Langevin Approach to Fractional Diffusion Equations Including Inertial Effects

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In recent years, several fractional generalizations of the usual Kramers−Fokker−Planck equation have been presented. Using an idea of Fogedby (Fogedby, H. C. *Phys. Rev. E* **1994**, *50*, 041103), we show how these equations are related to Langevin equations via the procedure of subordination.

Introduction

Some 70 years ago, Kramers[1] considered the motion of a Brownian particle subject to a space-dependent force $\mathbf{F}(\mathbf{x})$ per unit mass. His goal was to compute the joint probability distribution $f(\mathbf{x},\mathbf{u},t)$ for finding a particle at time t at the position $\mathbf{x}$ with the velocity $\mathbf{u}$. For this quantity, he could derive the famous Kramers−Fokker−Planck (KFP) equation[2,3]

$$\left[\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla_x + \mathbf{F}(\mathbf{x})\cdot\nabla_u\right] f(\mathbf{x},\mathbf{u},t) = \mathscr{L}_{\mathrm{FP}}\, f(\mathbf{x},\mathbf{u},t) \qquad (1)$$

where $\mathscr{L}_{\mathrm{FP}}$ is the Fokker−Planck collision operator

$$\mathscr{L}_{\mathrm{FP}} f = \gamma \nabla_u \cdot (\mathbf{u} f) + D\Delta_u f \qquad (2)$$

As is well-known, eq 1 corresponds to the Langevin equations (see, e.g., ref 2)

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) = \mathbf{u}(t) \quad \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{u}(t) = \mathbf{F}(\mathbf{x}) - \gamma\mathbf{u}(t) + \Gamma(t) \qquad (3)$$

where $\Gamma(t)$ obeys white noise statistics. It describes a Brownian particle which is subject to the relation $\langle \mathbf{x}^2\rangle \sim Dt$, where D is the diffusion coefficient. In many complex systems, this relation is violated, however. In fact, one often finds $\langle \mathbf{x}^2\rangle \sim D_\alpha t^\alpha$ with $\alpha \neq 1$, which is described as "anomalous" or "strange" diffusion. Here, D_α is a generalized diffusion coefficient with units of $[D_\alpha] = m^2 s^{-\alpha}$. Depending on α, such a process is called subdiffusive ($\alpha < 1$), superdiffusive ($1 < \alpha < 2$), ballistic ($\alpha = 2$), or turbulent-diffusive ($\alpha = 3$).

As was shown by several authors, strange diffusion may be described by fractional generalizations of eq 1 (for a review including discussions of various applications, see, e.g., ref 4). However, the latter may differ in the way the fractional character is incorporated. Thus, it comes as no surprise that three different types of fractional KFP equations may be found in the literature. For example, Metzler and Klafter[5−7] proposed the equation

$$\frac{\partial f(\mathbf{x},\mathbf{u},t)}{\partial t} = [-\mathbf{u}\cdot\nabla_x - \mathbf{F}(\mathbf{x})\cdot\nabla_u + \mathscr{L}_{\mathrm{FP}}]\gamma_\delta D_t^{1-\delta} f(\mathbf{x},\mathbf{u},t) \qquad (4)$$

which they obtained by means of a non-Markovian generalization of the Chapman−Kolmogorov equation. Another kind of fractional KFP equation has been proposed by Barkai and Silbey,[8] namely

$$\left[\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla_x + \mathbf{F}(\mathbf{x})\cdot\nabla_u\right] f(\mathbf{x},\mathbf{u},t) = \mathscr{L}_{\mathrm{FP}}\gamma_\delta D_t^{1-\delta} f(\mathbf{x},\mathbf{u},t) \qquad (5)$$

where γ_δ is a damping coefficient whose units are $[\gamma_\delta] = s^{\delta-1}$ and $D_t^{1-\delta}$ is the fractional time derivative whose Laplace space representation reads $D_t^{1-\delta} \leftrightarrow \lambda^{1-\delta}$. Finally, employing the concept of continuous-time random walks (CTRWs), Friedrich and co-workers[9,10] were able to derive the equation

$$\left[\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla_x + \mathbf{F}(\mathbf{x})\cdot\nabla_u\right] f(\mathbf{x},\mathbf{u},t) = \mathscr{L}_{\mathrm{FP}}\gamma_\delta \mathscr{D}_t^{1-\delta} f(\mathbf{x},\mathbf{u},t) \qquad (6)$$

Here, $\mathscr{D}_t^{1-\delta}$ denotes a fractional substantial derivative which can be written in Laplace space as $\mathscr{D}_t^{1-\delta} \leftrightarrow [\lambda + \mathbf{u}\cdot\nabla_x + \mathbf{F}(\mathbf{x})\cdot\nabla_u]^{1-\delta}$.

In this paper, we address the important question of how these three fractional KFP equations are connected to each other. As is well-known, fractional diffusion equations can be linked to CTRWs,[11] and according to Fogedby,[12] the latter can, in turn, be linked to sets of Langevin equations. This fact will be exploited below in order to gain insight into the nature of the stochastic processes underlying the three scenarios that were just described. For the sake of simplicity, we restrict ourselves to one-dimensional problems with no external force.

Langevin Approach to Fractional Diffusion Equations

In the spirit of Fogedby, let us first consider a stochastic process which is described by the following system of Langevin equations

$$\frac{\mathrm{d}}{\mathrm{d}s}u(s) = -\gamma u(s) + \Gamma(s) \quad \frac{\mathrm{d}}{\mathrm{d}s}t(s) = \eta(s) \qquad (7)$$

Here, $\Gamma(s)$ represents uncorrelated Gaussian noise with variance 1. The variable s is to be interpreted as an internal time, whereas t is the physical (wall-clock) time. The $\eta(s)$ are uncorrelated random numbers which are drawn from a one-sided Lévy distribution with a tail index δ [denoted by $L_\delta(x)$].[13] Mathematically speaking, the stochastic process $u(s)$ is subordinated by the $t(s)$ process. The latter is invertible, and the

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probability density of finding the internal time s at time t is given by

$$p(s,t) = \frac{d}{ds}[1 - L_\delta(t/(\gamma_\delta s)^{1/\delta})] \tag{8}$$

which is called the inverse one-sided Lévy stable distribution. It is a solution of the equation

$$\frac{\partial}{\partial t} p(s,t) = -\frac{\partial}{\partial s}\gamma_\delta D_t^{1-\delta}\, p(s,t) \tag{9}$$

and its Laplace transform reads $\hat{p}(s,\lambda) \propto \lambda^{\delta-1}\exp(-\gamma_\delta\lambda^\delta s)$. For details of mapping of the internal time s to the physical time t, the reader is referred to ref 14. Assuming that the stochastic processes $t(s)$ and $u(s)$ are statistically independent, the probability $P(u,t)$ of finding the velocity u at time t can be written as

$$P(u,t) = \int_0^\infty P_0(u,s)p(s,t)\mathrm{d}s \tag{10}$$

where the distribution function $P_0(u,s)$ is a solution of the standard diffusion equation

$$\frac{\partial P_0(u,s)}{\partial s} = \mathcal{L}_{\mathrm{FP}} P_0(u,s) \tag{11}$$

From eqs 9−11, it then follows that $P(u,t)$ satisfies the fractional diffusion equation

$$\frac{\partial P(u,t)}{\partial t} = \mathcal{L}_{\mathrm{FP}}\gamma_\delta D_t^{1-\delta}\, P(u,t) \tag{12}$$

The idea of representing the solution of a fractional diffusion equation like eq 12 as a superposition of Gaussians goes back to Barkai.[15] In the following, we will extend this method from velocity space to phase (position−velocity) space.

The Fractional KFP Equation by Metzler and Klafter

Let us now consider the Langevin system

$$\frac{d}{ds}x(s) = u(s)$$
$$\frac{d}{ds}u(s) = -\gamma u(s) + \Gamma(s) \qquad \frac{d}{ds}t(s) = \eta(s) \tag{13}$$

which is closely related to eq 3. Here, both $x(s)$ and $u(s)$ are subordinated by the same $t(s)$ process. In analogy with eq 10, the probability distribution $f(x,u,t)$ can be written as

$$f(x,u,t) = \int_0^\infty f_0(x,u,s)p(s,t)\mathrm{d}s \tag{14}$$

where $f_0(x,u,s)$ is the solution of the Fokker−Planck equation

$$\left[\frac{\partial}{\partial s} + u\frac{\partial}{\partial x}\right] f_0(x,u,s) = \mathcal{L}_{\mathrm{FP}}\, f_0(x,u,s) \tag{15}$$

Using these relations together with eq 9, one obtains

$$\frac{\partial f(x,u,t)}{\partial t} = \left[-u\frac{\partial}{\partial x} + \mathcal{L}_{\mathrm{FP}}\right]\gamma_\delta D_t^{1-\delta}\, f(x,u,t) \tag{16}$$

This is the fractional generalization of the usual KFP equation considered by Metzler and Klafter.[5−7]

We want to point out that, in this case, the relationship between $x(t)$ and $u(t)$ is not given by $\dot{x}(t) = u(t)$, and Galilean invariance is violated. Special arguments have to be given for the applicability of such an equation to physical problems. Interpreting the transformation $s(t)$ as a fluctuating quantity where $s(t)$ frequently "stops", the consequence for the process $x(t)$, $u(t)$ is that, during this period, the particle does not proceed in space. A numerical example for a trajectory is shown in the upper panel of Figure 1 where the behavior becomes evident.

The Fractional KFP Equation by Barkai and Silbey

Next, we want to consider the Langevin system

$$\frac{d}{ds}x(s) = u(s)\eta(s)$$
$$\frac{d}{ds}u(s) = -\gamma u(s) + \Gamma(s) \qquad \frac{d}{ds}t(s) = \eta(s) \tag{17}$$

For any specific realization of $\eta(s)$, one can view this as a stochastic process which only depends on the Gaussian variable $\Gamma(s)$. The corresponding probability distribution $f_0(x,u,s)$ is subject to the KFP-type equation

$$\left[\frac{\partial}{\partial s} + u\eta(s)\frac{\partial}{\partial x}\right] f_0(x,u,s) = \mathcal{L}_{\mathrm{FP}}\, f_0(x,u,s) \tag{18}$$

The solution of this equation is a Gaussian probability distribution with the second-order moments defined by

$$\frac{d}{ds}\langle u^2\rangle(s) = -2\gamma\langle u^2\rangle(s) + 2D$$
$$\frac{d}{ds}\langle xu\rangle(s) = -\gamma\langle xu\rangle(s) + \eta(s)\langle u^2\rangle(s)$$
$$\frac{d}{ds}\langle x^2\rangle(s) = 2\eta(s)\langle xu\rangle(s) \tag{19}$$

For simplicity, we first consider the case $\gamma = 0$ in which one obtains

$$\langle u^2\rangle(s(t)) = 2Ds(t)$$
$$\frac{d}{dt}\langle xu\rangle(s(t)) = \langle u^2\rangle(s(t))$$
$$\frac{d}{dt}\langle x^2\rangle(s(t)) = 2\langle xu\rangle(s(t)) \tag{20}$$

Introducing the auxiliary variables $\sigma(t)$ and $\Sigma(t)$ via

$$\frac{d}{dt}\sigma(t) = s(t) \qquad \frac{d}{dt}\Sigma(t) = \sigma(t) \tag{21}$$

one finds

$$\langle u^2\rangle(s(t)) = 2Ds(t)$$
$$\langle xu\rangle(s(t)) = 2D\sigma(t) \qquad \langle x^2\rangle(s(t)) = 4D\Sigma(t) \tag{22}$$

and the characteristic function

$$Z(k,\alpha,\cdot) = \int \mathrm{d}x \int \mathrm{d}u\, f(x,u,\cdot)\exp[ikx + i\alpha u] \tag{23}$$

of f_0 is obtained as

$$Z_0(k,\alpha,s,\sigma,\Sigma) = \exp[-D\alpha^2 s(t) - 2D\alpha k\sigma(t) - 2Dk^2\Sigma(t)] \tag{24}$$

Now, the stochastic process $\eta(s)$ defines a probability distribution $W(s,\sigma,\Sigma,t)$ where $s(t)$, $\sigma(t)$, and $\Sigma(t)$ are related to

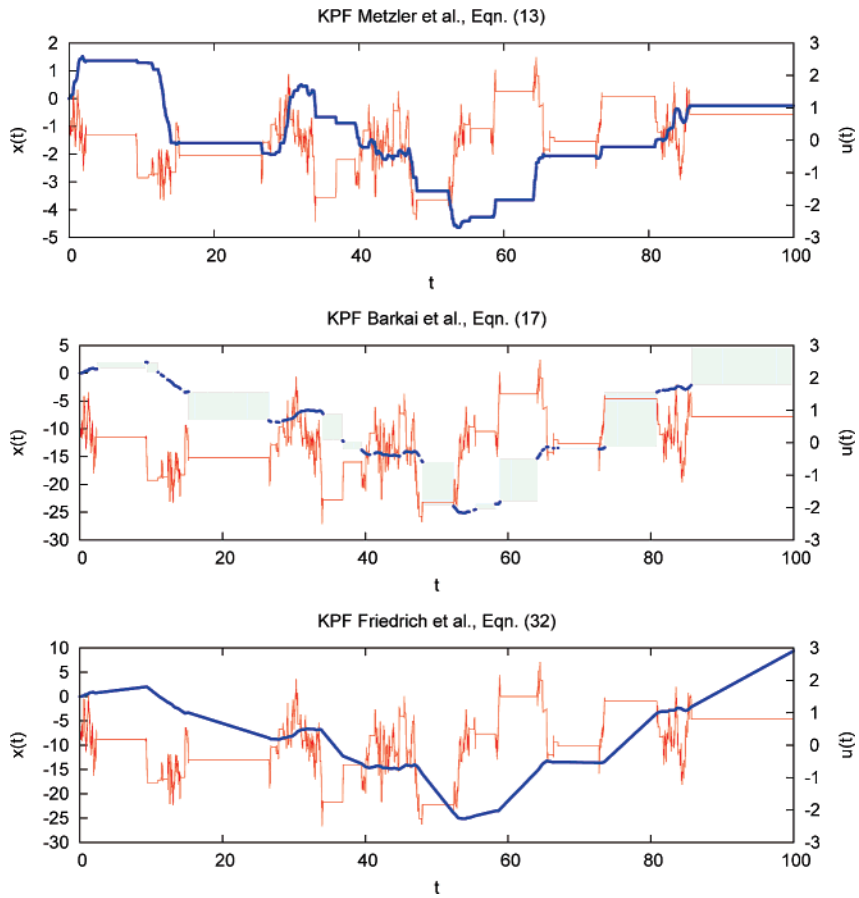

Figure 1. Numerical trajectories of the three different sets of Langevin equations for $\gamma = 1$ and $\delta = 0.85$ for equal realizations of $\eta(s)$ and $\Gamma(s)$. The blue and red lines represent the processes $x(t)$ and $u(t)$, respectively. For the case of Barkai and Silbey, the process $x(t)$ is not uniquely defined in the gray-shaded regions due the nonsteady character of $x(s)$.

$\eta(s)$ via eqs 17 and 21. We assume that this function satisfies the equation

$$\left[\frac{\partial}{\partial t} + \sigma \frac{\partial}{\partial \Sigma} + s \frac{\partial}{\partial \sigma}\right] W(s,\sigma,\Sigma,t) = -\frac{\partial}{\partial s} \gamma_\delta D_t^{1-\delta} W(s,\sigma,\Sigma,t) \quad (25)$$

which is the natural generalization of eq 9. In analogy with eq 10, the generic characteristic function of $f(x,u,t)$ can thus be written as

$$Z(k,\alpha,t) = \int \mathrm{d}s \int \mathrm{d}\sigma \int \mathrm{d}\Sigma\, Z_0(k,\alpha,s,\sigma,\Sigma) W(s,\sigma,\Sigma,t) \quad (26)$$

It is straightforward to show that the corresponding distribution function $f(x,u,t)$ obeys the fractional KFP equation

$$\left[\frac{\partial}{\partial t} + u \frac{\partial}{\partial x}\right] f(x,u,t) = \mathcal{L}_{\mathrm{FP}} \gamma_\delta D_t^{1-\delta} f(x,u,t) \quad (27)$$

with $\gamma = 0$.

The case $\gamma \neq 0$ is only slightly more difficult. Equation 27 yields

$$\left[\frac{\partial}{\partial t} - k \frac{\partial}{\partial \alpha}\right] Z(k,\alpha,t) = -\left[\gamma\alpha \frac{\partial}{\partial \alpha} + D\alpha^2\right] \gamma_\delta D_t^{1-\delta} Z(k,\alpha,t) \quad (28)$$

Using eq 24, we note that

$$\left[k \frac{\partial}{\partial \alpha}\right] Z_0 = \left[\sigma \frac{\partial}{\partial \Sigma} + s \frac{\partial}{\partial \sigma}\right] Z_0 \quad (29)$$

and

$$\left[\gamma\alpha \frac{\partial}{\partial \alpha} + D\alpha^2\right] Z_0 = \left[(2\gamma s - 1) \frac{\partial}{\partial s} + \gamma\sigma \frac{\partial}{\partial \sigma}\right] Z_0 \quad (30)$$

By means of eq 26, we then obtain

$$\left[\frac{\partial}{\partial t} + \sigma \frac{\partial}{\partial \Sigma} + s \frac{\partial}{\partial \sigma}\right] W(s,\sigma,\Sigma,t) = \left[\frac{\partial}{\partial s}(2\gamma s - 1) + \gamma \frac{\partial}{\partial \sigma}\sigma\right] \gamma_\delta D_t^{1-\delta} W(s,\sigma,\Sigma,t) \quad (31)$$

which is a generalization of eq 9. Therefore, starting with eq 17 and assuming that the stochastic process $\eta(s)$ defines a probability distribution $W(s,\sigma,\Sigma,t)$, which satisfies eq 31, the fractional KFP equation of Barkai and Silbey (eq 27) holds. In fact, the approach of Barkai and Silbey consists of the calculation of

$$x(s) = \int_0^s u(s')\eta(s')\mathrm{d}s'$$

and inserting $s = s(t)$ to obtain $x(t) = x(s(t))$. The latter step, however, is only well-defined if $x(s)$ is continuous. Here, $x(s)$ is not continuous, and the transformation is not uniquely defined. We conjecture that the fractional KFP equation by Barkai and Silbey assigns a certain interpretation to that transformation. This will be pursued in a further publication. A numerical example trajectory is given in the center panel of Figure 1.

The Fractional KFP Equation by Friedrich and Co-workers

Finally, we want to address the Langevin system

$$\frac{\mathrm{d}}{\mathrm{d}t}x(t) = u(t)$$
$$\frac{\mathrm{d}}{\mathrm{d}s}u(s) = -\gamma u(s) + \Gamma(s) \quad \frac{\mathrm{d}}{\mathrm{d}s}t(s) = \eta(s) \quad (32)$$

This set of equations describes a CTRW model for the velocity $u(t)$ that is connected to the space variable via $(\mathrm{d}/\mathrm{d}t)x(t) = u(t)$. Such a "random kick" CTRW model was shown to be described by the fractional KFP equation with retardation proposed in ref 9

$$\left[\frac{\partial}{\partial t} + u\frac{\partial}{\partial x}\right] f(x,u,t) = \mathcal{L}_{\mathrm{FP}}\gamma_\delta \mathcal{D}_t^{1-\delta} f(x,u,t) \quad (33)$$

where $\mathcal{D}_t^{1-\delta}$ is the fractional substantial derivative introduced above.

According to ref 10, eq 33 can also be written as

$$\left[\frac{\partial}{\partial t} + u\frac{\partial}{\partial x}\right] f(x,u,t) = \mathcal{L}_{\mathrm{FP}}\int_0^t Q(t-t')\mathrm{e}^{-(t-t')u\partial x} f(x,u,t')\mathrm{d}t' \quad (34)$$

if the memory kernel $Q(t - t')$ is chosen appropriately. In this case, the characteristic function satisfies the equation

$$\left[\frac{\partial}{\partial t} - k\frac{\partial}{\partial \alpha}\right] Z(k,\alpha,t) = -\int_0^t Q(t-t')\left[\gamma\alpha\frac{\partial}{\partial\alpha} + D\alpha^2\right] Z(k,\alpha + k(t-t'),t')\mathrm{d}t' \quad (35)$$

and one finds

$$Z_0(k,\alpha + k(t-t'),s,\sigma,\Sigma) = \exp[-D\alpha^2 s - 2D\alpha k\tilde{\sigma} - 2Dk^2\tilde{\Sigma}] \quad (36)$$

where we have introduced the new variables $\tilde{\sigma} = \sigma + s(t - t')$ and $\tilde{\Sigma} = \Sigma + \sigma(t - t') + s(t - t')^2/2$. Using relations similar to those in eqs 29 and 30 as well as the ansatz (eq 26), we obtain the evolution equation

$$\left[\frac{\partial}{\partial t} + \sigma\frac{\partial}{\partial\Sigma} + s\frac{\partial}{\partial\sigma}\right] W(s,\sigma,\Sigma,t) = \int_0^t Q(t-t')\left[\frac{\partial}{\partial s}(2\gamma s - 1) + \gamma\frac{\partial}{\partial\sigma}\sigma\right] \times W\left(s,\sigma - s(t-t'),\Sigma - \sigma(t-t') + \frac{s}{2}(t-t')^2,t'\right)\mathrm{d}t' \quad (37)$$

for $W(s,\sigma,\Sigma,t)$. The latter is simply a retarded version of eq 31.

To clarify the difference between eqs 31 and 37, we introduce the shifted variables $\hat{\sigma} = \sigma - st$ and $\hat{\Sigma} = \Sigma - \sigma t + (s/2)t^2$ in the sense that

$$W(s,\sigma,\Sigma,t) = \tilde{W}\left(s,\sigma - st,\Sigma - \sigma t + \frac{s}{2}t^2,t\right) \quad (38)$$

holds. Consequently eq 37 can be written as

$$\frac{\partial}{\partial t}\tilde{W}(s,\sigma,\Sigma,t) = \int_0^t Q(t-t')\left[\frac{\partial}{\partial s}(2\gamma s - 1) + \gamma\frac{\partial}{\partial\sigma}(\sigma + st)\right] \times \tilde{W}(s,\sigma,\Sigma,t')\mathrm{d}t' \quad (39)$$

A sample trajectory is presented in the lower panel of Figure 1.

Conclusions

Three different types of fractional generalizations of the KFP equation describing anomalous diffusion of inertial particles can be found in the literature. On the basis of the idea of subordination, which is equivalent to the introduction of an intrinsic, fluctuating time, we have clarified the meaning of these different equations. We have presented the corresponding sets of Langevin equations, which will be useful for a deeper understanding of the trajectories of the respective fractional processes with respect to applications.

We want to point out that single time probability distributions only give limited information. Thus, we suggest investigating multiple time probabilities, as has been put forward recently by in refs 14 and 16−18.

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