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Deriving fractional Fokker-Planck equations from a generalised master equation

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Abstract. – A generalised master equation is constructed from a non-homogeneous random walk scheme. It is shown how fractional Fokker-Planck equations for the description of anomalous diffusion in external fields, recently proposed in the literature, can be derived from this framework. Long-tailed waiting time distributions which cause slowly decaying memory effects, are demonstrated to give rise to a time-fractional Fokker-Planck equation that describes systems close to thermal equilibrium. An extension to include also Lévy flights leads to a generalised Laplacian in the corresponding fractional Fokker-Planck equation.

Anomalous diffusion is characterised through the power law form [1]

$$\langle(\Delta x)^2\rangle \propto K_\gamma t^\gamma \tag{1}$$

of the mean-square displacement deviating from the hallmark property $\langle(\Delta x)^2\rangle \propto K_1 t$ of Gaussian diffusion. According to the value of the anomalous diffusion coefficient γ, one distinguishes subdiffusion ($0 < \gamma < 1$) and superdiffusion ($\gamma > 1$). The dimension of the anomalous diffusion constant is $[K_\gamma] = \mathrm{cm}^2\mathrm{s}^{-\gamma}$.

Normal diffusion under the influence of an external force field is often described in terms of the *Fokker-Planck equation (FPE)*

$$\dot{W} = \left[-\frac{\partial}{\partial x}D^{(1)}(x) + \frac{\partial^2}{\partial x^2}D^{(2)}(x)\right] W(x,t)\,, \tag{2}$$

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where $D^{(1)}(x)$ is the external drift and $D^{(2)}(x)$ is the diffusion coefficient [2]. The one-dimensional FPE for one variable (2) is also referred to as Smoluchowski equation, and is discussed in terms of probability theory in ref. [3]. Equation (2) can be mapped onto the normalised FPE

$$\dot{W} = L_{\mathrm{FP}} W(x,t) \tag{3a}$$

through a transformation of variables [2] where the normalised FP-operator

$$L_{\mathrm{FP}} = \left[\frac{\partial}{\partial x}\frac{V'(x)}{m\eta_1} + K_1 \frac{\partial^2}{\partial x^2}\right] \tag{3b}$$

possesses a constant diffusion coefficient K_1. In eq. ($3b$), $V(x)$ is an external potential, m is the mass of the diffusing particle, and η_1 is the friction coefficient. Therefore, in what follows, we restrict our discussion to the normalised version of the FPE. We also limit the presentation to one dimension, with obvious generalisations to higher dimensions.

In analogy to the description of normal diffusion in an external field via the FPE (2) or its normalised version ($3a$), it has been suggested to model *anomalous diffusion under the influence of an external field* through *fractional Fokker-Planck equations* (*FFPEs*) which have been suggested for Lévy flights in random environments [4-6], for chaotic Hamiltonian systems [7], and for subdiffusive systems close to thermal equilibrium [8]. Apparently, these FFPEs differ considerably from each other. Here we demonstrate the derivation of the FFPE from a generalised master equation (GME) of the type [9]

$$\dot{W}(x,t) = \int_{-\infty}^{\infty} \mathrm{d}x' \int_0^t \mathrm{d}t' K(x,x';t-t') W(x',t'), \tag{4}$$

with the kernel $K(x,x';t)$ which, in general, introduces a non-Markovian memory and spatial correlations [2]. Note that we assumed that the kernel K depends only on the time difference $|t-t'|$. GMEs of the type (4) have been recently discussed in connection with the non-Markovian dynamics of protein folding [10].

In the following, we construct the GME (4) for a position-dependent external force field $F(x) = -V'(x)$ and a site-dependent and non-local transfer kernel $K(x,x',t)$ which decays slowly in space and time, on the basis of a non-homogeneous random walk scheme. This approach allows us to simultaneously consider both long-range transfer and waiting time statistics.

Following Weiss, we start off from the discrete master equation [11]

$$W_j(t+\Delta t) = A_{j-1}W_{j-1}(t) + B_{j+1}W_{j+1}(t), \tag{5}$$

describing the transfer properties of the system through the probability W_j to find the particle on site j after a jump during Δt, in dependence on the populations of the adjacent sites $j-1$ and $j+1$. A_{j-1} and B_{j+1} are the corresponding jump probabilities fulfilling the constraint $A_j + B_j = 1$. Upon Taylor expansions in time and space one recovers the FPE ($3a$) with the FP-operator ($3b$) in the continuum limit [11]. The lattice spacing Δx and the time step Δt assumed to be small parameters going to zero such that the ratio $(\Delta x)^2/\Delta t$ is finite, the coefficients in the FP-operator are given by

$$\frac{V'(x)}{m\eta_1} \equiv \lim_{\Delta x\to 0, \Delta t\to 0} \frac{\Delta x}{\Delta t}\left[B(x) - A(x)\right], \tag{6a}$$

$$K_1 \equiv \lim_{\Delta x\to 0, \Delta t\to 0} \frac{(\Delta x)^2}{\Delta t}. \tag{6b}$$

For taking the limits in eqs. (6*a*) and (6*b*) we impose the normalisation $A(x) + B(x) = 1$ and note that $\frac{A(x-\Delta x)}{B(x+\Delta x)} \sim 1 + \frac{2\Delta x V'(x)}{k_{\mathrm{B}}T}$ for $\Delta x \ll 1$, assuming that the inhomogeneity in jumping left or right on a site, $A(x) - B(x)$, follows the Boltzmann distribution, $k_{\mathrm{B}}T$ being the Boltzmann temperature.

The GME (5) describes Markovian systems with *local* jumps; thus justifying the Taylor expansions in t and x. Anomalous diffusion is intimately related to long-range temporal memory effects or jump length statistics. In the following we develop a framework which allows for the consideration of both temporal and spatial anomalies. At first, we consider the non-locality in space by allowing for jumps from any site $j \pm n$ to j, according to the GME $W_j(t+\Delta t) = \sum_{n=1}^{\infty} A_{j,n} W_{j-n}(t) + \sum_{n=1}^{\infty} B_{j,n} W_{j+n}(t)$ where now the transition matrix elements $A_{j,n}$ and $B_{j,n}$ underlie the normalisation condition $\sum_{n=1}^{\infty} (A_{j,n} + B_{j,n}) = 1$. In order to obtain the continuum limit of this GME, accounting for the non-locality of the transfer statistics, we employ the idea of a direction-dependent jump length distribution developed in ref. [12] for the description of random walks in a constant force field. As an x-dependent force field $F(x) = -V'(x)$ destroys the spatial homogeneity, the transfer statistics, as already implied by the matrices $(A_{j,n})$ and $(B_{j,n})$, must depend on the departure site x', as well as on the arrival site x. We assume that the transfer kernel $\Lambda(x, x')$ accounting for the *distance* between departure site x' and arrival site x, and the *spatial asymmetry* due to the force $F(x)$, is given through the functional form

$$\Lambda(x, x') \equiv \lambda(x - x')[A(x')\Theta(x - x') + B(x')\Theta(x' - x)] , \tag{7}$$

where $\Theta(x)$ is the Heaviside jump function. Thus, $\Lambda(x, x') = \Lambda(x' || x - x')$, *i.e.* the terms determining the jump length $|x - x'|$ and the dependence on x' separate. We impose the normalisation $\int_{-\infty}^{\infty} \mathrm{d}\delta \Lambda(x'||\delta) = 1$. Thus, on each site x', $A(x')$ and $B(x')$ are local weights for going right or left, and $\lambda(x)$ is the jump length or transfer distance probability density function. In order to include the above-mentioned temporal memory effects, we introduce a memory function $\psi(t)$, an example for which is the waiting time probability density function from continuous time random walk theory [13] which ascribes the time interval between successive jumps a waiting time t drawn from this waiting time probability density function. In the following, we adopt this term even for the more general case of an arbitrary memory for which the following derivations are valid. The non-local, continuous time-continuous space version of the GME (5) is, accordingly, given through

$$W(x, t) = \int_{-\infty}^{\infty} \mathrm{d}x' \int_0^t \mathrm{d}t' \psi(t - t') \Lambda(x, x') W(x', t') + \Phi(t) W_0(x) , \tag{8}$$

which explicitly involves the initial condition $W_0(x) = W(x, 0)$, as via the introduction of the waiting time probability density function $\psi(t)$ the particle can rest on a given site according to the probability $\Phi(t) = 1 - \int_0^t \mathrm{d}t' \psi(t')$. It is easy to show that eq. (8) is equivalent to the GME (4), with the kernel

$$K(x, x'; u) = u\psi(u) \frac{\Lambda(x, x') - \delta(x)}{1 - \psi(u)} \tag{9}$$

which generalises a result reported in ref. [14].

The GME (4) with the kernel (9) is a general description of a random walk process underlying only the assumption of the special form (7) of the transfer kernel.

Random walks defined through the functions $\Lambda(x, x')$ and $\psi(t)$ introduced above are an extension of homogeneous random walk schemes [11, 15], and they can be categorised by the existence or divergence of a finite transfer distance variance $\Sigma^2 \equiv \int_{-\infty}^{\infty} \mathrm{d}x \lambda(x) x^2$ and characteristic waiting time $T \equiv \int_0^\infty \mathrm{d}t'\psi(t')t'$. The cases in which we are interested can be described by Lévy-type jump length densities of index $\mu \in (1,2)$, following the asymptotic behaviour [16] $\lambda(x) \sim c_1\sigma^\mu/|x|^{1+\mu}$, or the waiting time density $\psi(t) \sim c_2\tau^\gamma/t^{1+\gamma}$. In Fourier and Laplace space, in the $k \to 0$ and $u \to 0$ limits, we find the asymptotic forms $\lambda_{\mathcal{C}}(k) \sim 1 - \sigma^\mu|k|^\mu$ and $\lambda_{\mathcal{S}}(k) \sim \frac{2}{\mu}\sigma k$ for the cosine and sine transforms, and $\psi(u) \sim 1-(u\tau)^\gamma$. In the k and u representations for $(\mu,\gamma) = (2,1)$, the expansions correspond to those of a Gaussian $\lambda(x)$ and Poissonian $\psi(t)$, and thus this case denotes Brownian diffusion in the force field $F(x)$.

To introduce these anomalous statistics into eq. (8) (or, equivalently, into the GME (4) with the kernel (9)), we rewrite it in Fourier-Laplace space:

$$uW(k,u) - W_0(k) = u\psi(u)\Lambda(k)W(k,u) - \psi(u)W_0(k). \tag{10}$$

Due to its definition (7), the Fourier transform of the transfer kernel $\Lambda(k)$ in eq. (10) is an operator in k, according to the observation that $\Lambda(x,x')W(x,t)$ transforms to

$$\Lambda(k)W(k,t) \equiv \lambda_{\mathcal{C}}(k)W(k,t) + i\lambda_{\mathcal{S}}(k)\{[A(k)-B(k)] * W(k,t)\}\,, \tag{11}$$

where the asterisk denotes a Fourier convolution which is to be taken within the braces [17].

Subdiffusion is characterised by a finite transfer variance Σ^2 and a diverging characteristic waiting time T. This corresponds to $\mu = 2$ and $\gamma < 1$. Taking into account the expansions for small k and the usual long-time limit [13], we arrive at the relation

$$W(k,u) - \frac{W_0(k)}{u} = u^{-\gamma}L_{\mathrm{FP}}(k)W(k,u). \tag{12}$$

Employing the definition of the Riemann-Liouville fractional derivative ${}_0D_t^{1-\gamma} = \frac{\partial}{\partial t}\,{}_0D_t^{-\gamma}$ given through [18]

$${}_0D_t^{1-\gamma}W(x,t) = \frac{1}{\Gamma(\gamma)}\frac{\partial}{\partial t}\int_0^t \mathrm{d}t'\frac{W(x,t')}{(t-t')^{1-\gamma}} \tag{13}$$

and the corresponding theorem $\mathcal{L}\{\,{}_0D_t^{-\gamma}W(x,t)\} = u^{-\gamma}W(x,u)$, we obtain the FFPE

$$\dot{W} = {}_0D_t^{1-\gamma}L_{\mathrm{FP}}W(x,t)\,, \tag{14}$$

which we recently proposed in ref. [8], with the FP-operator L_{FP} (3*b*). It involves the coefficients

$$\frac{V'(x)}{m\eta_\gamma} \equiv \frac{2\sigma}{\mu\tau^\gamma}[B(x)-A(x)]\,, \tag{15a}$$

$$K_\gamma^\mu \equiv \frac{\sigma^\mu}{\tau^\gamma}\,, \tag{15b}$$

with $\mu = 2$, the generalised friction coefficient η_γ being of dimension $[\eta_\gamma] = \mathrm{s}^{\gamma-2}$. In the FFPE (14) single modes decay in a Mittag-Leffler pattern with an asymptotic power law behaviour (see below), and this replaces the ordinary exponential decay found in the normal FPE. For systems relaxing towards thermal equilibrium, we find that the FFPE (14) obeys the *generalised Einstein-Stokes relation* $K_\gamma = \frac{k_{\mathrm{B}}T}{m\eta_\gamma}$ relating the generalised coefficients $K_\gamma = \sigma^2/\tau^\gamma$ and η_γ via the Boltzmann temperature. Furthermore, eq. (14) fulfils the *generalised Einstein relation* [19] $\langle x\rangle_{F_0} = \frac{1}{2}\frac{F_0\langle x^2\rangle_0}{k_{\mathrm{B}}T}$, connecting the drift $\langle x\rangle_{F_0}$ in the presence of a constant force F_0 with the second moment $\langle x^2\rangle_0 = \frac{2K_\gamma}{\Gamma(1+\gamma)}t^\gamma$ in the absence of the force [8].

The divergence of the characteristic waiting time T has been shown to lead to the Riemann-Liouville time fractional operator ${}_0D_t^{1-\gamma}$. We now go a step further and investigate the additional divergence of the jump length variance Σ^2, *i.e.* we assume a Lévy distribution with $\mu < 2$ for the jump distance distribution $\lambda(x)$ which is typical for *Lévy flights*. Then, the Fourier transform of the transfer kernel $\Lambda(x, x')$ contains the factor $|k|^\mu$ in the diffusive term *whereas the drift term is not modified*. The last point is at variance with the generalised drift occurring in the FFPE obtained in [7] from a generalised Kramers-Moyal expansion for chaotic systems. Recalling the definition of the Riesz fractional derivative $\mathcal{F}\left\{\nabla^\mu W(x,t)\right\} = -|k|^\mu W(k,t)$ [20], we obtain, after some manipulations, the FFPE

$$\dot{W} = {}_0D_t^{1-\gamma} L_{\mathrm{FFP}} W(x,t) \tag{16a}$$

with the fractional FP-operator

$$L_{\mathrm{FFP}} = \left[\frac{\partial}{\partial x}\frac{V'(x)}{m\eta_\gamma} + \nabla^\mu K_\gamma^\mu\right], \tag{16b}$$

for Lévy flights in an external potential. The drift and diffusion coefficients are defined in eqs. (15a) and (15b).

The FFPE (16a) describes the *interplay between subdiffusion and Lévy flights*. This can be seen as follows. Through the separation ansatz $W_n(x,t) = T_n(t)\varphi_n(x)$ for the eigenvalue $\lambda_{n,\gamma}$, the FFPE (16a) can be reduced to the spatial eigenequation $L_{\mathrm{FFP}}\varphi_n(x) = -\lambda_{n,\gamma}\varphi_n$, whereas the temporal eigenequation is solved by the Mittag-Leffler function: $T_n(t) = E_\gamma\left(-\lambda_{n,\gamma}t^\gamma\right) = \sum_{l=0}^{\infty}\frac{(-\lambda_{n,\gamma}t^\gamma)^l}{\Gamma(1+\gamma l)}$ with the power law asymptotic behaviour $T_n(t) \sim \lambda_{n,\gamma}^{-1}t^{-\gamma}$. The complete solution is then given by the sum over all eigensolutions [6, 8]. Thus, single modes decay in the slow Mittag-Leffler pattern, whereas the spatial eigensolutions $\varphi_n(x)$ are Lévy stable distributions of Lévy index μ. Due to the generalised central-limit theorem [16], also the full solution $W(x,t)$ is a Lévy distribution in x which causes the divergence of the mean-square displacement [6]. An alternative method of solution which can be applied to certain FFPEs is the method of characteristics [6]. A formal solution of eq. (16a) can be written in the form $W(x,t) = E_\gamma\left(L_{\mathrm{FFP}}t^\gamma\right)W(x,0)$.

Let us now discuss the connection of the FFPE (16a) to the equations proposed in literature. Equation (16a) reduces to the normal FPE (3a) for $\mu = 2$ and $\gamma = 1$. The Markovian (*i.e.* for $\gamma = 1$) version of the FFPE (16a) was derived in ref. [4] from a Langevin equation in a random environment. The general form of eq. (16a) corresponds to the result introduced in ref. [5] through the parametrisation of the trajectory. For a finite jump length variance Σ^2, the FFPE (14) was introduced in ref. [8]. It is interesting to note that the k-space equivalent of the FFPE (16a) for $\gamma = 1$ was derived in ref. [21].

The stationary solution of the FFPE (16a) is obtained through the usual requirement $\frac{\partial W}{\partial t} = 0$. If a stationary solution exists, *i.e.* iff the lowest eigenvalue $\lambda_0 = 0$, this corresponds to a vanishing probability current [2]. The expectation that drift and diffusion should give independent contributions to the probability current is mirrored in the fact that the first-order spatial derivative in the drift term in the FFPE (16a) is not changed for the case $\mu < 2$.

To conclude, we have introduced a new, non-homogeneous random walk model which explicitly takes into account the symmetry breaking of the space through the external field $V(x)$. Anomalous diffusion statistics in time and space are simultaneously incorporated. From this extended random walk scheme we constructed a generalised master equation which involves temporal memory effects and non-locality in space. It was shown how a diverging characteristic waiting time T and a diverging transfer distance variance Σ^2 give rise to the occurrence of a time-fractional Riemann-Liouville operator, and a generalised Laplacian, respectively. Our derivation further corroborates the use of fractional Fokker-Planck equations for the description of systems whose dynamics is governed by anomalous diffusion, *i.e.* generalised statistics of the microscopic motion underlying the process, averaged in some sense. The established connection between the extended random walk scheme, the generalised master equation, and fractional Fokker-Planck equations, besides their connection to the Langevin equation, will lead to a deeper physical understanding of systems exhibiting anomalous dynamics. The toolbox incorporating the approaches listed above offers a broad and unique approach to complex systems, and the solution for given potential types, such as a bistable potential used to model chemical or biological systems, will enrich the theoretical modelling. The advantage of the FFPE approach over the other approaches mentioned is, alike the situation for normal diffusion, that explicit solutions for a given external potential $V(x)$ or boundary value problems are obtained in a straightforward manner from this equation.

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