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The fractional Fokker–Planck equation: dispersive transport in an external force field

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Abstract. The fractional Fokker–Planck equation which has recently been established, is presented as a model for dispersive transport under the influence of an external force field. Special attention is paid to the subexponential, Mittag–Leffler pattern of the mode–relaxation, and the explicit solution of the dispersive analogue of the Ornstein–Uhlenbeck process. © 2000 Elsevier Science B.V. All rights reserved.

Key words: fractional Fokker–Planck equation, anomalous diffusion, fractional diffusion equation, fractional relaxation equation.

I INTRODUCTION

Brownian motion in the presence of an external force field $F(x) = -V'(x)$ is usually described in terms of the Fokker–Planck equation (FPE) [1–6]

$$\frac{\partial W}{\partial t} = \left[\frac{\partial}{\partial x}\frac{V'(x)}{m\eta_1} + K_1\frac{\partial^2}{\partial x^2}\right] W(x,t) \tag{1}$$

which defines the probability density function (pdf) $W(x,t)$ to find the test particle at a certain position x at a given time t. In Eq. (1), m denotes the mass of the particle, K_1 the diffusion constant associated with the transport process, and the friction coefficient η_1 is a measure for the interaction of the particle with its environment. The FPE (1) fulfils the following properties [5–8]:

(i.) In the force–free case, i.e. $V(x) = const$, the corresponding diffusion process is governed by Fick's second law, leading to the linear time dependence

$$\langle x^2 \rangle = 2K_1 t \tag{2}$$

of the mean square displacement; this hallmark of Gaussian diffusion is a consequence of the central limit theorem.

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(ii.) The stationary solution $W_{st}(x) \equiv \lim_{t\to\infty} W(x,t)$ is given by the Gibbs–Boltzmann distribution

$$W_{st}(x) = N \exp\{-\beta V(x)\} \tag{3}$$

with the normalisation constant N, and the Boltzmann factor $\beta \equiv (k_B T)^{-1}$.

(iii.) The diffusion and friction coefficients are connected by the Einstein–Stokes–Smoluchowski relation

$$K_1 = \frac{k_B T}{m\eta_1}, \tag{4}$$

an outcome of the fluctuation–dissipation theorem.

(iv.) From linear response, one recovers the generalised Einstein relation

$$\langle x \rangle_F = \frac{1}{2}\frac{F\langle x^2\rangle}{k_B T} \tag{5}$$

between the first moment in presence of the constant force F, $\langle x \rangle_F$, and the second moment in its absence, $\langle x^2 \rangle$ given by Eq. (2).

(v.) The temporal relaxation of single modes is exponential, as is discussed in section III.

In a variety of systems one finds that Eq. (2) is violated. Instead, diffusion in such systems is characterised by the power–law time dependence

$$\langle x^2 \rangle \propto t^\alpha, \quad \alpha \neq 1 \tag{6}$$

of the mean square displacement [8–12]. This form is connected with broad, Lévy-type transport statistics, ruled by the paramount generalised central limit theorem [8,13,14]. According to the value of the anomalous diffusion exponent α, one distinguishes subdiffusion ($0 < \alpha < 1$) and superdiffusion ($\alpha > 1$). In what follows, the first case is considered which is also referred to as dispersive transport [15]. Experimental evidence for such slow diffusion has been found for transport on percolation clusters [16], a bead immersed in a polymeric network [17], or for charge carrier transport in amorphous semiconductors [18,19], just to mention a few [8–12].

II THE FRACTIONAL FOKKER–PLANCK EQUATION

As a model for subdiffusion in an external potential field $V(x)$, the fractional Fokker–Planck equation (FFPE)

$$\frac{\partial W}{\partial t} = {}_0D_t^{1-\alpha}\left[\frac{\partial}{\partial x}\frac{V'(x)}{m\eta_\alpha} + K_\alpha\frac{\partial^2}{\partial x^2}\right]W(x,t) \tag{7}$$

has recently been suggested [20]. Here, K_α denotes the generalised diffusion coefficient of dimension $[K_\alpha] = \mathrm{cm}^2\mathrm{sec}^{-\alpha}$, and η_α is the generalised friction coefficient with $[\eta_\alpha] = \mathrm{sec}^{\alpha-2}$. Note that both K_α and η_α are time–independent. The FFPE (7) can be derived from a generalised master equation which follows from a non–homogeneous random walk model, in the diffusion limit [21]. In an alternative phase space derivation, the FFPE (7) corresponds to the high–friction limit of the velocity–averaged fractional Klein–Kramers equation resulting from a Chapman–Kolmogorov equation with broad waiting time statistics [22]. In the latter derivation, the non–integer dimensions of K_α and η_α follow naturally from the introduction of a non–Markovian integral kernel.

The fractional Riemann–Liouville operator ${}_0D_t^{1-\alpha} = \frac{d}{dt}\,{}_0D_t^{-\alpha}$ featuring in Eq. (7) is defined through the convolution integral [23]

$${}_0D_t^{1-\alpha}W(x,t) = \frac{1}{\Gamma(\alpha)}\frac{\partial}{\partial t}\int_0^t dt'\frac{W(x,t')}{(t-t')^{1-\alpha}}. \tag{8}$$

Its fundamental property is the fractional "differintegration" (differentiation or integration) of a power,

$${}_0D_t^p t^q = \frac{\Gamma(1+q)}{\Gamma(1+q-p)}t^{q-p} \tag{9}$$

for any real p, q. Thus, the fractional derivative of a constant,

$${}_0D_t^p 1 = \frac{1}{\Gamma(1-p)}t^{-p}, \quad p > 0 \tag{10}$$

reproduces an inverse power–law. Of course, for integer–valued p, the Γ–function diverges, and one recovers the standard result $d^n 1/dt^n = 0$. For the derivation of fractional equations, the generalised integration theorem [23]

$$\mathcal{L}\{\,{}_0D_t^{-\alpha}W(x,t)\} = u^{-\alpha}W(x,u) \tag{11}$$

of the Laplace transformation is useful. Note that due to the convolution nature of the fractional operator, Eq. (8), the FFPE (7) is non–Markovian and it incorporates memory effects [26].

Comparing to its Brownian analogue, Eq. (1), which corresponds to the limit $\alpha = 1$, the FFPE (7) fulfils the following properties [20,21]:

(i.) The force–free limit is described by the fractional diffusion equation which was originally established by Schneider and Wyss [25], and is characterised by the mean square displacement

$$\langle x^2\rangle = \frac{2K_\alpha}{\Gamma(1+\alpha)}t^\alpha, \tag{12}$$

in agreement with Eq. (6).

(ii.) The stationary limit distribution defined by $\frac{\partial W}{\partial t} = 0$ is given by the Gibbs–Boltzmann form (3). This means that the FFPE (7) describes systems close to thermal equilibrium: irrespectively of a different dynamical evolution, systems governed by both the FPE (1) and the FFPE (7) tend to the same limit distribution.

(iii.) A generalisation of the Einstein–Stokes–Smoluchowski relation,

$$K_\alpha = \frac{k_B T}{m\eta_\alpha}, \tag{13}$$

holds for the generalised coefficients K_α and η_α.

(iv.) For a constant force F, the generalised Einstein relation (5) is equally valid for the fractional case.

(v.) The relaxation of modes is subexponential, as is shown now.

III SEPARATION ANSATZ AND MITTAG–LEFFLER RELAXATION OF MODES

A standard method of solution for the FPE is the separation of variables [5]. Consider the separation ansatz

$$W_n(x,t) = T_n(t)\varphi_n(x) \tag{14}$$

for a given eigenvalue $\lambda_{n,\alpha}$. Introducing this ansatz into the FFPE (7), one obtains the two eigenequations

$$\frac{dT_n(t)}{dt} = -\lambda_{n,\alpha}\, {}_0D_t^{1-\alpha} T_n(t), \tag{15}$$

$$\left[\frac{d}{dx}\frac{V'(x)}{m\eta_\alpha} + K_\alpha \frac{d^2}{dx^2}\right]\varphi_n(x) = -\lambda_{n,\alpha}\varphi_n(x). \tag{16}$$

The spatial eigenequation (16) has the same structure as the one encountered for the standard FPE. The temporal eigenequation (15) is but the fractional relaxation equation [24], the solution of which is given in terms of the Mittag–Leffler function [27],

$$T_n(t) = E_\alpha(-\lambda_{n,\alpha}t^\alpha) \equiv \sum_{j=0}^{\infty} \frac{(-\lambda_{n,\alpha}t^\alpha)^j}{\Gamma(1+\alpha j)}. \tag{17}$$

As can be seen from the series expansion, the exponential form $E_1(-\lambda_{n,1}t) = \exp\{-\lambda_{n,1}t\}$ can be recovered in the Brownian limit $\alpha = 1$. For the case $\alpha = 1/2$, another simple representation can be found in terms of the complementary error function: $E_{1/2}(-\lambda_{n,1/2}t^{1/2}) = \exp\{\lambda_{n,1/2}^2 t\}\mathrm{erfc}(\lambda_{n,1/2}t^{1/2})$. A very interesting

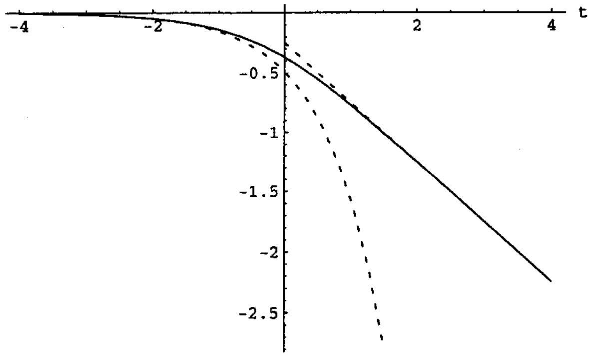

FIGURE 1. Mittag–Leffler relaxation on a double–logarithmic scale. The full line represents the Mittag–Leffler function for index 1/2. The dashed lines demonstrate the initial stretched exponential behaviour, and the final inverse power–law pattern.

property of the Mittag–Leffler function lies in the observation that it interpolates between an initial stretched exponential behaviour

$$E_\alpha(-\lambda_{n,\alpha}t^\alpha) \sim \exp\left\{-\frac{\lambda_{n,\alpha}t^\alpha}{\Gamma(1+\alpha)}\right\}, \quad \lambda_{n,\alpha}t^\alpha \ll 1 \tag{18}$$

and a long–time inverse power–law pattern

$$E_\alpha(-\lambda_{n,\alpha}t^\alpha) \sim \frac{1}{\lambda_{n,\alpha}t^\alpha}, \quad \lambda_{n,\alpha}t^\alpha \gg 1. \tag{19}$$

This behaviour is portrayed in Fig. 1.

A Subdiffusive Ornstein–Uhlenbeck process

In order to demonstrate the usefulness of the separation of variables method, it is worth while considering the subdiffusive generalisation of the Ornstein–Uhlenbeck process [6]. This process describes dispersive motion, for $0 < \alpha < 1$, in the parabolic potential $V(x) = \frac{1}{2}m\omega^2x^2$ which exerts a restoring force on the test particle. From the corresponding FFPE

$$\frac{\partial W}{\partial \tilde{t}} = {}_0D_{\tilde{t}}^{1-\alpha}\left[\frac{\partial}{\partial \tilde{x}}\tilde{x} + \frac{\partial^2}{\partial \tilde{x}^2}\right]W, \tag{20}$$

written in reduced variables $\tilde{t} \equiv t/\tau$, $\tau \equiv \omega^2/\eta_\alpha$ and $\tilde{x} \equiv x\sqrt{m\omega^2/[k_BT]}$, and the separation ansatz, Eq. (14), one infers the solution [28]

$$W(x,t) = \sqrt{\frac{m\omega^2}{2\pi k_B T}} \sum_{n=0}^{\infty} \frac{1}{2^n n!} E_\alpha(-n\tilde{t}^\alpha) H_n(\tilde{x}'/\sqrt{2}) H_n(\tilde{x}/\sqrt{2}) \exp\{-\tilde{x}^2/2\}. \quad (21)$$

Here, the initial condition $W_0(x) \equiv \lim_{t\to 0} W(x,t) = \delta(x-x')$ was assumed, and $H_n(z)$ denote the Hermite polynomials. The solution (21) corresponds to the result by Weiss [29] in respect to the spatial part, and the exponential decay of the modes is replaced by the Mittag–Leffler pattern. This solution (21) is plotted, for $\alpha = 1/2$ in Fig. 2a. From the initially asymmetric distribution, the centred, stationary solution is approached. Fig. 2b depicts the Brownian counterpart, demonstrating the considerably faster relaxation towards the thermal equilibrium state given by the Gibbs–Boltzmann distribution

$$\begin{aligned} W_{\text{st}}(x) &= \sqrt{\frac{m\omega^2}{2\pi k_B T}} H_0(\tilde{x}'/\sqrt{2}) H_0(\tilde{x}/\sqrt{2}) \exp\{-\tilde{x}^2/2\} \\ &\equiv \sqrt{\frac{m\omega^2}{2\pi k_B T}} \exp\left\{-\frac{m\omega^2 x^2}{2k_B T}\right\} \end{aligned} \quad (22)$$

the first term ($n=0$) from Eq. (21). The slow relaxation dynamics of the single modes, $T_n(t) = E_\alpha(-n\tilde{t}^\alpha)$, is mirrored in the temporal evolution of the first moment,

$$\langle x\rangle(t) = \langle x\rangle(0) E_\alpha(-[t/\tau]^\alpha), \quad (23)$$

which describes the Mittag–Leffler decay of the initial asymmetry, i.e. the equilibration towards the potential minimum. Equation (23) can be easily obtained from the FFPE (20) by integration, leading to the fractional relaxation equation $\frac{d}{dt}\langle x\rangle = {}_0D_t^{1-\alpha}\frac{\omega^2}{\eta_\alpha}\langle x\rangle$ for $\langle x\rangle$. In the same manner, the slightly more complicated, inhomogeneous fractional differential equation

$$\frac{d\langle x^2\rangle}{d\tilde{t}} = {}_0D_{\tilde{t}}^{1-\alpha}\left[-2\langle x^2\rangle + 2\right] = -2\,{}_0D_{\tilde{t}}^{1-\alpha}\langle x^2\rangle + \frac{2t^{\alpha-1}}{\Gamma(\alpha)} \quad (24)$$

for the second moment $\langle x^2\rangle$ is obtained. Laplace transformation and rearrangement of terms leads to the final result

$$\langle x^2\rangle(t) = \langle x^2\rangle_{\text{th}} + \left[\langle x^2\rangle(0) - \langle x^2\rangle_{\text{th}}\right] E_\alpha(-2[t/\tau]^\alpha). \quad (25)$$

Thus, the initial deviation from the thermal equilibrium value $\langle x^2\rangle_{\text{th}} \equiv \frac{k_B T}{m\omega^2}$, $\langle x^2\rangle(0) - \langle x^2\rangle_{\text{th}}$, relaxes according to a Mittag–Leffler pattern, with the characteristic time $2^{-1/\alpha}\tau$. According to Eq. (25) and the properties of the Mittag–Leffler function, one finds the initially potential–independent subdiffusion behaviour

$$\langle x^2\rangle(t) \sim \langle x^2\rangle(0) - 2\left[\langle x^2\rangle(0) - \langle x^2\rangle_{\text{th}}\right] \frac{(t/\tau)^\alpha}{\Gamma(1+\alpha)} + O([t/\tau]^{2\alpha}), \quad (26)$$

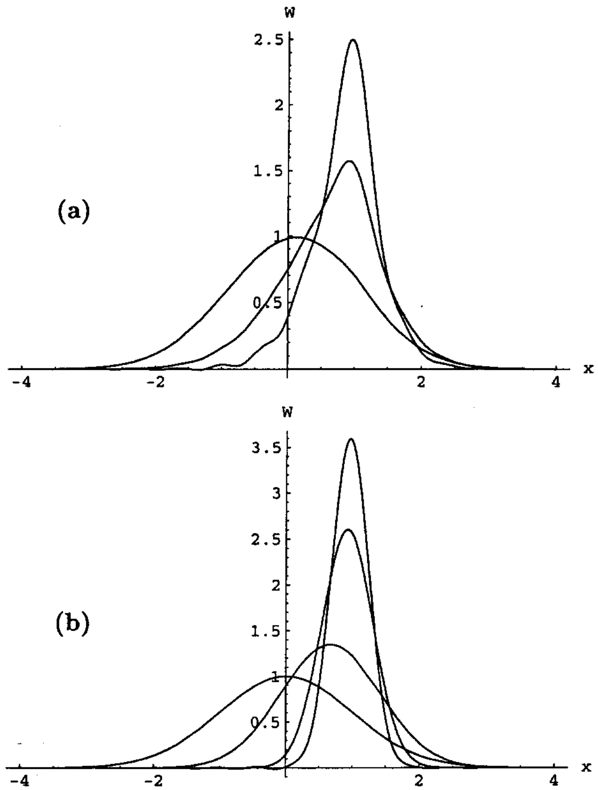

FIGURE 2. Pdf $W(x,t)$, Eq. (21), in the case of the subdiffusive Ornstein–Uhlenbeck process, for the anomalous diffusion exponent $\alpha = 1/2$ (a), and the Brownian case ($\alpha = 1$) (b). The initial value is chosen to be $W_0(x) = \delta(x-1)$. The maximum clearly shifts towards the origin, acquiring an inversion symmetric shape. (a) The curves are drawn for the times $t = 0.02, 0.2$, and 40, taking along the first 101 terms in the sum (21). (b) The curves are drawn for the times $t = 0.04$, 0.4, and 4. The centred curve represents the stationary state. Comparison to the subdiffusive solution demonstrates that the curve for $t = 40$ has almost reached stationarity. The small wiggles visible in the left flanks for the two shorter times are due to numerical inaccuracy due to the truncation in the summation.

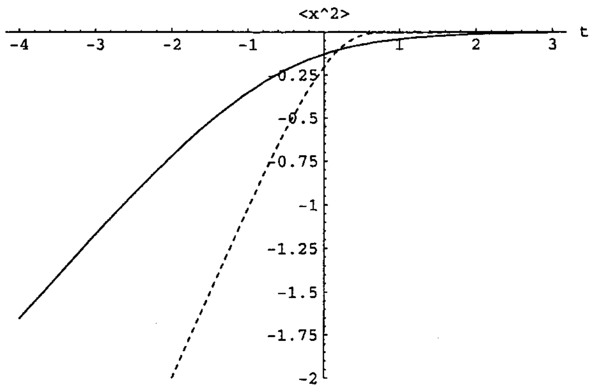

FIGURE 3. Mean square displacement for the subdiffusive ($\alpha = 1/2$, full line) and Brownian Ornstein–Uhlenbeck (dashed line) processes. The Brownian case shows the typical proportionality to t for small times, and approaches the saturation value much faster than its subdiffusive analogue which starts off with the $t^{1/2}$ behaviour and approaches the thermal equilibrium value by a power–law, Eq. (27).

or $\langle x^2\rangle(t) \sim 2\frac{K_\alpha t^\alpha}{\Gamma(1+\alpha)}$ for $\langle x\rangle(0) = 0$. This turns over to the final approach

$$\langle x^2\rangle(t) \sim \langle x^2\rangle_{\rm th}\left(1-\frac{\tau^\alpha}{2t^\alpha}\right)+\langle x^2\rangle(0)\frac{\tau^\alpha}{2t^\alpha} \tag{27}$$

of the equilibrium value. This slow power–law approximation is shown in Fig. 3. Note from Eq. (27) that the initial value $\langle x^2\rangle(0)$ decays slowly with the power–law $\propto t^{-\alpha}$.

IV CONCLUSIONS

The FFPE has been presented as a model equation for dispersive transport in an external force field. It has been shown that this equation is close to thermal equilibrium and fulfils the generalised Einstein–Stokes and the generalised Einstein relations. Being an alternative approach to asymmetric continuous time random walk models, generalised Langevin equations, or the generalised master equation, the subdiffusive FFPE offers a similar advantage as does the ordinary FPE in respect to equivalent Brownian models: a relatively straightforward calculation of its solution, the pdf $W(x,t)$, or the related moments of the transport process, as was exemplified for the subdiffusive Ornstein–Uhlenbeck process. Therefore, the FFPE constitutes a framework for the description of transport dynamics in complex systems whose temporal evolution is governed by slowly decaying memory effects leading to a phenomenologically subdiffusive behaviour. In this context it is worth mentioning that a generalised master equation of the type related to the FFPE, has been used recently in the modelling of non–Markovian dynamical processes in protein folding [30].

The fractional Riemann–Liouville operator which leads to the slow diffusion, has been shown to give rise to the Mittag–Leffler relaxation pattern of single modes. This relaxational behaviour which has been derived via the method of separation of variables, interestingly interpolates between an initial stretched exponential and a final inverse power–law relaxation patterns.

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