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Fractional master equations and fractal time random walks

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Fractional master equations containing fractional time derivatives of order $0<\omega\leq 1$ are introduced on the basis of a recent classification of time generators in ergodic theory. It is shown that fractional master equations are contained as a special case within the traditional theory of continuous time random walks. The corresponding waiting time density $\psi(t)$ is obtained exactly as $\psi(t)=(t^{\omega-1}/C)E_{\omega,\omega}(-t^{\omega}/C)$, where $E_{\omega,\omega}(x)$ is the generalized Mittag-Leffler function. This waiting time distribution is singular both in the long time as well as in the short time limit.

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I. INTRODUCTION AND STATEMENT OF THE PROBLEM

A recent classification theory [1–3] has derived fractional equations of motion from abstract ergodic theory. Fractional equations of motion contain fractional rather than integer order time derivatives as generators of the time evolution. Fractional equations of motion arise at anequilibrium phase transitions [1,2] or whenever a dynamical system is restricted to subsets of measure zero of its state space [3].

Master equations in which the time derivative is replaced with a derivative of fractional order form the subject of the present paper. Such fractional master equations arise as special cases of the more general *fractional Liouville equations* introduced in [1–3], and they contain the fractional diffusion equation as a special case. A fractional master equation for a translationally invariant d-dimensional system may be written formally, but in suggestive notation, as

$$\frac{\partial^{\omega}}{\partial t^{\omega}}p(\mathbf{r},t)=\sum_{\mathbf{r}'}w(\mathbf{r}-\mathbf{r}')p(\mathbf{r}',t), \tag{1.1}$$

where $p(\mathbf{r},t)$ denotes the probability density of finding the diffusing entity at the position $\mathbf{r}\in\mathbb{R}^d$ at time t if it was at the origin $\mathbf{r}=\mathbf{0}$ at time $t=0$. The positions $\mathbf{r}\in\mathbb{R}^d$ may be discrete or continuous. The fractional transition rates $w(\mathbf{r})$ measure the propensity for a displacement $\mathbf{r}$ in units of $[1/(\text{time})]^{\omega}$, and obey the relation $\Sigma_{\mathbf{r}}w(\mathbf{r})=0$. The fractional order ω plays the role of a dynamical critical exponent. Equation (1.1) can be made precise by applying the fractional Riemann-Liouville integral as

$$p(\mathbf{r},t)=\delta_{\mathbf{r}0}+\frac{1}{\Gamma(\omega)}\int_0^t(t-t')^{\omega-1}\sum_{\mathbf{r}'}w(\mathbf{r}-\mathbf{r}')p(\mathbf{r}',t')dt' \tag{1.2}$$

where the initial condition $p(\mathbf{r},0)=\delta_{\mathbf{r}0}$ has been incorporated.

Diffusion in a d-dimensional Euclidean space is contained in the fractional master equations (1.1) or (1.2) as the special case in which $\omega=1$ and $w(\mathbf{r})$ is the discretized Laplacian on a d-dimensional regular lattice. The integral form (1.2) suggests a relation with the well known theory of continuous time random walks [4–10]. It is the purpose and objective of the present paper to show that there exists a precise and rigorous relation between the fractional master equation and the theory of continuous time random walks. It will be shown that the fractional master equation describes a fractal time process [11,10]. Fractal time processes (see [10] for a review) are defined here as continuous time random walks whose waiting time density has an infinite first moment [12–16].

Given the existence of an exact relation between fractional master equations and fractal time random walks, it might seem that (1.1) or (1.2) also describe diffusion on fractals. Dimensional analysis suggests anomalous subdiffusive behavior of the form $\langle\mathbf{r}^2(t)\rangle\propto t^{\bar{d}/\tilde{d}}$, where $\bar{d}$ is the fractal dimension, and $\tilde{d}$ is the spectral or fracton dimension [17–19], and indeed some authors have suggested that $\omega=\tilde{d}/\bar{d}$. It must be clear, however, that while the relation between fractional master equations and fractal time random walks established in this paper is exact, the relation with diffusion on fractals is not. It appears doubtful that the latter relation can exist beyond superficial scaling similarities because exactly solvable cases show that the spectral properties as well as the eigenfunctions for fractal time walks and walks on fractals are radically different [20–23].

II. RELATION BETWEEN FRACTIONAL AND FRACTAL WALKS

Let us start by recalling briefly the general theory of continuous time random walks [5,7,8] The basic equation of motion is the continuous time random walk (CTRW) integral equation [16]

$$p(\mathbf{r},t)=\delta_{\mathbf{r}0}\Phi(t)+\int_0^t\psi(t-t')\sum_{\mathbf{r}'}\lambda(\mathbf{r}-\mathbf{r}')p(\mathbf{r}',t')dt' \tag{2.1}$$

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describing a random walk in continuous time without correlation between its spatial and temporal behavior. Here, as in (1.2), $p(\mathbf{r},t)$ denotes the probability density of finding the diffusing entity at the position $\mathbf{r} \in \mathbb{R}^d$ at time t if it started from the origin $\mathbf{r}=\mathbf{0}$ at time $t=0$. $\lambda(\mathbf{r})$ is 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 $\Sigma_{\mathbf{r}}\lambda(\mathbf{r})=1$. The function $\Phi(t)$ is the survival probability at the initial position which is related to the waiting time distribution through

$$\Phi(t)=1-\int_0^t \psi(t')dt'. \tag{2.2}$$

The objective of this paper which was defined in the introduction is to show that the fractional master equation (1.2) is a special case of the CTRW equation (2.1), and to find the appropriate waiting time density.

The translation invariant form of the transition probabilities in (2.1) allows a solution through Fourier-Laplace transformation. Let

$$\psi(u)=\mathscr{L}\{\psi(t)\}(u)=\int_0^\infty e^{-ut}\psi(t)dt \tag{2.3}$$

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

$$\lambda(\mathbf{q})=\mathscr{F}\{\lambda(\mathbf{r})\}(\mathbf{q})=\sum_{\mathbf{r}} e^{i\mathbf{q}\cdot\mathbf{r}}\lambda(\mathbf{r}) \tag{2.4}$$

the Fourier transform of $\lambda(\mathbf{r})$, which is also called the structure function of the random walk [5]. Then the Fourier-Laplace transform $p(\mathbf{q},u)$ of the solution to (2.1) is given as [5,7,8,16]

$$p(\mathbf{q},u)=\frac{1}{u}\frac{1-\psi(u)}{1-\psi(u)\lambda(\mathbf{q})}=\frac{\Phi(u)}{1-\psi(u)\lambda(\mathbf{q})}, \tag{2.5}$$

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

Similarly the fractional master equation (1.2) can be solved in Fourier-Laplace space with the result

$$p(\mathbf{q},u)=\frac{u^{\omega-1}}{u^{\omega}-w(\mathbf{q})}, \tag{2.6}$$

where $w(\mathbf{q})$ is the Fourier transform of the kernel $w(\mathbf{r})$ in (1.2). Eliminating $p(\mathbf{q},u)$ between (2.5) and (2.6) gives the result

$$\frac{1-\psi(u)}{u^{\omega}\psi(u)}=\frac{\lambda(\mathbf{q})-1}{w(\mathbf{q})}=C, \tag{2.7}$$

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

From (2.7) it is seen that the fractional master equation characterized by the kernel $w(\mathbf{r})$ and the order ω corresponds to a special case of space time decoupled continuous time random walks characterized by $\lambda(\mathbf{r})$ and $\psi(t)$. This correspondence is given precisely as

$$\psi(u)=\frac{1}{1+Cu^{\omega}} \tag{2.8}$$

and

$$\lambda(\mathbf{q})=1+Cw(\mathbf{q}) \tag{2.9}$$

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 (2.8) and exhibit the form of the waiting time density $\psi(t)$ in the time domain it is convenient to introduce the Mellin transformation

$$f(s)=\mathscr{M}\{f(x)\}(s)=\int_0^\infty x^{s-1}f(x)dx \tag{2.10}$$

for a function $f(x)$. The Mellin transformed waiting time density is obtained as

$$\psi(s)=\mathscr{M}\{\psi(t)\}(s)$$
$$=\frac{1}{\omega C^{1/\omega}}\left(\frac{1}{C^{1/\omega}}\right)^{-s}\frac{\Gamma\left(\frac{1}{\omega}-\frac{s}{\omega}\right)\Gamma\left(1-\frac{1}{\omega}+\frac{s}{\omega}\right)}{\Gamma(1-s)}, \tag{2.11}$$

where $\Gamma(x)$ denotes the gamma function. To obtain (2.11) from (2.8) the relation between Laplace and Mellin transforms

$$\mathscr{M}\{\mathscr{L}\{f(t)\}(u)\}(s)=\Gamma(s)\mathscr{M}\{f(t)\}(1-s), \tag{2.12}$$

the special result

$$\mathscr{M}\left\{\frac{1}{1+x}\right\}(s)=\Gamma(s)\Gamma(1-s), \tag{2.13}$$

and the general relation

$$\mathscr{M}\{f(ax^b)\}(s)=\frac{1}{b}a^{-s/b}\mathscr{M}\{f(x)\}(s/b), \tag{2.14}$$

valid for $a,b>0$, have been employed. Using the definition of the general H function given in the appendix one obtains the result

$$\psi(t)=\psi(t;\omega,C)$$
$$=\frac{1}{\omega C^{1/\omega}}H^{11}_{12}\left(\frac{t}{C^{1/\omega}}\left|\begin{matrix}\left(1-\frac{1}{\omega},\frac{1}{\omega}\right) & \\ \left(1-\frac{1}{\omega},\frac{1}{\omega}\right) & (0,1)\end{matrix}\right.\right), \tag{2.15}$$

which may be rewritten as

$$\psi(t;\omega,C)=\frac{1}{t}H^{11}_{12}\left(\frac{t}{C^{1/\omega}}\left|\begin{matrix}(1,1) & \\ (1,1) & (1,\omega)\end{matrix}\right.\right) \tag{2.16}$$

with the help of general relations for H functions [24]. The dependence on the parameters ω and C has been indicated explicitly. From the series expansion of H functions given in the appendix one finds

$$\psi(t;\omega,C)=\frac{t^{\omega-1}}{C}\sum_{k=0}^{\infty}\frac{1}{\Gamma(\omega k+\omega)}\left(-\frac{t^{\omega}}{C}\right)^{k}, \qquad (2.17)$$

showing that $\psi(t)$ behaves as

$$\psi(t)\propto t^{-1+\omega} \qquad (2.18)$$

for small $t\to 0$. Because $0<\omega\leq 1$ the waiting time density is singular at the origin except for $\omega=1$. The series representation (2.17) shows that the waiting time density is a natural generalization of an exponential waiting time density to which it reduces for $\omega=1$, i.e., $\psi(t;1,C)=(1/C)\exp(t/C)$. The series in (2.17) is recognized as the generalized Mittag-Leffler function $E_{\omega,\omega}(x)$, [25] and $\psi(t)$ may thus be written alternatively as

$$\psi(t;\omega,C)=\frac{t^{\omega-1}}{C}E_{\omega,\omega}\left(-\frac{t^{\omega}}{C}\right). \qquad (2.19)$$

Of course the result (2.17) can also be obtained more directly, but we have presented here a method using Mellin transforms because it remains applicable in cases where a direct inversion fails [23]. The asymptotic expansion of the Mittag-Leffler function for large argument [25] yields

$$\psi(t)\propto t^{-1-\omega} \qquad (2.20)$$

for large $t\to\infty$ and $0<\omega<1$. This result shows that the waiting time distribution has an algebraic tail of the kind usually considered in the theory of random walks [12–16].

III. DISCUSSION

In Fig. 1 we display the function $\psi(t;\omega,C)$ for $C=1$ and $\omega=0.01,0.1,0.5,0.9,0.99$ in a log-log plot. The asymptotic behavior (2.18) and (2.20) is clearly visible from the figure. The fractional order ω of the time derivative in (1.1) is restricted to $0<\omega\leq 1$ as a result of the general theory [3]. This and the behavior of $\psi(t)$ in Fig. 1 attributes special significance to the two limits $\omega\to 1$ and $\omega\to 0$.

In the limit $\omega\to 1$ the fractional master equation (1.2) reduces to the ordinary master equation, and the waiting time density becomes exponential $\psi(t;1,1)=\exp(-t)$. In the limit $\omega\to 0$, on the other hand, Eq. (1.1) reduces to an eigenvalue or fixed point equation for the operator on the right hand side by virtue of $\partial^0 f/\partial t^0=f$. While this is interesting in itself, an even more interesting aspect is that the corresponding waiting time density $\psi(t)$ approaches the form $\psi(t;\omega\to 0,1)\propto 1/t$ for which the normalization becomes logarithmically divergent. This signals an onset of localization in this singular limit. It is hoped that our results will stimulate further research into the fractal time concept.

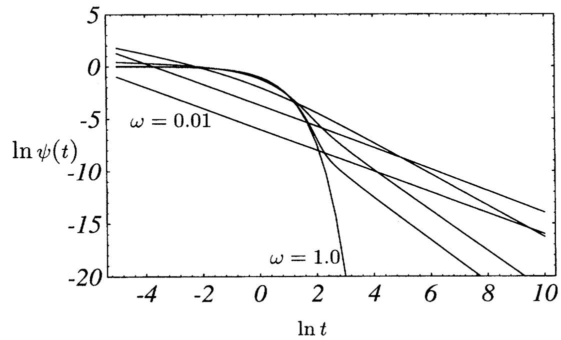

FIG. 1. Log-log plot of the waiting time density $\psi(t;\omega,1)$ for $\omega=0.01,0.1,0.5,0.9,0.99,1.0$. The curves for $\omega=1.0$ and $\omega=0.01$ have been labeled in the figure; the other curves interpolate between them. For $\omega=1$ the waiting time density is exponential $\psi(t)=\exp(-t)$ and for $\omega\to 0$ it approaches $\psi(t)\to 1/t$.

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APPENDIX: DEFINITION OF H FUNCTIONS

The general H function is defined as the inverse Mellin transform [24]

$$H_{PQ}^{mn}\left(z\,\middle|\,\begin{matrix}(a_1,A_1)\cdots(a_P,A_P)\\(b_1,B_1)\cdots(b_Q,B_Q)\end{matrix}\right)=\frac{1}{2\pi i}\int_{\mathscr{C}}\frac{\prod_{j=1}^{m}\Gamma(b_j+B_js)\prod_{j=1}^{n}\Gamma(1-a_j-A_js)}{\prod_{j=m+1}^{Q}\Gamma(1-b_j-B_js)\prod_{j=n+1}^{P}\Gamma(a_j+A_js)}z^{-s}ds, \qquad (A1)$$

where the contour $\mathscr{C}$ runs from $c-i\infty$ to $c+i\infty$ separating the poles of $\Gamma(b_j+B_js)$ $(j=1,\ldots,m)$ from those of $\Gamma(1-a_j-A_js)$ $(j=1,\ldots,n)$. Empty products are interpreted as unity. The integers m,n,P,Q satisfy $0\leq m\leq Q$ and $0\leq n\leq P$. The coefficients A_j and B_j are positive real numbers and the complex parameters a_j,b_j are such that no poles in the integrand coincide. If

$$\Omega=\sum_{j=1}^{n}A_j-\sum_{j=n+1}^{P}A_j+\sum_{j=1}^{m}B_j-\sum_{j=m+1}^{Q}B_j>0 \qquad (A2)$$

then the integral converges absolutely and defines the H function in the sector $|\arg z|<\Omega\pi/2$. The H function is also well defined when either

$$\delta=\sum_{j=1}^{Q} B_j-\sum_{j=1}^{P} A_j>0 \quad \text{with} \quad 0<|z|<\infty \tag{A3}$$

or

$$\delta=0 \quad \text{and} \quad 0<|z|<R=\prod_{j=1}^{P} A_j^{-A_j}\prod_{j=1}^{Q} B_j^{B_j}. \tag{A4}$$

For $\delta\geqslant 0$ the H function has the series representation

$$H_{PQ}^{mn}\left(z\left|\begin{matrix}(a_1,A_1)\cdots(a_P,A_P)\\(b_1,B_1)\cdots(b_Q,B_Q)\end{matrix}\right.\right)=\sum_{i=1}^{m}\sum_{k=0}^{\infty}\frac{\prod\limits_{\substack{j=1\\j\neq i}}^{m}\Gamma\left(b_j-(b_i+k)\frac{B_j}{B_i}\right)\prod\limits_{j=1}^{n}\Gamma\left(1-a_j+(b_i+k)\frac{A_j}{B_i}\right)}{\prod\limits_{j=m+1}^{Q}\Gamma\left(1-b_j+(b_i+k)\frac{B_j}{B_i}\right)\prod\limits_{j=n+1}^{P}\Gamma\left(a_j-(b_i+k)\frac{A_j}{B_i}\right)}\frac{(-1)^k z^{(b_i+k)/B_i}}{k!B_i}, \tag{A5}$$

provided that $B_k(b_j+l)\neq B_j(b_k+s)$ for $j\neq k$, $1\leqslant j,k\leqslant m$ and $l,s=0,1,\ldots$. The H function is a generalization of Meijers G function and many of the known special functions are special cases of it.

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