{J}_\alpha(x, s) = -D_\alpha s^{1-\alpha} \frac{d\hat{C}_\alpha(x, s)}{dx}, \quad (15)$$

$$L_\alpha(\hat{C}_\alpha) \equiv \delta_1 \hat{C}_\alpha(x_M^-, s) + \delta_2 \hat{C}_\alpha(x_M^+, s) + \delta_3 \hat{J}_\alpha(x_M^-, s) + \delta_4 \hat{J}_\alpha(x_M^+, s) = 0. \quad (16)$$

The solution of equation (14) for the initial condition $C_\alpha(x, 0) = \delta(x - x_0)$ is computed as

$$\begin{aligned} \hat{G}_\alpha(x, s; x_0) &= A_\alpha(s) \exp(x\sqrt{s^\alpha/D_\alpha}) + B_\alpha(s) \exp(-x\sqrt{s^\alpha/D_\alpha}) \\ &+ \frac{1}{2\sqrt{D_\alpha s^{1-\frac{\alpha}{2}}}} \exp(-|x - x_0|\sqrt{s^\alpha/D_\alpha}), \end{aligned} \quad (17)$$

where the coefficients $A_\alpha(s)$ and $B_\alpha(s)$ are determined, as previously, by the boundary conditions (16).

2.3. From the diffusion to the subdiffusion equation

Let us note that substitution

$$D_1 = D_\alpha s^{1-\alpha} \quad (18)$$

maps the Laplace transforms of the normal diffusion equation $EQ_1(\hat{G}_1) = 0$ (9), and flux $\hat{J}_1(x, s; x_0)$ (11) onto the subdiffusion ones $EQ_\alpha(\hat{G}_\alpha) = 0$ (14) and $\hat{J}_\alpha(x, s; x_0)$ (15), respectively. Assuming that the coefficients $\delta_1, \delta_2, \delta_3$ and δ_4 are the same for the normal diffusion and for the subdiffusion boundary conditions (10) and (16), the substitution (18) also transforms the diffusion boundary condition $L_1(\hat{G}_1) = 0$ (10) into the subdiffusion one $L_\alpha(\hat{G}_\alpha) = 0$ (16). Since Green's functions are uniquely determined by the subdiffusion equation, boundary conditions and initial condition (which are assumed to be the same for normal diffusion and subdiffusion), it is clear that the substitution (18) transforms Green's function for normal diffusion (12) into Green's function for subdiffusion (17). Comparing equations (12) and (17) we deduce that the coefficients $A_\alpha(s)$ and $B_\alpha(s)$ can be obtained from $A_1(s)$ and $B_1(s)$ by means of the replacement (18).

2.4. Inverse Laplace transform

As Green’s function is given by equation (17), with the functions $A_\alpha(s)$ and $B_\alpha(s)$ of rather complicated structure (as we will see in section 3.2), the calculation of the inverse Laplace transform is far from simple. Therefore, we expand the function into the following series:

$$\hat{G}_\alpha(x, s; x_0) = \sum_{n=0}^\infty a_n s^{\beta+nv} \exp(x\sqrt{s^\alpha/D_\alpha}) + \sum_{n=0}^\infty b_n s^{\gamma+n\sigma} \exp(-x\sqrt{s^\alpha/D_\alpha}) + \frac{1}{2\sqrt{D_\alpha} s^{1-\frac{\alpha}{2}}} \exp(-|x-x_0|\sqrt{s^\alpha/D_\alpha}).$$

When the Laplace transform is in such a form, the inverse transformation can be easily calculated, using the formula derived by means of the method based on the Mellin transform [19] (for details of the derivation see the appendix)

$$f_{v,\beta}(t; a) \equiv L^{-1}(s^\nu e^{-as^\beta}) = \frac{1}{\beta a^{\frac{1+\nu}{\beta}}} H_{1,1}^{1,0} \left(\frac{a^{\frac{1}{\beta}}}{t} \left| \begin{matrix} 1 & 1 \\ \frac{1+\nu}{\beta} & \frac{1}{\beta} \end{matrix} \right. \right), \tag{19}$$

where H denotes the Fox function, $a, \beta > 0$, and the parameter ν is not limited. Due to formula (19), we obtain Green’s function as a series of Fox functions. As shown in the appendix, the function $f_{v,\beta}$ is given by the formula

$$f_{v,\beta}(t; a) = -\frac{1}{\pi t^{1+\nu}} \sum_{k=0}^\infty \frac{\sin[\pi(k\beta + \nu)]\Gamma(1 + k\beta + \nu)}{k!} \left(-\frac{a}{t^\beta}\right)^k. \tag{20}$$

The domain of applicability of equation (20) appears to be limited [19, 20]. The Fox function (19) is analytical and has its series expansion (20) for every non-zero value of the variable $\frac{a^{\frac{1}{\beta}}}{t}$ when $\frac{1}{\beta} - 1 > 0$. Otherwise, the additional restrictions should be imposed. For example, when $\beta = 1$, equation (20) is still valid under the condition $a < t$. In the following, we consider the cases where $\beta < 1$, so we will not further discuss the domain of applicability of formula (20).

3. Green’s functions for subdiffusive systems

To illustrate the considerations of the previous section, we find here Green’s function for the homogeneous system, which is well known, and next we discuss a composite system containing two parts where, respectively, normal diffusion and subdiffusion occur. As far as we know, such a system has not yet been considered. Leaving the detailed analysis of this system to the next paper, we derive here the respective Green’s functions.

3.1. The homogeneous system

Since the subdiffusive homogeneous system has already been described in detail, we only show here that the procedure presented above gives the same results as that of [2]. For the homogeneous system of normal diffusion, the functions $A(s)$ and $B(s)$ from equation (12) vanish. So, the Laplace transform of GF is

$$\hat{G}_1(x, s; x_0) = \frac{1}{2\sqrt{D_1 s}} \exp(-|x-x_0|\sqrt{s/D_1}), \tag{21}$$

and the inverse Laplace transform of (21) gives the Gaussian function

$$G_1(x, t; x_0) = \frac{1}{2\sqrt{\pi D_1 t}} \exp(-(x-x_0)^2/4Dt).$$

The replacement (18) transforms the GF for normal diffusion into the following function:

$$\hat{G}_\alpha(x, s; x_0) = \frac{1}{2\sqrt{D_\alpha s^{1-\frac{\alpha}{2}}}} \exp(-|x - x_0| \sqrt{s^\alpha/D_\alpha}),$$

and due to equation (19) we obtain

$$\begin{aligned} G_\alpha(x, t; x_0) &= \frac{1}{2\sqrt{D_\alpha}} f_{\frac{\alpha}{2}-1, \frac{\alpha}{2}}^\alpha \left(t; \frac{|x - x_0|}{\sqrt{D_\alpha}} \right) \\ &= \frac{1}{\alpha|x - x_0|} H_{1\ 1}^{1\ 0} \left(\left(\frac{(x - x_0)^2}{D_\alpha t} \right)^{\frac{1}{\alpha}} \middle| \begin{array}{c} 1\ 1 \\ 1\ \frac{\alpha}{2} \end{array} \right). \end{aligned} \quad (22)$$

Let us note that the Fox function has several different representations equivalent to each other. Using formula [20]

$$\begin{aligned} H_{1\ 1}^{1\ 0} \left(\left(\frac{(x - x_0)^2}{D_\alpha t} \right)^{\frac{1}{\alpha}} \middle| \begin{array}{c} 1\ 1 \\ 1\ \frac{\alpha}{2} \end{array} \right) &= \frac{\alpha}{2} H_{1\ 1}^{1\ 0} \left(\frac{x - x_0}{\sqrt{D_\alpha t^\alpha}} \middle| \begin{array}{c} 1\ \frac{\alpha}{2} \\ 1\ 1 \end{array} \right) \\ &= \frac{\alpha}{2} \frac{|x - x_0|}{\sqrt{D_\alpha t^\alpha}} H_{1\ 1}^{1\ 0} \left(\frac{|x - x_0|}{\sqrt{D_\alpha t^\alpha}} \middle| \begin{array}{c} 1 - \frac{\alpha}{2}\ \frac{\alpha}{2} \\ 0\ 1 \end{array} \right), \end{aligned}$$

we transform Green's function (22) to that derived in [2].

3.2. The two-part system

As a second example, we consider a system composed of two parts: L ($x < x_M$) where normal diffusion occurs with the diffusion coefficient D_{1L} and R ($x > x_M$) where there is subdiffusion with the subdiffusion coefficient $D_{\alpha R}$. We assume the following boundary conditions at x_M :

$$J_1(x_M^-, t) = J_\alpha(x_M^+, t), \quad (23)$$

$$G_1(x_M^-, t) = G_\alpha(x_M^+, t). \quad (24)$$

To use the procedure presented in the previous section, we temporarily assume that in the region R normal diffusion occurs with the diffusion coefficient D_{1R} . Assuming that $x_0 < x_M$, the solutions of the diffusion equation with the boundary conditions (23) and (24) can be written in terms of the Laplace transform as follows:

$$\begin{aligned} \hat{G}_{11--}(x, s; x_0) &= \left(\frac{1}{2\sqrt{D_{1L}s}} - \frac{1}{\sqrt{D_{1L}s}(\sqrt{D_{1L}/D_{1R}} + 1)} \right) \exp(-(2x_M - x - x_0)\sqrt{s/D_{1L}}) \\ &\quad + \frac{1}{2\sqrt{D_{1L}s}} \exp(-|x - x_0| \sqrt{s/D_{1L}}), \end{aligned} \quad (25)$$

for $x < x_M$, and

$$\hat{G}_{11+-}(x, s; x_0) = \frac{1}{\sqrt{D_{1L}s} + \sqrt{D_{1R}s}} \exp(-(x_M - x_0)\sqrt{s/D_{1L}} - (x - x_M)\sqrt{s/D_{1R}}), \quad (26)$$

for $x > x_M$ (index 11 of Green's function is assigned to the system where normal diffusion occurs in both parts, index 1α corresponds to the system with normal diffusion and subdiffusion, the indices $+$, $-$ refer to the signs of $x - x_M$ and $x_0 - x_M$, respectively).

In the next step we pass from 11 to 1α functions. Let us note that for the homogeneous system, the substitution (18) has been done for the whole system. However, for the composite one the substitution should be performed only with respect to the part where subdiffusion

occurs. Thus,

$$D_{1R} = D_{\alpha R} s^{1-\alpha}, \tag{27}$$

whereas the coefficient D_{1L} remains unchanged. Substituting (27) in the functions (25) and (26) we obtain

$$\begin{aligned} \hat{G}_{1\alpha--}(x, s; x_0) &= \left(\frac{1}{2\sqrt{D_{1L}s}} - \frac{1}{\sqrt{D_{1L}s}(\sqrt{D_{1L}s^{\alpha-1}/D_{\alpha R}} + 1)} \right) \\ &\times \exp(-(2x_M - x - x_0)\sqrt{s/D_{1L}}) + \frac{1}{2\sqrt{D_{1L}s}} \exp(-|x - x_0|\sqrt{s/D_{1L}}), \end{aligned} \tag{28}$$

and

$$\hat{G}_{1\alpha+-}(x, s; x_0) = \frac{1}{\sqrt{D_{1L}s} + \sqrt{D_{\alpha R}s^{2-\alpha}}} \exp(-(x_M - x_0)\sqrt{s/D_{1L}} - (x - x_M)\sqrt{s^\alpha/D_{\alpha R}}). \tag{29}$$

It is easy to see that the functions (28) and (29) fulfil the Laplace transforms of the boundary conditions (23) and (24). Expanding these functions into series, we obtain

$$\begin{aligned} \hat{G}_{1\alpha--}(x, s; x_0) &= \frac{1}{2\sqrt{sD_{1L}}} (\exp(-|x - x_0|\sqrt{s/D_{1L}}) + \exp(-(2x_M - x - x_0)\sqrt{s/D_{1L}})) \\ &+ \frac{1}{\sqrt{D_{1L}}} \sum_{n=0}^{\infty} \left(-\sqrt{\frac{D_{\alpha R}}{D_{1L}}} \right)^{n+1} s^{\frac{(1-\alpha)n-\alpha}{2}} \exp(-(2x_M - x - x_0)\sqrt{s/D_{1L}}), \end{aligned} \tag{30}$$

$$\begin{aligned} \hat{G}_{1\alpha+-}(x, s; x_0) &= \frac{1}{\sqrt{D_{1L}}} \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \left(-\sqrt{\frac{D_{\alpha R}}{D_{1L}}} \right)^n \frac{1}{k!} \left(-\frac{x_M - x_0}{\sqrt{D_{1L}}} \right)^k s^{\frac{(1-\alpha)n+k-1}{2}} \\ &\times \exp(-(x - x_M)\sqrt{s^\alpha/D_{\alpha R}}). \end{aligned} \tag{31}$$

Using formula (19), we obtain from equations (30) and (31) Green's functions for the considered system

$$\begin{aligned} G_{1\alpha--}(x, t; x_0) &= \frac{1}{2\sqrt{\pi D_{1L}t}} (\exp(-(x - x_0)^2/4D_{1L}t) + \exp(-(2x_M - x - x_0)^2/4D_{1L}t)) \\ &+ \frac{1}{\sqrt{D_{1L}}} \sum_{n=0}^{\infty} \left(-\sqrt{\frac{D_{\alpha R}}{D_{1L}}} \right)^{n+1} f_{\frac{(1-\alpha)n-\alpha}{2}, \frac{1}{2}} \left(t; \frac{2x_M - x - x_0}{\sqrt{D_{1L}}} \right), \end{aligned} \tag{32}$$

$$\begin{aligned} G_{1\alpha+-}(x, t; x_0) &= \frac{1}{\sqrt{D_{1L}}} \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \left(-\sqrt{\frac{D_{\alpha R}}{D_{1L}}} \right)^n \frac{1}{k!} \left(-\frac{x_M - x_0}{\sqrt{D_{1L}}} \right)^k \\ &\times f_{\frac{(1-\alpha)n+k-1}{2}, \frac{\alpha}{2}} \left(t; \frac{x - x_M}{\sqrt{D_{1L}}} \right). \end{aligned} \tag{33}$$

For $x_0 > x_M$, the calculations are very similar to those presented above. In this case Green's functions are

$$G_{1\alpha-+}(x, t; x_0) = \frac{1}{\sqrt{D_{1L}}} \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \left(-\sqrt{\frac{D_{\alpha R}}{D_{1L}}} \right)^n \frac{1}{k!} \left(\frac{x_M - x_0}{\sqrt{D_{1L}}} \right)^k f_{\frac{(1-\alpha)n+k-1}{2}, \frac{1}{2}} \left(t; \frac{x_M - x}{\sqrt{D_{1L}}} \right), \tag{34}$$

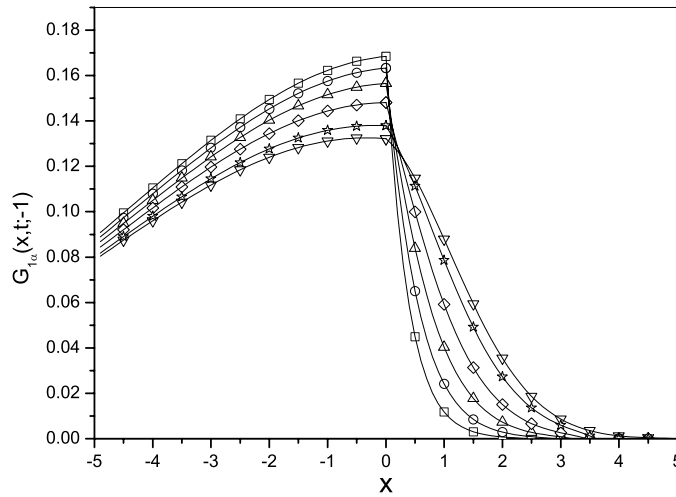


Figure 1. Green's functions for the two-part system for $x_0 = -1$ and several values of the parameter α : \square corresponds to $\alpha = 0.1$, \circ to $\alpha = 0.3$, \triangle to $\alpha = 0.5$, \diamond to $\alpha = 0.7$, \star to $\alpha = 0.9$ and ∇ to $\alpha = 1, 0$ (the normal diffusion case).

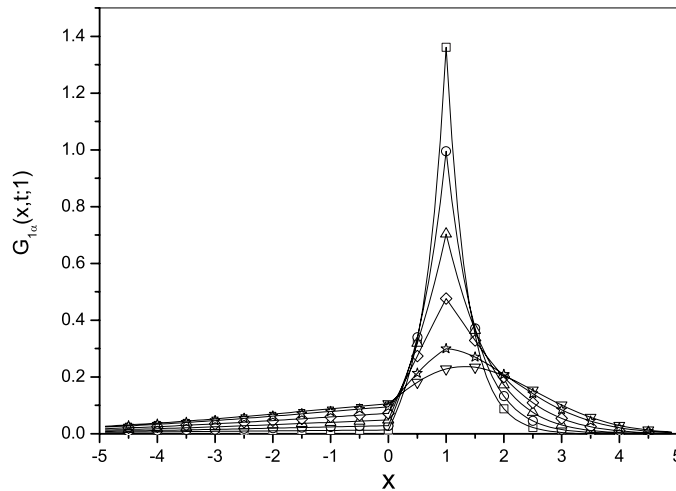


Figure 2. Green's functions for the two-part system for $x_0 = 1$ and several values of the parameter α (the description of the symbols is the same as for figure 1).

$$G_{1\alpha++}(x, t; x_0) = \frac{1}{2\sqrt{D_{\alpha R}t}} \left[f_{\frac{\alpha}{2}-1, \frac{\alpha}{2}} \left(t; \frac{|x-x_0|}{\sqrt{D_{\alpha R}}} \right) + f_{\frac{\alpha}{2}-1, \frac{\alpha}{2}} \left(t; \frac{x+x_0-2x_M}{\sqrt{D_{\alpha R}}} \right) \right] - \frac{1}{\sqrt{D_{\alpha R}}} \sum_{n=0}^{\infty} \left(-\sqrt{\frac{D_{\alpha R}}{D_{1L}}} \right)^n f_{\frac{(1-\alpha)n+\alpha-1}{2}, \frac{\alpha}{2}} \left(t; \frac{x+x_0-2x_M}{\sqrt{D_{\alpha R}}} \right). \tag{35}$$

To illustrate the above results we present two plots of Green's functions for several values of α . Figure 1 presents Green's functions (32) and (33) when the initial point x_0 is placed at the region L (with $x_0 = -1$). In figure 2 there are plots of Green's functions (34) and (35) when the initial point is located in the region R (with $x_0 = 1$); here $x_M = 0$. We use the

arbitrary units and the values of the parameters are: $D_{1L} = 1$, $D_{1R} = 0.1$, $D_{\alpha R} = 0.1$ and $t = 10$. For the double series occurring in the functions (33) and (34), and for the function $f_{v,\beta}$ given by equation (20), the first 20 terms are taken in each of the series. For the functions (32) and (35) given by the single series the first 40 terms are taken and for the function $f_{v,\beta}$ we have taken the first 70 terms in the numerical calculations. We have checked that increasing these numbers does not change our results noticeably.

Let us briefly discuss the main qualitative differences between Green's functions for normal diffusion and those for $\alpha < 1$. For the case of $x_0 < x_M$, the inflection point of Green's functions is located at x_M for $\alpha < 1$ whereas for normal diffusion this point is placed in the region R a finite distance from the border between L and R . For the case of $x_0 > x_M$, the differences between the considered Green's functions are very similar to those between Green's functions for homogeneous diffusive and subdiffusive systems studied in [2].

4. Final remarks

The procedure presented above allows one to solve the subdiffusion equations for non-homogeneous systems such as a membrane system, layered system etc. The procedure uses the fact that the normal diffusion equation is simpler to solve than the subdiffusive one and relation (18) transforms Green's functions, the diffusive equation and boundary conditions from the normal to the subdiffusive case. Thus, knowing the Laplace transform of \hat{G}_1 one immediately obtains the Laplace transform of \hat{G}_α .

Summarizing our considerations, the procedure to obtain Green's functions for the subdiffusive system with linear boundary conditions is presented as a do list:

1. find the Laplace transforms of Green's functions for the analogous system for normal diffusion,
2. obtain the Laplace transform of Green's functions for the subdiffusive system using the replacement (18); when the system is divided into several parts, the replacement should be applied only to the part where subdiffusion occurs,
3. expand the Laplace transform of Green's function \hat{G}_α into the power series of s^ν multiplied by e^{-as^β} ,
4. use formula (19) to calculate the inverse Laplace transform.

The numerical calculations performed in section 3.2, which give Green's functions presented in figures 1 and 2, show the usefulness of the method. It gives explicitly analytic solutions of subdiffusive equations which are appropriate for numerical calculations.

Finally we return to the method of mapping Green's function for normal diffusion to the subdiffusive one by relation (3), which has been mentioned in the introduction. Let us observe that substituting expression (4) into equation (3) we obtain

$$\begin{aligned}\hat{G}_\alpha(x, s) &= \frac{D_1}{D_\alpha s^{1-\alpha}} \int_0^\infty e^{-\frac{D_1 s^\alpha}{D_\alpha} u} G_1(x, u) \\ &= \frac{D_1}{D_\alpha s^{1-\alpha}} \hat{G}_1\left(x, \frac{D_1}{D_\alpha} s^\alpha\right).\end{aligned}\quad (36)$$

If we apply the replacement (18) to the rhs of equation (36), we get the identity. So, the procedure presented in this paper is consistent with the procedure discussed in [9] for the homogeneous system.

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Appendix

We derive here relations (19) and (20). Let us consider the Laplace transform

$$\hat{f}_{\nu,\beta}(s; a) \equiv L[f(t)](s) = s^\nu e^{-as^\beta}. \quad (\text{A1})$$

The Mellin transform

$$M[f(x)](p) \equiv \int_0^\infty x^{p-1} f(x) dx,$$

applied to relation (A1) gives

$$M[\hat{f}_{\nu,\beta}(s; a)](p) = \frac{1}{\beta a^{\frac{p+\nu}{\beta}}} \Gamma\left(\frac{p+\nu}{\beta}\right). \quad (\text{A2})$$

Using the well-known formula

$$M[L[f(t)](s)](1-p) = \Gamma(1-p)M[f(t)](p),$$

we obtain

$$f(t) = M^{-1} \left[\frac{1}{\Gamma(1-p)} M[L[f(t)](s)](1-p) \right]. \quad (\text{A3})$$

Putting equation (A2) in (A3) and using the inverse Mellin transform we get

$$f(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} t^{-p} \frac{1}{\beta a^{\frac{1-p+\nu}{\beta}}} \frac{\Gamma\left(\frac{1-p+\nu}{\beta}\right)}{\Gamma(1-p)} dp.$$

Comparing the above equation with the definition of the Fox H -function

$$H_{PQ}^{mn} \left(z \left| \begin{matrix} (a_1, A_1) & \cdots & (a_P, A_P) \\ (b_1, B_1) & \cdots & (b_Q, B_Q) \end{matrix} \right. \right) = \frac{1}{2\pi i} \int_C z^p \frac{A(p)B(p)}{C(p)D(p)} dp,$$

where $A(p) = \prod_{j=1}^m \Gamma(b_j - B_j p)$, $B(p) = \prod_{j=1}^n \Gamma(1 - a_j + A_j p)$, $C(p) = \prod_{j=1}^Q \Gamma(1 - b_j + B_j p)$, $D(p) = \prod_{j=1}^P \Gamma(a_j - A_j p)$, and the circle C separates the poles of $A(p)$ and $B(p)$, we obtain

$$H_{PQ}^{mn} = - \sum_{\text{poles of } A(p)} \text{Res} \left(\frac{A(p)B(p)}{C(p)D(p)} \right).$$

To get the poles of $A(p)$ we take the relation $b_j - B_j p = -k$, with $k = 0, 1, 2, \dots$, which gives

$$p_{j,k} = \frac{b_j + k}{B_j}. \quad (\text{A4})$$

Using the relation

$$\begin{aligned} \lim_{p \rightarrow p_{j,k}} (b_j - B_j p + k) \Gamma(b_j - B_j p) &= \lim_{p \rightarrow p_{j,k}} \frac{\Gamma(b_j - B_j p + k + 1)}{(b_j - B_j p)(b_j - B_j p + 1) \cdots (b_j - B_j p + k)} \\ &= \frac{\Gamma(1)}{(-k)(-k+1)(-k+2) \cdots (-1)} = \frac{(-1)^k}{k!}, \end{aligned}$$

we find

$$\operatorname{Res}_{p=p_{j,k}} \left(\frac{A(p)B(p)}{C(p)D(p)} \right) = -\frac{(-1)^k A'_j(p_{j,k})B(p_{j,k})}{B_j k! C(p_{j,k})D(p_{j,k})} z^{p_{j,k}},$$

where $A'_j(p) = \frac{A(p)}{\Gamma(b_j - B_j p)}$. So, we obtain

$$H_{PQ}^{mn}(z) = \sum_{j=1}^m \frac{1}{B_j} \sum_{k=0}^{\infty} \frac{(-1)^k A'_j(p_{j,k})B(p_{j,k})}{B_j k! C(p_{j,k})D(p_{j,k})} z^{p_{j,k}}. \quad (\text{A5})$$

Additionally, we use the relation $\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin(\pi z)}$, which gives

$$\frac{1}{\Gamma(-\alpha k)} = -\frac{\sin(\pi \alpha k)\Gamma(1 + \alpha k)}{\pi}.$$

From the above equation and formulae (A4) and (A5), we get relation (20).

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