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.

CONTENTS

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[page 1, §1]

1. Introduction

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

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

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

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

are in some sense asymptotically equivalent to a fractional diffusion equation [3, 4, 5, 6, 7, 8]. *[1.1.2]* Let me first explain the symbols in these two equations. *[1.1.3]* Of course the fractional time derivative of order α in (1) is only a symbolic notation (a *[page 2, §0]* definition is given in eq. (13) below). *[2.0.4]* 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]. *[2.0.5]* 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 [1, 2] for details). *[2.0.6]* As usual Δ denotes the Laplacian and the constant $C_\alpha \geq 0$ denotes the fractional diffusion coefficient.

[2.1.1] Despite early doubts, formulated e.g. in [11, p. 78], many authors [3, 4, 5, 6, 7, 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. *[2.1.2]* Equivalence between propositions A and B requires that A implies B and further that B implies A. *[2.1.3]* One implication, namely that A implies B, was shown to be false in Refs. [12] and [13, p. 116ff] by showing that fractional diffusion equations of order α and type $\beta \neq 1$ $(0 \leq \beta \leq 1)$ do not have a probabilistic interpretation.

[2.2.1] 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). *[2.2.2]* Naturally, the idea underlying the example can be widely generalized.

2. Definition of Models

[2.3.1] Consider first the integral equation of motion for the CTRW-model [9, 10]. *[2.3.2]* The probability density $p(\mathbf{r},t)$ obeys the integral equation

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

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. *[2.3.3]* 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

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

[page 3, §0] 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.

[3.1.1] Two lattice models with different waiting time density will be considered. *[3.1.2]* In the first model the waiting time density is chosen as the one found in [1, 2]

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

where $0 < \alpha \le 1, 0 < \tau < \infty$ 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]. *[3.1.3]* 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 $0 < \alpha \le 1$, $0 < \tau < \infty$ and $c > 0$ is a suitable dimensional constant.

[3.2.1] The waiting time density $\psi_2(t)$ differs only little from $\psi_1(t)$ as shown graphically in Figure 1. *[3.2.2]* 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.

[3.3.1] 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 j-th 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 $\mathbf{r} \neq \mathbf{s}$.

[page 4, §1]

3. Results

[4.1.1] 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 intitial condition

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

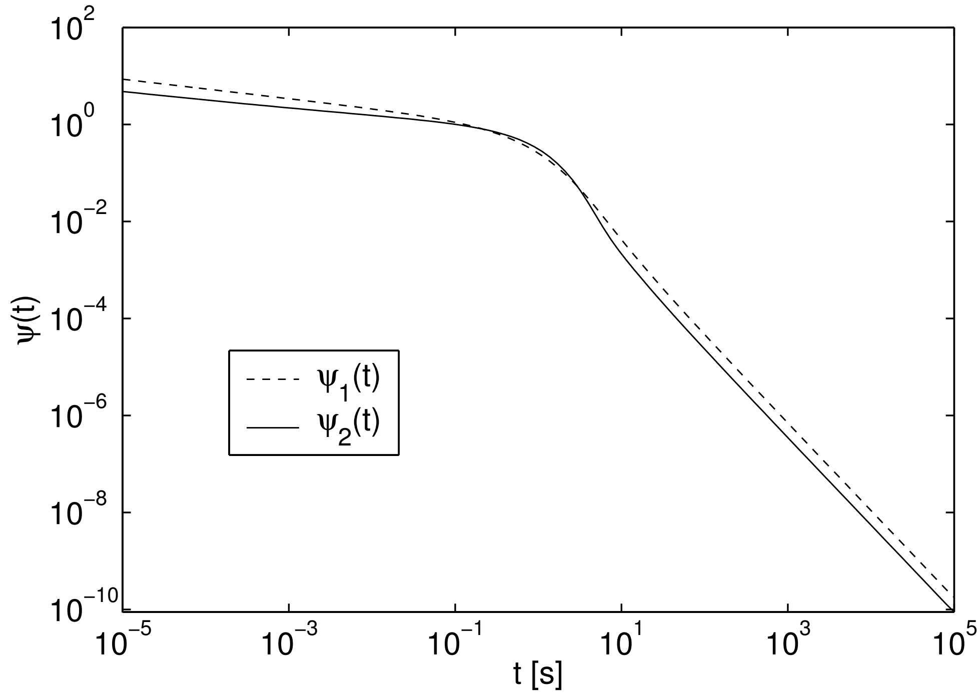

FIGURE 1. Waiting time densities $\psi_1(t)$ for model 1 and $\psi_2(t)$ for model 2 with $\alpha = 0.8$, $\tau = 1$ s and $c = 1\ \mathrm{s}^{-1.2}$.

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).

[page 5, §1] *[5.1.1]* 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). *[5.1.2]* 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. *[5.1.3]* Equation (16) equals the result obtained from Fourier-Laplace transformation of the fractional Cauchy problem defined by equations (10) and

(11). *[5.1.4]* 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.

[5.2.1] The continuum limit $\sigma,\tau\to 0$ was the background and motivation for the discussion in Ref. [2]. *[5.2.2]* 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

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

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

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

[5.2.3] Here the expansion $\cos(x) = 1 - x^2/2 + x^4/24 - ...$ has been used. *[5.2.4]* 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

$$\mathrm{D}^{\alpha,1}_{0+}\overline{p_1}(\mathbf{r},t) = C_\alpha\Delta\overline{p_1}(\mathbf{r},t) \tag{19}$$

with initial condition analogous to eq. (11).

[5.3.1] Consider now the second model with waiting time density $\psi_2(t)$ given by eq. (8). *[5.3.2]* In this case

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

and

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

From this follows

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

showing that the continuum limit as in eq. (17) with finite C_α does not give rise to the propagator of fractional diffusion. *[5.3.3]* On the other hand the conventional continuum limit with $C_1 = \lim_{\substack{\tau\to 0\\ \sigma\to 0}} \sigma^2/(2d\tau)$ exists and yields

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

the Gaussian propagator of ordinary diffusion with diffusion constant C_1.

4. **Discussion**

[5.4.1] The idea underlying the construction of the counterexample can be generalized. *[5.4.2]* The freedom in the choice of the input functions $\psi(t)$ and $\lambda(\mathbf{r})$ allows to construct a wide variety of continuum limits. *[5.4.3]* This shows that the claims in [3, 4, 5, 6, 7, 8] are too general.

[5.5.1] 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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