On Fractional Diffusion and its Relation with Continuous Time Random Walks

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ABSTRACT

Time evolutions whose infinitesimal generator is a fractional time derivative arise generally in the long time limit. Such fractional time evolutions are considered here for random walks. An exact relationship is established between the fractional master equation and a separable continuous time random walk of the Montroll-Weiss type. The waiting time density can be expressed using a generalized Mittag-Leffler function. The first moment of the waiting density does not exist.

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1 Fractional Time Evolution

A series of recent investigations \([1, 2, 3, 4, 5]\) has found that, in a suitable long time limit, the macroscopic time evolution \(T^t\) of a physical observable \(X(t)\) is given as a convolution of the form

\[
T^t_\alpha X(t_0) = \int_0^\infty X(t_0 - s) h_\alpha \left( \frac{s}{t} \right) \frac{ds}{t}
\]

(1)

where \(t \geq 0, 0 < \alpha \leq 1\) and

\[
h_\alpha(x) = \frac{1}{x^\alpha} H_{11}^{10} \left( \left| \frac{1}{x} \right| \frac{(0, 1)}{(0, 1/\alpha)} \right)
\]

(2)

is defined through its Mellin transform \([2]\)

\[
\int_0^\infty H_{11}^{10} \left( x \frac{(0, 1)}{(0, 1/\alpha)} \right) x^{s-1} dx = \frac{\Gamma(s/\alpha)}{\Gamma(s)}
\]

(3)

For \(\alpha = 1\)

\[
h_1(x) = \lim_{\alpha \to 1^-} h_\alpha(x) = \delta(x - 1)
\]

(4)

and hence eq. (1) reduces to

\[
T^t_1 X(t_0) = X(t_0 - t)
\]

(5)

a simple translation. For fixed \(\alpha\) the operators \(T^t_\alpha, t \geq 0\) form a one-parameter semigroup on a Banach space (e.g. the space of all continuous functions vanishing at infinity).
Much interest in the semigroups $T^t_\alpha$ derives from the fact that their infinitesimal generators are proportional to

$$
(\partial^\alpha_t X)(t) = \lim_{s \to 0} \frac{T^s_\alpha X(t) - X(t)}{s} = \frac{1}{\Gamma(-\alpha)} \int_0^\infty \frac{X(t) - X(t-s)}{s^{\alpha+1}} ds, \quad (6)
$$

i.e. to fractional time derivatives of order $\alpha$. This may be seen from Ref. [7] (p. 302), and the fact that the kernels $h_\alpha(s/t)/t$ in eq. (1) are stable probability densities (see also [5]).

Derivatives of noninteger order $0 < \alpha \leq 1$ with respect to time are in this way found to furnish an important generalization for the infinitesimal generator of the macroscopic time evolution of physical observables.

Given the generality of the results above it is natural to consider specific examples by replacing the integer order time derivative with a fractional derivative. A particularly interesting example is given by diffusion and random walks [8, 9]. The fractional generalization of the familiar master equation for random walks turns out to be intimately related to the theory of continuous time random walks with power-law tails in the waiting time density [10]. It is the purpose of this note to exhibit an exact relationship between a fractional master equation and continuous time random walks [8].

Let me conclude this introduction with the remark that only a special subclass of separable continuous time random walks with algebraically decaying waiting time distributions corresponds exactly to a generalized master equation with Riemann-Liouville-type fractional time derivative. It would be interesting to specify precisely whether, and under which conditions, other waiting time densities with a power-law tail lead to the same result [11, 12].

2 Fractional Master Equation

Consider a random walk and let $p(\vec{r}, t)$ denote the probability density to find the walker at the position $\vec{r} \in \mathbb{R}^d$ at time $t$ if it was at the origin $\vec{r} = 0$.
at time $t = 0$. The positions $\vec{r} \in \mathbb{R}^d$ may be discrete or continuous. The conventional master equation for the random walk reads
\begin{equation}
\frac{\partial}{\partial t} p(\vec{r}, t) = \sum_{\vec{r}'} w(\vec{r} - \vec{r}') p(\vec{r}', t) \tag{7}
\end{equation}
with initial condition $p(\vec{r}, 0) = \delta_{\vec{r}0}$. To establish the fractional generalization of this initial value problem one must respect the nonlocal nature of the fractional derivatives. This leads to the fractional master equation
\begin{equation}
\partial_{0+}^\alpha p(\vec{r}, t) = \delta_{\vec{r}0} \frac{1}{\Gamma(1 - \alpha) t^\alpha} + \sum_{\vec{r}'} w(\vec{r} - \vec{r}') p(\vec{r}', t) \tag{8}
\end{equation}
where $0 < \alpha \leq 1$, $t \geq 0$, and the initial condition $p(\vec{r}, 0) = \delta_{\vec{r}0}$ has been incorporated. Note that the fractional transition rates $w(\vec{r})$ have units of $(1/\text{time})^\alpha$. They obey the relation $\sum_{\vec{r}} w(\vec{r}) = 0$. Applying a fractional integral of order $\alpha$ to equation (8) yields an integral equation
\begin{equation}
p(\vec{r}, t) = \delta_{\vec{r}0} + \frac{1}{\Gamma(\alpha)} \int_0^t (t - t')^{\alpha-1} \sum_{\vec{r}'} w(\vec{r} - \vec{r}') p(\vec{r}', t') \, dt' \tag{9}
\end{equation}
reminiscent of the integral equation for continuous time random walks [13, 14, 15, 16, 17, 18].

3 Continuous Time Random Walks

The basic integral equation for separable continuous time random walks describes a random walker in continuous time without correlation between its spatial and temporal behaviour, and reads [16, 10]
\begin{equation}
p(\vec{r}, t) = \delta_{\vec{r}0} \Phi(t) + \int_0^t \psi(t - t') \sum_{\vec{r}'} \lambda(\vec{r} - \vec{r}') p(\vec{r}', t') \, dt' \tag{10}
\end{equation}
Here, as in (9), \( p(\vec{r}, t) \) denotes the probability density to find the walker at the position \( \vec{r} \in \mathbb{R}^d \) at time \( t \) if it started from the origin \( \vec{r} = 0 \) at time \( t = 0 \). \( \lambda(\vec{r}) \) is the probability for a displacement \( \vec{r} \) in each single step, and \( \psi(t) \) is the waiting time distribution giving the probability density for the occurrence of a time interval \( t \) between two consecutive steps. The transition probabilities obey \( \sum_{\vec{r}} \lambda(\vec{r}) = 1 \). The function \( \Phi(t) \) in eq. (10) is the survival probability at the initial position. It is related to the waiting time distribution through

\[
\Phi(t) = 1 - \int_0^t \psi(t') \, dt'.
\]

(11)

Note that in equation (10) the system is prepared with the walker at position \( \vec{r} = 0 \), and it develops from there according to \( \psi(t) \).

4 Relation between equations (9) and (10)

The similarity between equations (9) and (10) suggests that the former is a special case of the latter. To show that this is true let

\[
\psi(u) = \mathcal{L}\{\psi(t)\}(u) = \int_0^\infty e^{-ut} \psi(t) \, dt
\]

(12)

denote the Laplace transform of \( \psi(t) \) and write

\[
\lambda(\vec{q}) = \mathcal{F}\{\lambda(\vec{r})\}(\vec{q}) = \sum_{\vec{r}} e^{i\vec{q} \cdot \vec{r}} \lambda(\vec{r})
\]

(13)

for the Fourier transform of \( \lambda(\vec{r}) \). Then the Fourier-Laplace transform \( p(\vec{q}, u) \) of the solution to (10) is given as

\[
p(\vec{q}, u) = \frac{\Phi(u)}{u 1 - \psi(u) \lambda(k)}
\]

(14)
where $\Phi(u)$ is the Laplace transform of the survival probability.

Similarly the fractional master equation (9) can be solved in Fourier-Laplace space with the result

$$p(\vec{q}, u) = \frac{u^{\alpha-1}}{u^\alpha - w(\vec{q})}$$  \hspace{1cm} (15)$$

where $w(\vec{q})$ is the Fourier transform of the kernel $w(\vec{r})$ in (9). Eliminating $p(\vec{q}, u)$ between (14) and (15) gives the result

$$\frac{1 - \psi(u)}{w^\alpha \psi(u)} = \frac{\lambda(\vec{q}) - 1}{w(\vec{q})} = C$$  \hspace{1cm} (16)$$

where $C$ is a constant. The last equality holds because the left hand side of the first equality is $\vec{q}$-independent while the right hand side is independent of $u$.

From (16) it is seen that the fractional master equation characterized by the kernel $w(\vec{r})$ and the order $\alpha$ corresponds to a special class of space time decoupled continuous time random walks characterized by $\lambda(\vec{r})$ and $\psi(t)$. This correspondence is given precisely as

$$\psi(u) = \frac{1}{1 + Cu^\alpha}$$  \hspace{1cm} (17)$$

and

$$\lambda(\vec{q}) = 1 + Cw(\vec{q})$$  \hspace{1cm} (18)$$

with the same constant $C$ appearing in both equations. Not unexpectedly the correspondence defines the waiting time distribution uniquely up to a constant while the structure function is related to the Fourier transform of the transition rates.
To invert the Laplace transformation in (17) and exhibit the form of the waiting time density $\psi(t)$ in the time domain one rewrites eq. (17)

$$\psi(u) = \frac{u^{-\alpha}}{C} \frac{1}{1 + \frac{u}{C}} = \sum_{k=0}^{\infty} \frac{(-1)^k}{C^{k+1}} u^{-\alpha(k+1)}$$

(19)

and inverts the series term by term. This yields the result

$$\psi(t; \alpha, C) = \frac{t^{\alpha-1}}{C} \sum_{k=0}^{\infty} \frac{1}{\Gamma(\alpha k + \alpha)} \left(-\frac{t^\alpha}{C}\right)^k.$$  

(20)

First one notes that for $\alpha = 1$ the result reduces to

$$\psi(t; 1, C) = \frac{1}{C} \exp(-t/C)$$

(21)

the familiar exponential form. For $0 < \alpha < 1$ the result is recognized as

$$\psi(t; \alpha, C) = \frac{t^{\alpha-1}}{C} E_{\alpha, \alpha} \left(-\frac{t^\alpha}{C}\right).$$

(22)

where the function

$$E_{\alpha, \beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}$$

(23)

is the generalized Mittag-Leffler function [19].

The asymptotic behaviour of $\psi(t)$ for $t \to 0$ is readily obtained by noting that $E_{\alpha, \alpha}(0) = 1$. Hence $\psi(t)$ behaves as

$$\psi(t) \propto t^{-1+\alpha}$$

(24)
for $t \to 0$. For $0 < \alpha < 1$ the waiting time density becomes singular at the origin.

The asymptotic behaviour for large waiting times $t \to \infty$ is obtained from the asymptotic series expansion for the Mittag-Leffler function [19]

$$E_{\alpha,\beta}(z) = -\sum_{n=1}^{N} \frac{z^{-n}}{\Gamma(\beta - \alpha n)} + O(|z|^{-N})$$

valid for $|\arg(-z)| < (1 - (\alpha/2))\pi$ and $z \to \infty$. It follows from this that $E_{\alpha,\beta}(-x) \propto x^{-2}$ for $x \to \infty$ and hence that

$$\psi(t) \propto t^{-1-\alpha}$$

for large $t \to \infty$ and $0 < \alpha < 1$. This result shows that the waiting time distribution has an algebraic tail as it is usually assumed in the theory of continuous time random walks [20, 21, 22, 23, 10].

In summary it has been shown that the master equation with a Riemann-Liouville fractional time derivative of order $\alpha$ corresponds exactly to a continuous time random walk whose waiting time density is related to the generalized Mittag-Leffler function and exhibits a power-law tail. It would be interesting to know the precise conditions under which the more general class of separable continuous time random walks obeying eq. (26) “approximates” [11] this result.

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