PHYSICAL REVIEW E VOLUME 53, NUMBER 4 APRIL 1996

Stochastic foundations of fractional dynamics

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(Received 5 September 1995)

It is shown that fractional diffusion equations arise very naturally as the limiting dynamic equations of all continuous time random walks with decoupled temporal and spatial memories and with either temporal or spatial scale invariance (fractal walks), thus enlarging their stochastic foundations hitherto restricted to a particular case of fractal walk [R. Hilfer and L. Anton, Phys. Rev. E **51**, R848 (1995)].

PACS number(s): 05.60.+w, 05.40.+j, 02.50.−r, 44.30.+v

Fractional diffusion equations have been the subject of several recent papers where it has been found that they provide a natural dynamic framework for the description of anomalous diffusion phenomena, such as diffusion on fractal structures [1] or Lévy flights [2]. Some efforts have been made as well in order to give some stochastic justification both of anomalous diffusion [3] and of fractional dynamic equations [4], in both cases under the framework of continuous time random walks (CTRW). The aim of this paper is to show that the relation of CTRW with fractional dynamics is much deeper than previously shown [4].

In [4] a relation was established between fractional diffusion equations and fractal walks, according to which fractional equations describe a CTRW with a very precise form in terms of H functions of the waiting time distribution $\phi(t)$. Here it will be shown that we do not need to restrict so much the form of $\phi(t)$ in order to obtain in the long-time limit a behavior described by a fractional diffusion equation. Furthermore, we shall see that, quite generally, fractional dynamics are to be considered as the long-time limit of any CTRW with decoupled spatial and temporal memories and that they are particularly well suited for all CTRW lacking a characteristic measure of length or time, hence the name *fractal walks.*

As reviewed in [5], the statistics of a CTRW presenting anomalous diffusive behavior ultimately relies on the failure of the central limit theorem. This may be due to three reasons: the CTRW is governed by a wide waiting time distribution $\phi(t)$ [wide in the sense that the distribution has an infinite first moment, that is to say, $\phi(t)$ is such that $\phi(t) \sim t^{-1-\gamma}$ as $t \to \infty$ with $0 < \gamma < 1$], by a wide displacement per step distribution $\lambda(\mathbf{r})$ [or, equivalently, having $\lambda(\mathbf{r}) \sim r^{-3-\beta}$ as $r \to \infty$ with $0 < \beta < 2$, which is a distribution with an infinite second moment] or having long-range correlations.

In the first two cases (either no characteristic time scale or no characteristic length), no knowledge of the precise functional form of $\phi(t)$ or $\lambda(\mathbf{r})$ for intermediate times or distances is needed in order to establish the limiting probability distribution of the resulting CTRW (the mathematical foundations of this are to be found in the Lévy distributions (Ref. [6] Chap. VIII) as limit distributions in a generalized central limit theorem). Therefore, these cases provide the easiest generalization of the normal diffusive random walk.

It is a well-known result of the stochastic theory of CTRW's [7] that if $\psi(\mathbf{r},t)$ is the probability distribution of making a step of length $\mathbf{r}$ in the time interval from t to $t+dt$ for a random particle starting at $t=0$ from $r=0$, the probability $\rho(\mathbf{r},t)$ that the particle is at $\mathbf{r}$ at time t satisfies the following equation:

$$\rho(\mathbf{r},t) = \sum_{\mathbf{r}'} \int_0^t \rho(\mathbf{r}',\tau)\psi(\mathbf{r}-\mathbf{r}',t-\tau)d\tau + \left(1 - \int_0^t \psi(\tau)d\tau\right)\delta_{\mathbf{r},0}. \tag{1}$$

As tangentially noted in [3], this result is formally equivalent to a generalized master equation

$$\frac{\partial \rho}{\partial t} = \sum_{\mathbf{r}'} \int_0^t K(\mathbf{r}-\mathbf{r}',t-\tau)\rho(\mathbf{r}',\tau)d\tau \tag{2}$$

when one takes, in Fourier-Laplace space,

$$K(\mathbf{k},u) = \frac{\psi(\mathbf{k},u) - \phi(u)}{1-\phi(u)}u. \tag{3}$$

In our scheme, Eqs. (2) and (3) will play a major role, in contrast to [3], and they will lead us to more general results.

Now, we restrict ourselves to CTRW's with decoupled temporal and spatial memories, so that one may write $\psi(\mathbf{r},t) = \phi(t)\lambda(\mathbf{r})$, and where either the waiting time distribution $\phi(t)$ or the displacement per step distribution $\lambda(\mathbf{r})$ is wide in the sense exposed previously, namely, that either the first or the second moment of the distribution is infinite, respectively. This approach leads immediately, as shown in [3], to the following $(\mathbf{k},u) \to (\mathbf{0},0)$ limiting $\psi(\mathbf{k},u)$ distributions in the Fourier-Laplace domain, respectively:

$$\psi(\mathbf{k},u) \sim 1 - C_1 u^\gamma - \frac{\sigma^2}{2}k^2, \tag{4}$$

$$\psi(\mathbf{k},u) \sim 1 - \tau u - C_2 k^\beta, \tag{5}$$

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1063-651X/96/53(4)/4191(3)/$10.00

where $0 < \gamma < 1$ and $0 < \beta < 2$. By introducing these results in Eq. (3) one finds the behavior for small $(\mathbf{k}, u)$ of the generalized master equation's kernel $K(\mathbf{k}, u)$ for CTRW's lacking characteristic measures:

$$K(\mathbf{k}, u) \sim -\frac{\sigma^2}{2\tau} u^{1-\gamma} k^2, \quad (6)$$

$$K(\mathbf{k}, u) \sim -\frac{C_2}{\tau} k^{\beta}. \quad (7)$$

Now, if we are interested in dynamics showing anomalous diffusive properties it may be shown that, in the long-time limit, these anomalous properties arise exclusively from the limiting behavior of the kernel $K(\mathbf{r}, t)$ at large distances or long times. More specifically, if one studies a diffusive phenomenon with strong memory effects (for nonlocal effects one would proceed similarly), one may split the kernel into two different functions containing the long-time behavior on the one hand and the intermediate- and short-time behavior on the other hand:

$$K(\mathbf{r}, t) = \begin{cases} K_1(\mathbf{r}, t), & t < T \\ K_2(\mathbf{r}, t), & t > T. \end{cases} \quad (8)$$

Using this notation, the generalized master equation (2) turns, in the limit $t \gg T$, into

$$\frac{\partial \rho}{\partial t} = \sum_{\mathbf{r}'} F_1(\mathbf{r} - \mathbf{r}')\rho(\mathbf{r}', t) + \sum_{\mathbf{r}'} \int_0^t K_2(\mathbf{r} - \mathbf{r}', t - \tau)\rho(\mathbf{r}', \tau) d\tau, \quad (9)$$

where $F_1(\mathbf{r}) = \int_0^T K_1(\mathbf{r}, \tau) d\tau$. Equation (9) makes clear that the kernel at short and intermediate times $K_1(\mathbf{r}, t)$ is only responsible for a conventional diffusive motion without memory, whereas all memory effects are accounted for by the long-time kernel $K_2(\mathbf{r}, t)$.

Since we are interested in diffusion features largely departing from conventional diffusion properties, one may assume that the first summand in (9) can be neglected in front of the second summand and we are finally led to the conclusion that strongly anomalous diffusion is described, in the long-time (or long-distance) limit, only by the limiting behavior of the generalized master equation's kernel. However, these limiting kernels are already known [(6) and (7)] for the stochastic movements that we are considering, and we arrive then at the following dynamic equations in Fourier-Laplace space:

$$u\rho(\mathbf{k}, u) - \rho(\mathbf{k}, t = 0) = -\frac{\sigma^2}{2C_1} k^2 u^{1-\gamma} \rho(\mathbf{k}, u), \quad (10)$$

$$u\rho(\mathbf{k}, u) - \rho(\mathbf{k}, t = 0) = -\frac{C_2}{\tau_1} k^{\beta} \rho(\mathbf{k}, u). \quad (11)$$

When inverting the transforms in order to recover the $(\mathbf{r}, t)$ picture, one finds the following unusual inversions:

$$\mathcal{L}^{-1}\left\{u^{1-\gamma}\rho\right\}, \quad \mathcal{F}^{-1}\left\{k^{\beta}\rho\right\}, \quad (12)$$

which have been seen in [8] to correspond to the Riemann-Liouville and the Riesz fractional derivatives, respectively. Using these mathematical tools we can now invert Eqs. (10) and (11) to get

$$\frac{\partial \rho}{\partial t} = \frac{\sigma^2}{2C_1} \nabla^2 \frac{\partial^{1-\gamma}\rho}{\partial t^{1-\gamma}}, \quad (13)$$

$$\frac{\partial \rho}{\partial t} = \frac{C_2}{2\tau_1} \nabla^{\beta} \rho, \quad (14)$$

where $\partial^{1-\gamma}/\partial t^{1-\gamma}$ stands for the $1 - \gamma$ order temporal Riemann-Liouville fractional derivative and ∇^{β} is the β order three-dimensional spatial Riesz fractional derivative (for an integral representation of them see the Appendix). Assuming a sufficiently good behavior of the probability density ρ (Ref. [8], Sec. 2.7), one can finally recast these two fractional equations in a more suggestive form:

$$\frac{\partial^{\gamma} \rho}{\partial t^{\gamma}} = D_2 \nabla^2 \rho, \quad (15)$$

$$\frac{\partial \rho}{\partial t} = D_1 \nabla^{\beta} \rho. \quad (16)$$

Thus, we have shown that fractional dynamic equations describe not only a particular case of CTRW, with a very definite waiting time distribution $\phi(t)$ or displacement per step distribution $\lambda(\mathbf{r})$ as observed in [4], but provide a limiting macroscopic dynamic description for all CTRW's with decoupled temporal and spatial memories and without characteristic measures of either time or distance (fractal walks). Fractional diffusion equations must thus be viewed not as exotic and pathologic dynamics but as a general limiting description of all scale invariant diffusion processes.

ACKNOWLEDGMENTS

Professor David Jou, Professor José Casas-Vázquez, and Professor Josep M. Burgués are gratefully acknowledged for useful discussions and for their interest in this work. The author has received financial support from the Programa de Formació d'Investigadors of the Direcció General de Recerca of the Generalitat de Catalunya. Financial support from the Dirección General de Investigación Científica y Técnica of the Spanish Ministry of Education under Grant No. PB94-0718 is acknowledged as well.

APPENDIX: FRACTIONAL DERIVATIVES

Here we shall briefly define, by means of their integral representation, the fractional derivatives that have been brought up in the text. For a more thorough explanation of their motivations and implications refer to [8] and references therein.

1. Riemmann-Liouville fractional derivative

This is historically the first sound definition of a fractional derivative of just one variable, it arises naturally from the formula for n-fold integration. Its integral representation is

$$\frac{\partial^{\alpha} f}{\partial t^{\alpha}} = \frac{1}{\Gamma(n - \alpha)} \frac{d^n}{dt^n} \int_0^t \frac{f(\tau) d\tau}{(t - \tau)^{\alpha - n + 1}}, \quad (A1)$$

where n is the smallest integer larger than α ($n = [\alpha]+1$).

2. Riesz fractional derivative

This is a definition for fractional derivatives in higher dimensional spaces $\mathbb{R}^n$. Its motivation is the generalization of the Laplacian ∇^2 to an arbitrary order "Laplacian" ∇^β:

$$\nabla^\beta f = d_{n,l}(\beta) \int_{\mathbb{R}^n} \sum_{k=0}^{l} (-1)^k \binom{l}{k} \frac{f(\mathbf{x} - k\mathbf{y})}{|\mathbf{y}|^{n+\beta}} d\mathbf{y}, \tag{A2}$$

where $d_{n,l}(\beta)$ is a constant depending on the dimension of the space n, the integer l, and the real number β in such a way that definition (A2) is independent of l as long as $l > \beta$.

The cumbersome aspect of these definitions disappears when one computes their Laplace or Fourier integral transforms, respectively. When performed, these transformations yield very elegant and natural definitions, namely,

$$\widetilde{\frac{\partial^\alpha f}{\partial t^\alpha}}(u) = u^\alpha \tilde{f}(u),$$
$$\widehat{\nabla^\beta f}(\mathbf{k}) = k^\beta \hat{f}(\mathbf{k}).$$

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