Subdiffusion in a system with a thin membrane

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XII Polish Workshop on Relativistic Heavy-Ion Collisions
4-6 November 2016
Institute of Physics, Jan Kochanowski University in Kielce

Subdiffusion in a membrane system

First step

- T. Kosztołowicz, K. Dworecki, and S. Mrówczyński, *How to measure subdiffusion parameters*, Phys. Rev. Lett. **94**, 170602 (2005)
- T. Kosztołowicz, K. Dworecki, and S. Mrówczyński, *Measuring subdiffusion parameters*, Phys. Rev. E **71**, 041105 (2005)

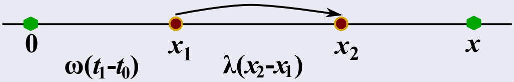
Random walk model

- T. Kosztołowicz, *Random walk model of subdiffusion in a system with a thin membrane*, Phys. Rev. E **91**, 022102 (2015)
- T. Kosztołowicz, *Subdiffusive random walk in a membrane system. The generalized method of images approach*, J. Stat. Mech. P10021 (2015)
- T. Kosztołowicz, K.D. Lewandowska, *Subdiffusion–absorption process in a system with a thin membrane*, Math. Model. Nat. Phenom. **11 (3)** 128 (2016)

Outline

1. Anomalous diffusion
2. How to measure subdiffusion parameters
3. Subdiffusion and slow subdiffusion in a system with a thin membrane - new boundary conditions at thin membrane
4. Normal diffusion in a membrane system as a long memory process: theory + experimental verification

Diffusion



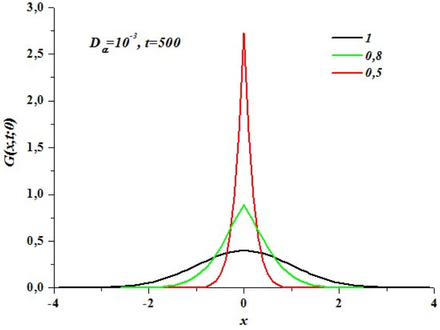
$\langle\lambda^2(x)\rangle < \infty$ $\langle\omega(t)\rangle < \infty$	$\langle\lambda^2(x)\rangle < \infty$ $\langle\omega(t)\rangle = \infty$	$\langle\lambda^2(x)\rangle = \infty$ $\langle\omega(t)\rangle < \infty$
normal diffusion	subdiffusion	superdiffusion
$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$	$\frac{\partial C}{\partial t} = D_\alpha \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\frac{\partial^2 C}{\partial x^2}$	$\frac{\partial C}{\partial t} = D_\beta \frac{\partial^\beta C}{\partial x^\beta}$
$\lambda(x) \sim e^{-x^2/2\sigma}$	$\lambda(x) \sim e^{-x^2/2\sigma}$	$\lambda(x) \sim \left(\frac{\sigma}{\lvert x\rvert}\right)^{1+\beta}$ $\lvert x\rvert \gg \sigma,\ 1 < \beta < 2$
$\omega(t) \sim e^{-t/\tau}$	$\omega(t) \sim \left(\frac{\tau}{t}\right)^{1+\alpha},\ t \gg \tau,\ 0 < \alpha < 1$	$\omega(t) \sim e^{-t/\tau}$

Mean square displacement $\langle x^2(t)\rangle$ for subdiffusion

$$\langle x^2(t)\rangle = \frac{2D_\alpha}{\Gamma(1+\alpha)} t^\alpha\ , \quad \text{for} \quad 0 < \alpha < 1\ ,$$

where

- D_α – subdiffusion coefficient,
- $\Gamma(z)$ – Gamma function.



$$G(x,t;x_0)=\frac{1}{2\sqrt{\pi Dt}}\exp\left(-\frac{(x-x_0)^2}{4Dt}\right) \qquad \alpha=1$$

$$G(x,t;x_0)=\frac{1}{\alpha|x-x_0|}H_{11}^{10}\left(\left(\frac{(x-x_0)^2}{D_\alpha t}\right)^{1/\alpha}\middle|\begin{matrix}1 & 1\\ 1 & \alpha/2\end{matrix}\right) \qquad \alpha<1$$

$\langle \tau \rangle = -\left.\frac{d\hat{\omega}(s)}{ds}\right|_{s=0}$, $\hat{\omega}(0) = 1$, $\hat{\omega}(s) = 1 - \mu v(s)$

Normal diffusion

$\langle \tau \rangle := \int_0^\infty \tau \omega(\tau) d\tau < \infty$

$$\hat{\omega}(s) = 1 - \mu s \;,$$

Subdiffusion

$\langle \tau^\rho \rangle := \int_0^\infty \tau^\rho \omega(\tau) d\tau = \infty$ for $\rho > \alpha$, $0 < \alpha < 1$, and $\langle \tau^\rho \rangle < \infty$ for $\rho \leq \alpha$

$$\hat{\omega}(s) = 1 - \mu s^\alpha \;, \; 0 < \alpha < 1 \;,$$

Slow subdiffusion

$\langle \tau^\rho \rangle = \infty$ for $\rho > 0$

$$\hat{\omega}(s) = 1 - \mu v(s);$$

$v(s)$ is a slowly varying function $v(as)/v(s) \longrightarrow 1$, $a > 0$, and $v(s) \to 0$ when $s \to 0^+$.

PRL **94,** 170602 (2005) PHYSICAL REVIEW LETTERS week ending 6 MAY 2005

How to Measure Subdiffusion Parameters

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We propose a method to measure the subdiffusion parameter α and subdiffusion coefficient D_α which are defined by means of the relation $\langle x^2 \rangle = \frac{2D_\alpha}{\Gamma(1+\alpha)} t^\alpha$, where $\langle x^2 \rangle$ denotes a mean square displacement of a random walker starting from $x = 0$ at the initial time $t = 0$. The method exploits a membrane system where a substance of interest is transported in a solvent from one vessel to another across a thin membrane which plays here only an auxiliary role. We experimentally study a diffusion of glucose and sucrose in a gel solvent, and we precisely determine the parameters α and D_α, using a fully analytic solution of the fractional subdiffusion equation.

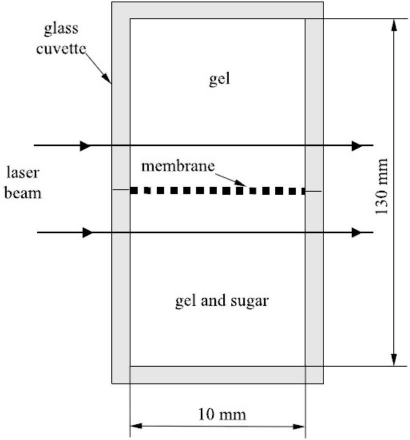
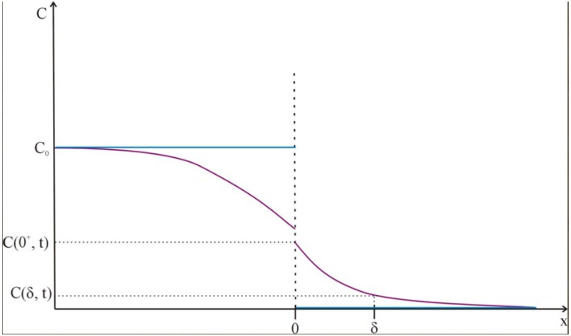


FIG. 1. Schematic view of the membrane system under study.



$$\frac{\partial C(x,t)}{\partial t} = D_\alpha \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \frac{\partial^2 C(x,t)}{\partial x^2} \quad , \quad C(\delta, t) = \kappa C(0^+, t)$$

$$\frac{d^\delta f(t)}{dt^\delta} = \frac{1}{\Gamma(k-\delta)} \frac{d^k}{dt^k} \int_0^t (t-t')^{k-\delta-1} f(t') dt' \ , \ k-1 \leq \delta < k$$

$$\delta(t) = A(\alpha, D_\alpha, \kappa) t^{\alpha/2}.$$

$$D_\alpha = \frac{A^2}{\left[\left(H^{1\,0}_{1\,1}\right)^{-1}\left(\frac{\alpha\kappa}{2} \,\middle|\, \begin{smallmatrix} 1 & 1 \\ 0 & \frac{2}{\alpha} \end{smallmatrix}\right)\right]^\alpha}.$$

Fitting the experimental $\delta(t)$ by the function At^γ, we have found the index $\alpha = 2\gamma = 0.90 \pm 0.01$. It does not much differ from unity, but it signals subdiffusion due to the small error [5]. With the numerical values of inverse Fox functions, we recalculate the coefficient A into D_α by means of the relation (16). Thus, we get $D_{0.90} = (9.8 \pm 1.0) \times 10^{-4}$ [$mm^2/s^{0.90}$] for glucose and $D_{0.90} = (6.3 \pm 0.9) \times 10^{-4}$ [$mm^2/s^{0.90}$] for sucrose.

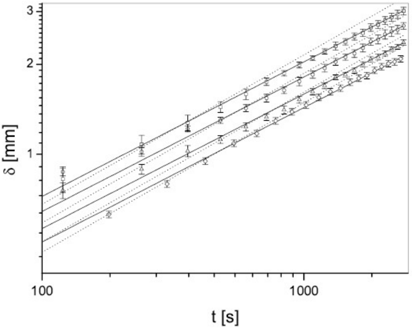


FIG. 2. The experimentally measured thickness of the near-membrane layer δ as a function of time t for glucose with $\kappa = 0.05$ (□), $\kappa = 0.08$ (○), $\kappa = 0.12$ (△), and for sucrose with $\kappa = 0.08$ (◇). The solid lines represent the power function $At^{0.45}$, while the dotted lines correspond to the function $A\sqrt{t}$.

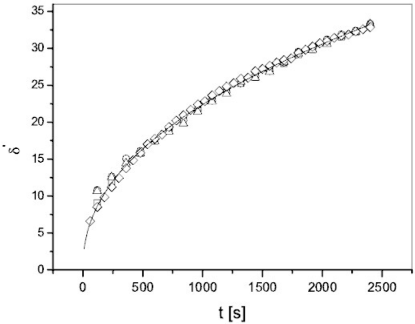
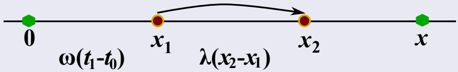


FIG. 3. The experimentally measured δ divided by the coefficient A from Eq. (15). The symbols are assigned as in Fig. 2 and the line represents the function $t^{0.45}$. For clarity of the plot the

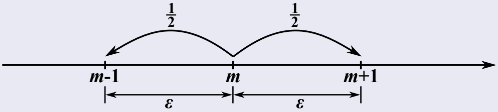
Continuous Time Random Walk

I version



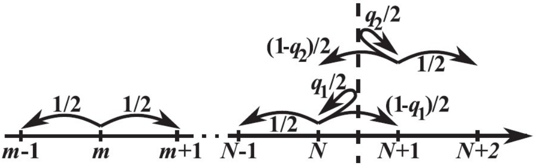
both $\tau = t_1 - t_0$ and $\epsilon = x_2 - x_1$ are random variables

II version



τ is a random variable, ϵ is a small parameter, $x = \epsilon m$

The simplest model of random walk in a membrane system



$$P_{n+1}(m; m_0) = \frac{1}{2} P_n(m-1; m_0) + \frac{1}{2} P_n(m+1; m_0)\ ,\ \ m \neq N, N+1\ ,$$

$$P_{n+1}(N; m_0) = \frac{1}{2} P_n(N-1; m_0) + \frac{1-q_2}{2} P_n(N+1; m_0) + \frac{q_1}{2} P_n(N; m_0)\ ,$$

$$P_{n+1}(N+1; m_0) = \frac{1-q_1}{2} P_n(N; m_0) + \frac{1}{2} P_n(N+2; m_0) + \frac{q_2}{2} P_n(N+1; m_0)\ ,$$

II version

The method

1. From discrete time n to continuous time t:
since $\hat{\omega}(0) = 1$ we suppose for small s

$$\hat{\omega}(s) \equiv \int_0^\infty \mathrm{e}^{-st} \omega(t) dt = 1 - \mu v(s),$$

$v(s) \to 0$ when $s \to 0$
2. From discrete position m to continuous space variable $x = \epsilon m$

Laplace transforms of the Green's functions

$$\hat{P}_-(x,s;x_0) = \frac{\sqrt{v(s)}}{2s\sqrt{D}}\left[e^{-\frac{|x-x_0|\sqrt{v(s)}}{\sqrt{D}}} + \left(\kappa_1 + \kappa_2\sqrt{\frac{v(s)}{D}}\right) e^{-\frac{(2x_N - x - x_0)\sqrt{v(s)}}{\sqrt{D}}} \right],$$

$$\hat{P}_+(x,s;x_0) = \frac{\sqrt{v(s)}}{2s\sqrt{D}} e^{-\frac{(x-x_0)\sqrt{v(s)}}{\sqrt{D}}} \left(1 - \kappa_1 - \kappa_2\sqrt{\frac{v(s)}{D}}\right),$$

$$\kappa_1 = \frac{\gamma_1 - \gamma_2}{\gamma_1 + \gamma_2}\ ,\ \kappa_2 = \frac{2/\gamma_1}{(1/\gamma_1 + 1/\gamma_2)^2}\ .$$

$$q_1(\epsilon) = e^{-\frac{\epsilon}{\gamma_1}}\ ,\ q_2(\epsilon) = e^{-\frac{\epsilon}{\gamma_2}}\ .$$

γ_1, γ_2 – reflection membrane coefficients for continuous system

Boundary condition at a thin membrane in terms of Laplace transform

$$\hat{P}_-(x_N, s; x_0) = \left(\frac{\gamma_1}{\gamma_2} + \gamma_1 \sqrt{\frac{v(s)}{D}} \right) \hat{P}_+(x_N, s; x_0) \; ,$$

$$\hat{J}_-(x_N, s; x_0) = \hat{J}_+(x_N, s; x_0) \; .$$

$$\hat{J}(x, s) = -D \frac{s}{v(s)} \frac{d\hat{P}(x, s)}{dx} \; .$$

$$\mathcal{L}^{-1}\left[s^{\delta} \hat{P}(x, s) \right] = \frac{\partial^{\delta} P(x, t)}{\partial t^{\delta}} \; , 0 < \delta < 1,$$

Boundary condition for normal diffusion, $v(s) = s$

$$P_-(x_N, t; x_0) = \frac{\gamma_1}{\gamma_2}\, P_+(x_N, t; x_0) + \frac{\gamma_1}{\sqrt{D}} \frac{\partial^{1/2} P_+(x_N, t; x_0)}{\partial t^{1/2}} \ ,$$

$$J_-(x_N, t; x_0) = J_+(x_N, t; x_0) \ .$$

Solutions to normal diffusion equation, $C(x,0) = C_0\Theta(-x)$

For the boundary condition 'with memory':

$$C(x,t) = C_0 - C_0\frac{(1-\kappa_1)}{2}\mathrm{erfc}\left(\frac{x_N - x}{2\sqrt{Dt}}\right)$$

$$+\frac{C_0\kappa_2}{2\sqrt{\pi Dt}}\left(1 - \frac{\kappa_2(x_N - x)}{2Dt(1-\kappa_1\kappa_2)^2}\right)\mathrm{e}^{-\frac{(x_N - x)^2}{4Dt}} \quad , x < 0 \; ,$$

$$C(x,t) = C_0\frac{(1-\kappa_1)}{2}\mathrm{erfc}\left(\frac{x - x_N}{2\sqrt{Dt}}\right) - \frac{C_0\kappa_2}{2\sqrt{\pi Dt}}\mathrm{e}^{-\frac{(x-x_N)^2}{4Dt}} \quad , \; x > 0 \; .$$

For the boundary condition 'without memory':

$$C(x,t) = C_0 - C_0\frac{(1-\kappa_1)}{2}\mathrm{erfc}\left(\frac{x_N - x}{2\sqrt{Dt}}\right) \quad , x < 0 \; ,$$

$$C(x,t) = C_0\frac{(1-\kappa_1)}{2}\mathrm{erfc}\left(\frac{x - x_N}{2\sqrt{Dt}}\right) \quad , \; x > 0.$$

Boundary condition 'with memory'

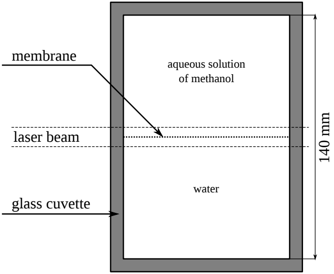
$$C(x_N^-, t) = \frac{\gamma_1}{\gamma_2}\, C(x_N^+, t) + \frac{\gamma_1}{\sqrt{D}} \frac{\partial^{1/2} C(x_N^+, t)}{\partial t^{1/2}}\ .$$

Boundary condition 'without memory'

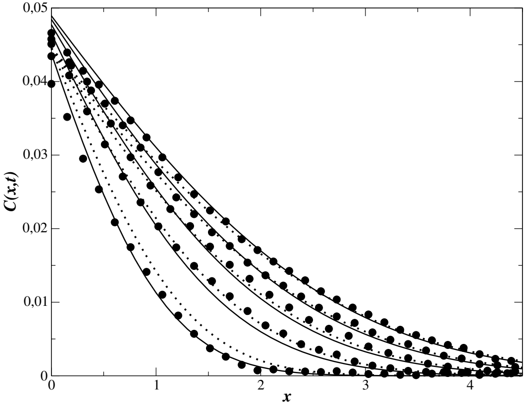
$$C(x_N^-, t) = \frac{\gamma_1}{\gamma_2}\, C(x_N^+, t)\ .$$

Experimental verification

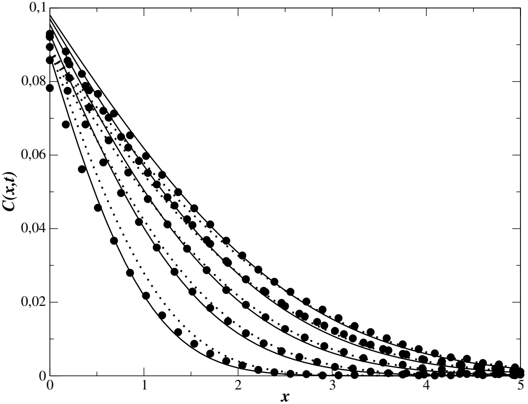
Normal diffusion of methanol in water, membrane thickness $\approx$ $0.2mm$



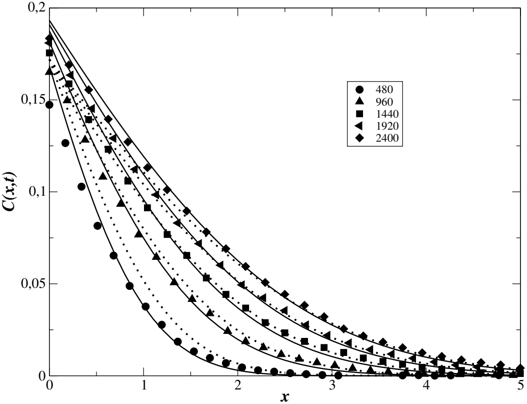
$$C(x,t) = \begin{cases} C_0, & x < 0, \\ 0, & x > 0. \end{cases}$$



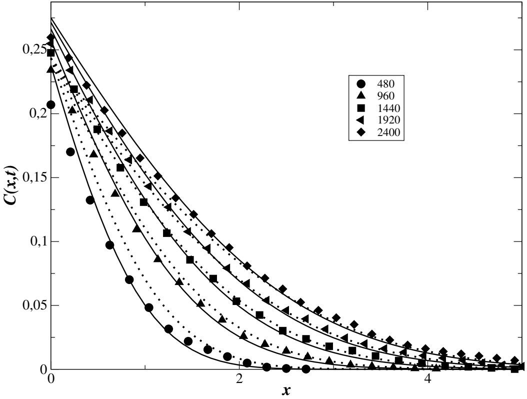
$C_0 = 0.125 mol/dm^3$, $\alpha = 1$, $D = 0.00097\ mm^2/s$, $\kappa_1 = 0.15$, $\kappa_2 = 0.185$, $t = 480, 960, 1440, 1920, 2400 s$, symbols – experimental results, solid lines – solutions for the bc with memory, dotted lines – solutions for the bc without memory



$C_0 = 0.250 mol/dm^3$, $\alpha = 1$, $D = 0.00097\ mm^2/s$, $\kappa_1 = 0.15$, $\kappa_2 = 0.185$, $t = 480, 960, 1440, 1920, 2400 s$, symbols – experimental results, solid lines – solutions for the bc with memory, dotted lines – solutions for the bc without memory

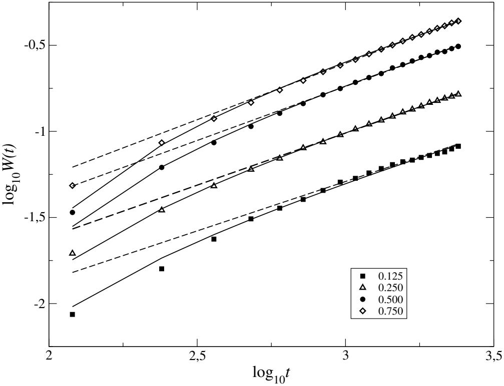


$C_0 = 0.500 mol/dm^3$, $\alpha = 1$, $D = 0.00097\ mm^2/s$, $\kappa_1 = 0.15$, $\kappa_2 = 0.185$, $t = 480, 960, 1440, 1920, 2400s$, symbols – experimental results, solid lines – solutions for the bc with memory, dotted lines – solutions for the bc without memory



$C_0 = 0.750 mol/dm^3$, $\alpha = 1$, $D = 0.00097\ mm^2/s$, $\kappa_1 = 0.15$, $\kappa_2 = 0.185$, $t = 480, 960, 1440, 1920, 2400 s$, symbols – experimental results, solid lines – solutions for the bc with memory, dotted lines – solutions for the bc without memory

Time evolution of the total amount of substance $W(t)$ in the region $x > 0$, $W(t) = \int_0^\infty C(x,t)dx$



$C_0 = 0.125, 0.250, 0.500, 0.750\ mol/dm^3$, $\alpha = 1$, $D = 0.00097\ mm^2/s$, $\kappa_1 = 0.15$, $\kappa_2 = 0.185$, symbols – experimental results, solid lines – solutions for the bc with memory, dotted lines – solutions for the bc without memory

The Green's functions for subdiffusion, $v(s) = s^\alpha$, $\alpha < 1$

$$P_-(x,t;x_0) = \frac{1}{2\sqrt{D_\alpha}}\left[f_{\alpha/2-1,\alpha/2}\left(t;\frac{|x-x_0|}{\sqrt{D_\alpha}}\right) + \kappa_1 f_{\alpha/2-1,\alpha/2}\left(t;\frac{2x_N-x-x_0}{\sqrt{D_\alpha}}\right)\right] + \frac{\kappa_2}{2D_\alpha} f_{\alpha-1,\alpha/2}\left(t;\frac{2x_N-x-x_0}{\sqrt{D_\alpha}}\right),$$

$$P_+(x,t;x_0) = \frac{1-\kappa_1}{2\sqrt{D_\alpha}}\, f_{\alpha/2-1,\alpha/2}\left(t;\frac{x-x_0}{\sqrt{D_\alpha}}\right) - \frac{\kappa_2}{2D_\alpha}\, f_{\alpha-1,\alpha/2}\left(t;\frac{x-x_0}{\sqrt{D_\alpha}}\right).$$

$$f_{\nu,\beta}(t;a) = \frac{1}{t^{\nu+1}}\sum_{k=0}^{\infty}\frac{1}{k!\Gamma(-k\beta-\nu)}\left(-\frac{a}{t^\beta}\right)^k,$$

$a, \beta > 0$ (the function $f_{\nu,\beta}$ can be treated as a special case of the Fox function)

Slow subdiffusion

$$\hat{\omega}(s) = 1 - \mu v(s) \quad , \quad v(s) = \left(\frac{1}{\ln(1/s)}\right)^{r-1} \; , \; r > 1 \; ,$$

$$P_{-}(x,t;x_0) = \frac{\kappa_0}{2\sqrt{D(\ln t)^{r-1}}} \mathrm{e}^{-\frac{|x-x_0|}{\sqrt{D(\ln t)^{r-1}}}}$$

$$+ \left[\frac{\kappa_0}{2\sqrt{D(\ln t)^{r-1}}} \mathrm{e}^{-\frac{(2x_N - x - x_0)}{\sqrt{D(\ln t)^{r-1}}}} + \frac{\kappa_G}{2D(\ln t)^{r-1}} \mathrm{e}^{-\frac{(2x_N - x - x_0)}{\sqrt{D(\ln t)^{r-1}}}} \right] ,$$

$$P_{+}(x,t;x_0) = \frac{1-\kappa_0}{2\sqrt{D(\ln t)^{r-1}}} \mathrm{e}^{-\frac{(x-x_0)}{\sqrt{D(\ln t)^{r-1}}}}$$

$$- \frac{\kappa_G}{2D(\ln t)^{r-1}} \mathrm{e}^{-\frac{(x-x_0)}{\sqrt{D(\ln t)^{r-1}}}} ,$$

$$\kappa_0 = \frac{\gamma_1 - \gamma_2}{\gamma_1 + \gamma_2} \; , \; \kappa_G = \frac{4\gamma_1}{(1+\gamma_1/\gamma_2)^2} \; , \; D = \frac{\epsilon^2}{2\mu} \; .$$

Subdiffusion

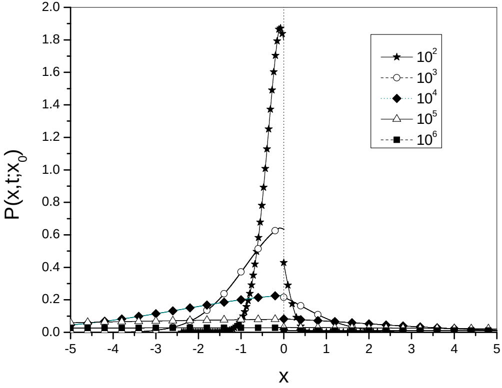


Figure : Plots of the Green's functions for subdiffusion occurring in the system with a thin membrane obtained for $\alpha = 0.9$, $D = 0.001$, $\gamma_1 = 0.8$, $\gamma_2 = 0.3$, $x_0 = -0.5$ for times given in the legend.

Slow subdiffusion

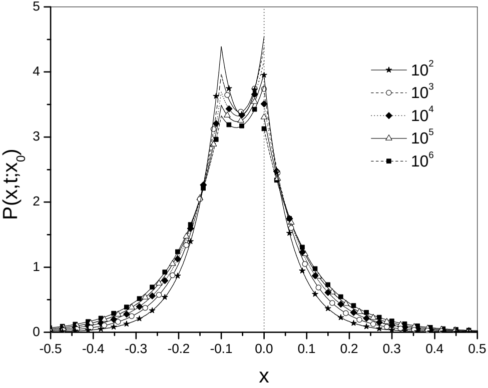


Figure : Plots of the Green's functions for 'slow subdiffusion' occurring in the system with a thin membrane, here $r = 1.9$, the other parameters are the same as in the previous figure.

Boundary condition at a thin membrane

for subdiffusion

$$P_-(x_N, t; x_0) = \frac{\gamma_1}{\gamma_2} P_+(x_N, t; x_0) + \frac{\gamma_1}{\sqrt{D}} \frac{\partial^{\alpha/2} P_+(x_N, t; x_0)}{\partial t^{\alpha/2}} ,$$

for slow subdiffusion

$$P_-(x_N, t; x_0) = \lambda_1 P_+(x_N, t; x_0) + \lambda_2 \frac{d}{dt} \int_0^t F(t-t') P_+(x_N, t'; x_0) dt' ,$$

where

$$F(t) = \frac{\mu(t, (r-1)/2)}{\Gamma(r/2)} ,$$

$\mu(t, (r-1)/2) = \int_0^\infty \frac{t^\zeta \zeta^{(r-1)/2}}{\Gamma(1+\zeta)} d\zeta$ is the Volterra–type function.

Final remarks

1. The presented model allows one to obtain the Green's functions for various kinds of diffusion.
2. The model is useful to describe diffusion in systems in which homogeneity can be broken at several points or which are composed of several parts.
3. The new boundary condition at a thin membrane contains a fractional time derivative; this derivative is present also in the boundary condition at a thin membrane located in a system in which normal diffusion occurs. Thus, **normal diffusion in a membrane system appears to be a process with a 'long memory' which is created by the membrane**.

Thank you for your attention

From discrete to continuous time

$$P_{n+1}(m; m_0) = \frac{1}{2} P_n(m-1; m_0) + \frac{1}{2} P_n(m+1; m_0)$$

Generating function

$$S(m, z; m_0) = \sum_{n=0}^{\infty} z^n P_n(m, m_0)$$

We use the following formula

$$P(m, t; m_0) = \sum_{n=0}^{\infty} P_n(m, m_0) \Phi_n(t) \; , \tag{1}$$

where $\Phi_n(t)$ is the probability that the particle takes n jumps in the time interval $(0, t)$.

$$\hat{\Phi}_n(s) = \frac{1 - \hat{\omega}(s)}{s} \left[\hat{\omega}(s)\right]^n \; . \tag{2}$$

From discrete to continuous time

Combining the Laplace transform of Eq. (1) with Eq. (2) we get

$$\hat{P}(m, s; m_0) = \frac{1 - \hat{\omega}(s)}{s} S\left(m, \hat{\omega}(s); m_0\right) . \qquad (3)$$

From discrete to continuous space variable

Supposing ϵ denotes the distance between discrete sites, and supposing

$$x = \epsilon m \ , \ x_0 = \epsilon m_0 \ , \ x_N = \epsilon N \ ,$$

taking into consideration the following relation valid for small ϵ

$$\frac{P(m, t; m_0)}{\epsilon} \approx P(x, t; x_0) \ ,$$

we pass from a discrete to a continuous space variable assuming that ϵ is small.

From discrete to continuous space variable

$$S(m,z;m_0) = \frac{[\eta(z)]^{|m-m_0|}}{\sqrt{1-z^2}}$$

$$\eta(z) = \frac{1-\sqrt{1-z^2}}{z} \ .$$

$$\hat{P}(x,s;x_0) = \frac{\sqrt{\mu}v(s)}{\epsilon s\sqrt{2v(s)-\mu v^2(s)}} \left[\frac{1-\sqrt{2\mu v(s)-\mu^2 v^2(s)}}{1-\mu v(s)}\right]^{\frac{|x-x_0|}{\epsilon}}$$

$$\hat{P}(x,s;x_0) \neq 0 \ , \ \hat{P}(x,s;x_0) < \infty \Rightarrow \epsilon \sim \sqrt{\mu}$$

$$D = \frac{1}{2}\frac{\epsilon^2}{\mu} \ ,$$

Subdiffusion equation and its fundamental solution (Green's function)

$$\hat{P}(x,s;x_0) = \frac{\sqrt{v(s)}}{2s\sqrt{D}} \mathrm{e}^{-|x-x_0|\sqrt{\frac{v(s)}{D}}}$$

$$s\hat{P}(x,s;x_0) - P(x,0;x_0) = \frac{Ds}{v(s)} \frac{\partial^2 \hat{P}(x,s;x_0)}{\partial x^2}$$

$$P_{n+1}(m;m_0) = \frac{1}{2}P_n(m-1;m_0) + \frac{1}{2}P_n(m+1;m_0),$$

$$\hat{P}(m,s;m_0) = \frac{1-\hat{\omega}(s)}{s} S\left(m, \hat{\omega}(s); m_0\right),$$

$$s\hat{P}(x,s;x_0) - P(x,0;x_0) = \frac{s\hat{\omega}(s)}{2(1-\hat{\omega}(s))} \frac{\partial^2 \hat{P}(x,s;x_0)}{\partial x^2}$$

Interpretation: approximation of $\hat{\omega}(s)$ for small ϵ, not for small s!

$$\hat{\omega}(s) = \frac{1}{1 + \frac{\epsilon^2}{2D} v(s)}$$

In the limit of small ϵ (for $s > 0$)

$$\hat{\omega}(s) \approx 1 - \frac{\epsilon^2}{2D} v(s)$$

Subdiffusion equation with fractional time derivative, $v(s) = s^{\alpha}$

$$s\hat{P}(x,s) - P(x,0) = Ds^{1-\alpha}\frac{\partial^2 \hat{P}(x,s)}{\partial x^2} \ ,$$

$$\mathcal{L}^{-1}\left[s\hat{P}(x,s) - P(x,0)\right] = \frac{\partial P(x,t)}{\partial t} \ , \ \mathcal{L}^{-1}\left[s^{\delta}\hat{P}(x,s)\right] = \frac{\partial^{\delta} P(x,t)}{\partial t^{\delta}} \ , 0 < \delta < 1,$$

$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\frac{\partial^2 P(x,t)}{\partial x^2} \ , \ 0 < \alpha < 1$$

The Riemann–Liouville derivative is defined as being valid for $\delta > 0$ (here k is a natural number which fulfils $k - 1 \leq \delta < k$)

$$\frac{d^{\delta} f(t)}{dt^{\delta}} = \frac{1}{\Gamma(k-\delta)}\frac{d^k}{dt^k}\int_0^t (t-t')^{k-\delta-1} f(t')dt' \ .$$

For $\alpha = 1$ one obtains a normal diffusion equation.

The particular forms of the generating function, hereafter denoted as S_i where the index i denote the signs of $m - N$, are the following (here $m_0 \leq N$)

$$S_-(m, z; m_0) = \frac{[\eta(z)]^{|m-m_0|}}{\sqrt{1-z^2}} + \left[\frac{q_1 - q_2\eta(z)}{1-(q_1+q_2-1)\eta(z)}\right] \frac{[\eta(z)]^{2N-m-m_0+1}}{\sqrt{1-z^2}} ,$$

$$S_+(m, z; m_0) = \frac{[\eta(z)]^{m-m_0}(1+\eta(z))(1-q_1)}{\sqrt{1-z^2}\,[1-(q_1+q_2-1)\eta(z)]} .$$

Basic relations for reflection membrane coefficients

However, a new problem arises within this limit. The mean number of steps $\langle n(t)\rangle$ over time interval $[0,t]$ is given by the following formula

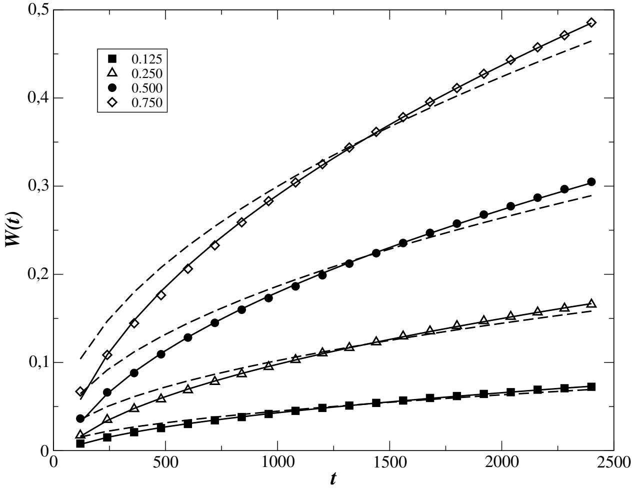
$$\langle n(t)\rangle = \mathcal{L}^{-1}\left[\frac{\hat{\omega}(s)}{s[1-\hat{\omega}(s)]}\right] = \frac{2D}{\epsilon^2}\mathcal{L}^{-1}\left[\frac{1}{v(s)}\right],$$

which provides $\langle n(t)\rangle \longrightarrow \infty$ when $\epsilon \longrightarrow 0$. Thus, for a very small ϵ, $\langle n(t)\rangle$ takes anomalous large values. Then, the probability that a particle which tries to pass the partially permeable wall 'infinite times' in every finite time interval passes through the wall, is equal to one. In order to avoid such a situation we assume that q_1 and q_2 are the functions of the parameter ϵ (for $q_1, q_2 > 0$) which fulfil $q_1(0) = q_2(0) = 1$. After calculations we get (T. Kosztołowicz, PRE 91, 022102 (2015))

$$q_1(\epsilon) = \mathrm{e}^{-\frac{\epsilon}{\gamma_1}}\ ,\ q_2(\epsilon) = \mathrm{e}^{-\frac{\epsilon}{\gamma_2}}\ .$$

γ_1, γ_2 – reflection membrane coefficients for continuous system

Time evolution of the total amount of substance $W(t)$ in the region $x > 0$, $W(t) = \int_0^\infty C(x,t)dx$



The problem

Parameters (probabilities) describing random walk in a discrete system, like the probability of jump $p_{m,m+1} = p_{m+1,m} = 1/2$, probability of stopping a particle by a membrane q, probability of particle's absorbing R etc., should be redefined in a system with continuous variables.
The parameters μ or/and ϵ can be involved into relation between 'discrete' and 'continuous' diffusion parameters.

Laplace transforms of the Green's functions

$$\hat{P}_-(m,s;m_0) = \frac{1-\hat{\omega}(s)}{s\sqrt{1-[\hat{\omega}(s)]^2}}\Bigg[[\eta(\hat{\omega}(s))]^{|m-m_0|} + \Lambda(s)[\eta(\hat{\omega}(s))]^{2N-m-m_0+1}\Bigg], \quad (4)$$

$$\hat{P}_+(m,s;m_0) = \frac{1-\hat{\omega}(s)}{s\sqrt{1-[\hat{\omega}(s)]^2}} \times M(s)[\eta(\hat{\omega}(s))]^{|m-m_0|}, \quad (5)$$

where

$$\Lambda(s) \equiv \frac{q_1 - q_2\eta(\hat{\omega}(s))}{1-(q_1+q_2-1)\eta(\hat{\omega}(s))}, \quad (6)$$

and

$$M(s) \equiv \frac{(1-q_1)(1+\eta(\hat{\omega}(s)))}{1-(q_1+q_2-1)\eta(\hat{\omega}(s))}. \quad (7)$$