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On fractional diffusion and continuous time random walks☆

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Abstract

A continuous time random walk model is presented with long-tailed waiting time density that approaches a Gaussian distribution in the continuum limit. This example shows that continuous time random walks with long time tails and diffusion equations with a fractional time derivative are in general not asymptotically equivalent.

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1. Introduction

Given the connection (established in Refs. [1,2]) between continuous time random walks (CTRW) and diffusion equations with fractional time derivative

$$\frac{\partial^\alpha}{\partial t^\alpha} p(\mathbf{r},t) = C_\alpha \Delta p(\mathbf{r},t) \quad 0 < \alpha \leqslant 1 \tag{1}$$

it has been subsequently argued in the literature that all continuous time random walks with long-tailed waiting time densities $\psi(t)$, i.e., with

$$\psi(t) \sim t^{-1-\alpha} \quad t \to \infty \tag{2}$$

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are in some sense asymptotically equivalent to a fractional diffusion equation [3–8]. Let me first explain the symbols in these two equations. Of course the fractional time derivative of order α in (1) is only a symbolic notation (a definition is given in Eq. (13) below). Random walks on a lattice in continuous time are described by $p(\mathbf{r}, t)$, the probability density to find a random walker at the (discrete) lattice position $\mathbf{r} \in \mathbb{R}^d$ at time t if it started from the origin $\mathbf{r} = \mathbf{0}$ at time $t = 0$ [9,10]. In Eq. (2) the waiting time distribution $\psi(t)$ gives the probability density for a time interval t between two consecutive steps of the random walker, and the long time tail exponent α is the same as the order of the fractional time derivative in (1) (see Refs. [1,2] for details). As usual Δ denotes the Laplacian and the constant $C_\alpha \geqslant 0$ denotes the fractional diffusion coefficient.

Despite early doubts, formulated, e.g. in Ref. [11, p. 78], many authors [3–8] consider it now an established fact that Proposition A "$p(\mathbf{r}, t)$ *satisfies a fractional diffusion equation*" and Proposition B "$p(\mathbf{r}, t)$ *is the solution of a CTRW with long time tail*" are in some sense asymptotically equivalent. Equivalence between propositions A and B requires that A implies B and further that B implies A. One implication, namely that A implies B, was shown to be false in Refs. [12] and [13, p. 116ff] by showing that all fractional diffusion equations of order α and type $\beta \neq 1\,(0 \leqslant \beta \leqslant 1)$ do not have a probabilistic interpretation.

In this paper an example of a CTRW is given whose waiting time density fulfills Eq. (2) but whose asymptotic continuum limit is not the fractional diffusion equation (1) (with the same α). Naturally, the idea underlying the example can be widely generalized.

2. Definition of models

Consider first the integral equation of motion for the CTRW-model [9,10]. The probability density $p(\mathbf{r}, t)$ obeys the integral equation

$$p(\mathbf{r}, t) = \delta_{\mathbf{r}\mathbf{0}} \Phi(t) + \int_0^t \psi(t - t') \sum_{\mathbf{r}'} \lambda(\mathbf{r} - \mathbf{r}') p(\mathbf{r}', t')\, \mathrm{d}t' \;, \tag{3}$$

where $\lambda(\mathbf{r})$ denotes the probability for a displacement $\mathbf{r}$ in each single step, and $\psi(t)$ is the waiting time distribution giving the probability density for the time interval t between two consecutive steps. The transition probabilities obey $\sum_{\mathbf{r}} \lambda(\mathbf{r}) = 1$, and the function $\Phi(t)$ is the survival probability at the initial position which is related to the waiting time distribution through

$$\Phi(t) = 1 - \int_0^t \psi(t')\, \mathrm{d}t' \;. \tag{4}$$

Fourier–Laplace transformation leads to the solution in Fourier–Laplace space given as [10]

$$p(\mathbf{k}, u) = \frac{1}{u} \frac{1 - \psi(u)}{1 - \psi(u)\lambda(\mathbf{k})} \;, \tag{5}$$

where $p(\mathbf{k}, u)$ is the Fourier–Laplace transform of $p(\mathbf{r}, t)$ and similarly for ψ and λ.

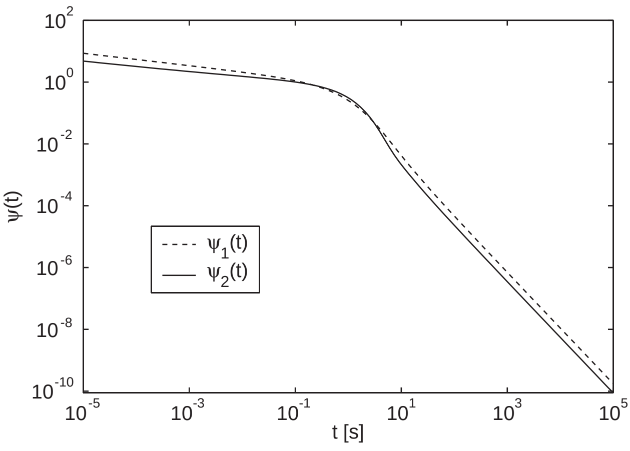

Fig. 1. Waiting time densities $\psi_1(t)$ for model 1 and $\psi_2(t)$ for model 2 with $\alpha = 0.8$, $\tau = 1$ s and $c = 1$ s$^{-1.2}$.

Two lattice models with different waiting time density will be considered. In the first model the waiting time density is chosen as the one found in Refs. [1,2]

$$\psi_1(t) = \frac{t^{\alpha-1}}{\tau^\alpha} E_{\alpha,\alpha}\left(-\frac{t^\alpha}{\tau^\alpha}\right) , \tag{6}$$

where $0 < \alpha \leqslant 1, 0 < \tau < \infty$ is the characteristic time, and

$$E_{a,b}(x) = \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(ak+b)} \qquad a > 0, \ \ b \in \mathbb{C} \tag{7}$$

is the generalized Mittag–Leffler function [14]. In the second model the waiting time density is chosen as

$$\psi_2(t) = \frac{t^{\alpha-1}}{2c\tau^2} E_{\alpha,\alpha}\left(-\frac{t^\alpha}{c\tau^2}\right) + \frac{1}{2\tau}\exp(-t/\tau) , \tag{8}$$

where $0 < \alpha \leqslant 1$, $0 < \tau < \infty$ and $c > 0$ is a suitable dimensional constant.

The waiting time density $\psi_2(t)$ differs only little from $\psi_1(t)$ as shown graphically in Fig. 1. Note that both models have a long time tail of the form given in Eq. (2), and the average waiting time $\int_0^\infty t\psi_i(t)\,\mathrm{d}t$ diverges.

For both models the spatial transition probabilities are chosen as those for nearest-neighbour transitions (Polya walk) on a d-dimensional hypercubic lattice given as

$$\lambda(\mathbf{r}) = \frac{1}{2d} \sum_{j=1}^{d} \delta_{\mathbf{r},-\sigma\mathbf{e}_j} + \delta_{\mathbf{r},\sigma\mathbf{e}_j} , \tag{9}$$

where $\mathbf{e}_j$ is the jth unit basis vector generating the lattice, $\sigma > 0$ is the lattice constant, and $\delta_{\mathbf{r},\mathbf{s}} = 1$ for $\mathbf{r} = \mathbf{s}$ and $\delta_{\mathbf{r},\mathbf{s}} = 0$ for $\mathbf{r} \neq \mathbf{s}$.

3. Results

It follows from the general results in Ref. [1] that the first model defined by Eqs. (6) and (9) is equivalent to the fractional master equation

$$\mathrm{D}_{0+}^{\alpha,1}\, p(\mathbf{r},t) = \sum_{\mathbf{r}'} w(\mathbf{r}-\mathbf{r}')\, p(\mathbf{r}',t) \tag{10}$$

with initial condition

$$p(\mathbf{r},0) = \delta_{\mathbf{r},\mathbf{0}} \tag{11}$$

and fractional transition rates

$$w(\mathbf{r}) = \frac{\lambda(\mathbf{r})-1}{\tau^\alpha}\ . \tag{12}$$

Here the fractional time derivative $\mathrm{D}_{0+}^{\alpha,1}$ of order α and type 1 in Eq. (10) is defined as [15]

$$\mathrm{D}_{0+}^{\alpha,1}\, p(\mathbf{r},t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-t')^{-\alpha} \frac{\partial}{\partial t}\, p(\mathbf{r},t')\,\mathrm{d}t' \tag{13}$$

thereby giving a more precise meaning to the symbolic notation in Eq. (1). The result is obtained from inserting the Laplace transform of $\psi_1(t)$,

$$\psi_1(u) = \frac{1}{1+(\tau u)^\alpha}\ , \tag{14}$$

and the Fourier transform of $\lambda(\mathbf{r})$, the so-called structure function

$$\lambda(\mathbf{k}) = \frac{1}{d}\sum_{j=1}^{d} \cos(\sigma k_j)\,, \tag{15}$$

into Eq. (5). This gives

$$p_1(\mathbf{k},u) = \frac{1}{u}\left(\frac{(\tau u)^\alpha}{1+(\tau u)^\alpha-\lambda(\mathbf{k})}\right) = \frac{u^{\alpha-1}}{u^\alpha - w(\mathbf{k})}\ , \tag{16}$$

where the Fourier transform of Eq. (12) was used in the last equality and the subscript refers to the first model. Eq. (16) equals the result obtained from Fourier–Laplace transformation of the fractional Cauchy problem defined by Eqs. (10) and (11). Hence a CTRW-model with $\psi_1(t)$ and the fractional master equation describe the same random walk process in the sense that their fundamental solutions are the same.

The continuum limit $\sigma,\ \tau \to 0$ was the background and motivation for the discussion in Ref. [2]. It follows from Eq. (1.9) in Ref. [2] by virtue of the continuity theorem [16] for characteristic functions that for the first model the continuum limit with

$$C_\alpha = \lim_{\substack{\tau\to 0\\ \sigma\to 0}} \frac{\sigma}{2\,d\tau^\alpha} \tag{17}$$

leads for all fixed $\mathbf{k}, u$ to

$$\bar{p}_1(\mathbf{k},u) = \lim_{\substack{\tau\to 0\\ \sigma\to 0\\ \sigma^2/\tau^\alpha \to 2\,dC_\alpha}} p_1(\mathbf{k},u) = \frac{u^{\alpha-1}}{u^\alpha + C_\alpha \mathbf{k}^2}\ . \tag{18}$$

Here the expansion $\cos(x) = 1 - x^2/2 + x^4/24 - \cdots$ has been used. Therefore, the solution of the first model with waiting time density $\psi_1(t)$ converges in the continuum limit to the solution of the fractional diffusion equation

$$\mathrm{D}_{0+}^{\alpha,1}\bar{p}_1(\mathbf{r},t) = C_\alpha \Delta \bar{p}_1(\mathbf{r},t) \tag{19}$$

with initial condition analogous to Eq. (11).

Consider now the second model with waiting time density $\psi_2(t)$ given by Eq. (8). In this case

$$\psi_2(u) = \frac{1}{2+2c\tau^2u^\alpha} + \frac{1}{2+2\tau u} \tag{20}$$

and

$$\begin{aligned} p_2(\mathbf{k},u) &= \frac{1}{u}\left(1-(\lambda(\mathbf{k})-1)\frac{\psi_2(u)}{1-\psi_2(u)}\right)^{-1} \\ &= \frac{1}{u}\left(1-(\lambda(\mathbf{k})-1)\frac{2+\tau u+c\tau^2u^\alpha}{\tau u+c\tau^2u^\alpha+2c\tau^3u^{\alpha+1}}\right)^{-1} \\ &= \frac{1}{u}\left\{1+\frac{1}{\tau^\alpha u^\alpha}\left(\frac{\sigma^2\mathbf{k}^2}{2d}-\frac{\sigma^4\mathbf{k}^4}{24d}+\cdots\right)\right. \\ &\qquad \left.\times\left(\frac{2+\tau u+c\tau^2u^\alpha}{(\tau u)^{1-\alpha}+c\tau^{2-\alpha}+2c\tau^{3-\alpha}u}\right)\right\}^{-1} . \end{aligned} \tag{21}$$

From this follows

$$\bar{p}_2(\mathbf{k},u) = \lim_{\substack{\tau\to 0\\ \sigma\to 0\\ \sigma^2/\tau^\alpha\to 2\,dC_\alpha}} p_2(\mathbf{k},u) = 0 \tag{22}$$

showing that the continuum limit as in Eq. (17) with finite C_α does not give rise to the propagator of fractional diffusion. On the other hand the conventional continuum limit with $C_1 = \lim_{\substack{\tau\to 0\\ \sigma\to 0}} \sigma/2d\tau$ exists and yields

$$\bar{p}_2(\mathbf{k},u) = \lim_{\substack{\tau\to 0\\ \sigma\to 0\\ \sigma^2/\tau\to 2dC_1}} p_2(\mathbf{k},u) = \frac{1}{u+C_1\mathbf{k}^2} , \tag{23}$$

the Gaussian propagator of ordinary diffusion with diffusion constant C_1.

4. Discussion

The idea underlying the construction of the counterexample can be generalized. The freedom in the choice of the input functions $\psi(t)$ and $\lambda(\mathbf{r})$ allows to construct a wide variety of continuum limits. This shows that the claims in [3–8] are too general.

In summary the counterexample shows that a power-law tail in the waiting time density is not sufficient to guarantee the emergence of the propagator of fractional diffusion in the continuum limit.

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References

[1] R. Hilfer, L. Anton, Fractional master equations and fractal time random walks, Phys. Rev. E 51 (1995) R848.
[2] R. Hilfer, Exact solutions for a class of fractal time random walks, Fractals 3 (1) (1995) 211.
[3] A. Compte, Stochastic foundations of fractional dynamics, Phys. Rev. E 55 (1996) 4191.
[4] I. Sokolov, J. Klafter, A. Blumen, Fractional kinetics, Physics Today Nov.2002 (2002) 48.
[5] R. Metzler, J. Klafter, I. Sokolov, Anomalous transport in external fields: Continuous time random walks and fractional diffusion equations extended, Phys. Rev. E 58 (1998) 1621.
[6] E. Barkai, R. Metzler, J. Klafter, From continuous time random walks to the fractional Fokker–Planck equation, Phys. Rev. E 61 (2000) 132.
[7] M. Meerschaert, D. Benson, H. Scheffler, B. Baeumer, Stochastic solution of space-time fractional diffusion equations, Phys. Rev. E 65 (2002) 041103.
[8] R. Gorenflo, F. Mainardi, Non-Markovian random walk models, scaling and diffusion limits, in: O. Nielsen (Ed.), 2nd Conference on Levy processes: Theory and Applications, University of Aarhus, Aarhus, 2003, p. 120.
[9] E. Montroll, G. Weiss, Random walks on lattices, II, J. Math. Phys. 6 (1965) 167.
[10] B. Hughes, Random Walks and Random Environments, Vol. 1, Clarendon Press, Oxford, 1995.
[11] R. Hilfer, On fractional diffusion and its relation with continuous time random walks, in: A.P.R. Kutner, K. Sznajd-Weron (Eds.), Anomalous Diffusion: From Basis to Applications, Springer, Berlin, 1999, p. 77.
[12] R. Hilfer, Fractional diffusion based on Riemann–Liouville fractional derivatives, J. Phys. Chem. B 104 (2000) 3914.
[13] R. Hilfer, Applications of Fractional Calculus in Physics, World Scientific Publ. Co., Singapore, 2000.
[14] A. Erdelyi, et al., Higher Transcendental Functions, Vol. III, McGraw-Hill Book Co., New York, 1955.
[15] R. Hilfer, Fractional time evolution, in: R. Hilfer (Ed.), Applications of Fractional Calculus in Physics, World Scientific, Singapore, 2000, p. 87.
[16] H. Bauer, Wahrscheinlichkeitstheorie, Walter de Gruyter, Berlin, 1991.