

# Non-homogeneous random walks, generalised master equations, fractional Fokker-Planck equations, and the generalised Kramers-Moyal expansion

R. Metzler<sup>a</sup>

Department of Physics and School of Chemical Sciences, University of Illinois at Urbana-Champaign, 600 S. Mathews MC-712 Box 24-6, Urbana, IL 61801, USA

Received 30 June 2000 and Received in final form 12 November 2000

**Abstract.** A generalised random walk scheme for random walks in an arbitrary external potential field is investigated. From this concept which accounts for the symmetry breaking of homogeneity through the external field, a generalised master equation is constructed. For long-tailed transfer distance or waiting time distributions we show that this generalised master equation is the genesis of apparently different fractional Fokker-Planck equations discussed in literature. On this basis, we introduce a generalisation of the Kramers-Moyal expansion for broad jump length distributions that combines multiples of both ordinary and fractional spatial derivatives. However, it is shown that the nature of the drift term is not changed through the existence of anomalous transport statistics, and thus to first order, an external potential  $\Phi(x)$  feeds back on the probability density function  $W$  through the classical term  $\propto \partial/\partial x \Phi'(x)W(x, t)$ , *i.e.*, even for Lévy flights, there exists a linear infinitesimal generator that accounts for the response to an external field.

**PACS.** 05.10.Gg Stochastic analysis methods (Fokker-Planck, Langevin, etc.) – 05.40.Fb Random walks and Lévy flights – 05.60.-k Transport processes – 02.50.Ey Stochastic processes

## 1 Introduction

Many physical systems show more or less pronounced correlations in their dynamical behaviour, these being either non-Markovian memory effects, or non-locality in space [1–3]. Often, these correlations are governed by long-tailed or Lévy-type statistics giving rise to the validity of some superordinate limit theorem [1–4]. The probability density function (pdf) to find the test particle under consideration at position  $x$  at time  $t$  of such systems can be described in terms of a generalised master equation (GME) of the form [5–12]

$$\frac{\partial W(x, t)}{\partial t} = \int_{-\infty}^{\infty} dx' \int_0^t dt' \mathfrak{K}(x, x'; t - t') W(x', t') \quad (1)$$

where the kernel  $\mathfrak{K}(x, x'; t - t')$  governs the transfer from a site  $x'$  to  $x$  and the dependence of the process on its history (memory), and thus causes, in general, temporal or spatial non-locality. It is our goal to investigate the generalisations of the kinetic equation corresponding to the

master equation (1) for self-similar temporal or spatial forms of the kernel  $\mathfrak{K}$ . Throughout this paper, we consider only systems which are homogeneous in time, *i.e.*, the kernel  $\mathfrak{K}$  depends only on the time difference  $|t - t'|$ . Moreover, we concentrate on such cases that assume spatial and temporal decoupling, *i.e.*, jump length and waiting time of the associated random walk process are assumed to be independent. The discussion is also restricted to the one-dimensional case.

Rather than *via* a master equation, the pdf  $W(x, t)$  of a Markovian system under the influence of the external force field  $F(x) = -\frac{d}{dx}\Phi(x)$  is usually described through the Fokker-Planck equation (FPE) [13]

$$\frac{\partial W}{\partial t} = L_{\text{FP}} W \quad (2a)$$

with the normalised FP-operator

$$L_{\text{FP}} = \frac{\partial}{\partial x} \frac{\Phi'(x)}{m\eta} + K \frac{\partial^2}{\partial x^2} \quad (2b)$$

where  $m$  is the mass of the diffusing particle,  $\eta$  denotes the friction coefficient, and  $K = k_{\text{B}}T/(m\eta)$  is the diffusion constant. The monovariate FPE for one variable (2a) is often referred to as Smoluchowski equation, and is discussed in probabilistic terms in reference [14].

<sup>a</sup> *Permanent address:* Department of Physics, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Rm 12-109, Cambridge, MA 02139, USA  
e-mail: metz@mit.edu

We note that the FPE

$$\frac{\partial W}{\partial t} = \left( -\frac{\partial}{\partial x} D^{(1)}(x) + \frac{\partial^2}{\partial x^2} D^{(2)}(x) \right) W(x, t) \quad (3)$$

with space-dependent coefficients can always be mapped onto the FPE (2a). Here,  $D^{(1)}(x)$  is an external drift caused through the force  $F(x)$ , and  $D^{(2)}(x)$  is a space-dependent diffusion coefficient [11,12]. The associated transformation of variables from equations (3) to (2a) is  $x \rightarrow \int_0^x dx' \sqrt{K/D^{(2)}(x')}$ , and  $W \rightarrow \sqrt{D^{(2)}(x)/KW}$  so that  $\Phi'(x) = -m\eta D^{(1)}(x)$  [15]. Due to this general transformation, equation (2a) is sometimes called normalised FPE [11].

The FPE (2a) for  $\Phi(x) = \text{const.}$  describes Gaussian diffusion, a hallmark property of which is the linear time dependence  $\langle(\Delta x)^2\rangle = 2Kt$  of the mean squared displacement. We are interested in systems whose dynamical evolution is based upon transport processes which exhibit anomalous diffusion behaviour of the power-law type [1,2,16]

$$\langle x^2(t) \rangle \propto K_\gamma t^\gamma, \quad \gamma \neq 1, \quad (4)$$

in the force-free limit. One distinguishes subdiffusion for  $0 < \gamma < 1$ , and superdiffusion for  $\gamma > 1$ , and for Lévy flights the mean squared displacement diverges [1–3]. In equation (4), the generalised diffusion constant  $K_\gamma$  is of dimension  $[K_\gamma] = \text{cm}^2 \text{sec}^{-\gamma}$ .

Instead of modelling the forced transport in systems whose dynamics is governed by a non-local temporal or spatial behaviour connected with Lévy-type statistics, through the GME (1), fractional Fokker-Planck equations (FFPEs) have been suggested [17–26]. Recently, we pointed out that such FFPEs can be constructed, as a natural generalisation of the standard FPE, from a modified, non-homogeneous random walk scheme [24], or from the Langevin equation with Gaussian,  $\delta$ -correlated noise in combination with broadly distributed multiple trapping [26].

The basic result of these derivations is the FFPE

$$\frac{\partial W}{\partial t} = {}_0D_t^{1-\gamma} \left( \frac{\partial}{\partial x} \frac{\Phi'(x)}{m\eta_\gamma} + {}_{-\infty}D_x^\mu K_\gamma^\mu \right) W(x, t) \quad (5)$$

which describes physical systems governed by a competition of subdiffusion and Lévy flights, leading to the time-fractional operator  ${}_0D_t^{1-\gamma}$  responsible for the non-Markovian character of equation (5), and the generalised Laplacian  ${}_{-\infty}D_x^\mu$  reminiscent of the Lévy distributed jump lengths. In what follows, we derive the FFPE (5) in a formal way from the GME (1). We then establish the non-homogeneous random walk model and derive the kernel  $\mathfrak{K}$  from equation (1) for this model, leading to the FFPE (5).

More specifically, we discuss two important points which so far have not been dealt with in detail. First, we address in depth the relation for different types of externally driven anomalous motion between the FFPE description and the associated generalised master equation, which leads to a better understanding of the meaning of the fractional transport equations. The second

important issue concerns the question of deriving a generalisation of the Kramers-Moyal expansion for the case of broad jump length statistics. It will be shown that both ordinary and fractional differential operators in the spatial coordinate emerge in growing order of the Kramers-Moyal index. However, for *any* Lévy index characterising the jump length distribution, the lowest order force term represents the classical first order, local gradient, *i.e.*, the standard drift term obtains. Moreover, the Pawula theorem, in essence, carries over to anomalous statistics so that either the expansion is terminated after the second term, or terms of all order have to be carried along to guarantee positivity.

## 2 Generalised master and fractional Fokker-Planck equations

In Fourier-Laplace space, the GME (1) takes on the form

$$uW(k, u) - W_0(k) = \mathfrak{K}(k, u) * W(k, u) \quad (6)$$

where  $k$  is the wave number,  $u$  the Laplace variable, and the asterisk denotes a Fourier convolution  $f(x) * g(x) \equiv \int_{-\infty}^{\infty} dx' f(x-x')g(x')$ . Dividing equation (6) by  $u$ , we obtain, after Laplace inversion and differentiation  $\frac{\partial}{\partial t}$ , the alternative representation

$$\frac{\partial W(x, t)}{\partial t} = \frac{\partial}{\partial t} \int_{-\infty}^{\infty} dx' \int_0^t dt' \tilde{\mathfrak{K}}(x, x', t-t') W(x, t') \quad (7)$$

of the GME (1) which will be more convenient in the forthcoming derivations. The new kernel is given through  $\tilde{\mathfrak{K}}(x, x'; u) = \mathfrak{K}(x, x'; u)/u$ , *i.e.*  $\tilde{\mathfrak{K}}(x, x'; t) = \int_0^t dt' \mathfrak{K}(x, x'; t')$ . Let us now assume that  $\tilde{\mathfrak{K}}$  can be written in the product form  $\tilde{\mathfrak{K}}(x, x'; t) = M(x, x')\Pi(t)$ . Then, the transfer kernel  $M(x, x')$  is responsible for spatial correlations, whereas the memory kernel  $\Pi(t)$  introduces the non-Markovian behaviour; and  $M$  and  $\Pi$  are independent. We proceed by considering long-tailed forms for the memory part  $\Pi$ , before dealing with the spatial part  $M$ .

If  $\Pi(t)$  follows the broad power-law form

$$\Pi(t) = \frac{(t/\tau)^{\gamma-1}}{\Gamma(\gamma)} \quad (8)$$

for  $0 < \gamma < 1$ , the solution  $W(x, t)$  of the GME (1) (or (7)) features a strong dependence on its prehistory, *i.e.*, on  $W(x, t')$ ,  $t' < t$ . The resulting equation

$$\frac{\partial W(x, t)}{\partial t} = \frac{1}{\Gamma(\gamma)} \frac{\partial}{\partial t} \int_0^t dt' \frac{\int_{-\infty}^{\infty} dx' M(x, x') W(x', t')}{(t-t')^{1-\gamma}} \quad (9)$$

includes the defining expression

$${}_0D_t^{1-\gamma} W(x, t) = \frac{1}{\Gamma(\gamma)} \frac{\partial}{\partial t} \int_0^t dt' \frac{W(x, t')}{(t-t')^{1-\gamma}} \quad (10)$$

of the Riemann-Liouville fractional derivative  ${}_0D_t^{1-\gamma}$  [28]. With this definition, the GME (1) for the power-law memory can be expressed in the form of the fractional master equation (compare [29])

$$\frac{\partial W(x, t)}{\partial t} = {}_0D_t^{1-\gamma} \int_{-\infty}^{\infty} dx' M(x, x') W(x', t). \quad (11)$$

In this equation, the kernel  $M$  describes the transfer of a particle from the departure site  $x'$  to the arrival site  $x$ , thereby covering the distance  $|x - x'|$ . We now consider special forms of this kernel  $M$ .

For the case when the transfer kernel depends only on the distance  $|x - x'|$  from departure to arrival site, and is given through  $M(k) = -K_\gamma k^2$  in Fourier space, the fractional diffusion equation [27]

$$\frac{\partial W}{\partial t} = {}_0D_t^{1-\gamma} K_\gamma \frac{\partial^2}{\partial x^2} W(x, t) \quad (12)$$

emerges. In the external field  $\Phi(x)$ , the choice (compare Risken [11]),

$$M(x, x') = \left( \frac{\partial \Phi'(x)}{\partial x} \frac{1}{m\eta_\gamma} + K_\gamma \frac{\partial^2}{\partial x^2} \right) \delta(x - x') \quad (13)$$

leads to the FFPE

$$\frac{\partial W}{\partial t} = {}_0D_t^{1-\gamma} \left( \frac{\partial \Phi'(x)}{\partial x} \frac{1}{m\eta_\gamma} + K_\gamma \frac{\partial^2}{\partial x^2} \right) W(x, t) \quad (14)$$

proposed in reference [23] for subdiffusive systems close to thermal equilibrium.

Conversely, assuming a Markovian dynamics corresponding to  $\Pi = 1$  in equation (7), and the transfer kernel  $M$  obeying the fractal form  $M(k) = -K^\mu |k|^\mu$ , we find the fractional diffusion equation for Lévy flights,

$$\frac{\partial W}{\partial t} = K^\mu {}_{-\infty}D_x^\mu W(x, t), \quad (15)$$

which was derived by Compte [30], and which features the fractional Riesz-Weyl derivative, defined through [31]

$$\mathcal{F} \left\{ {}_{-\infty}D_x^\mu W(x, t) \right\} = -|k|^\mu W(k, t). \quad (16)$$

The corresponding FFPE for Lévy flights in an external potential,

$$\frac{\partial W}{\partial t} = \left( \frac{\Phi'(x)}{m\eta} + K^\mu {}_{-\infty}D_x^\mu \right) W(x, t) \quad (17)$$

which was derived in reference [17] for Lévy flights in a random environment, is then obtained through the kernel

$$M(x, x') = \left( \frac{\partial \Phi'(x)}{\partial x} \frac{1}{m\eta} + K^\mu {}_{-\infty}D_x^\mu \right) \delta(x - x'). \quad (18)$$

Combining the slowly decaying memory leading to the operator  ${}_0D_t^{1-\gamma}$  with the Lévy flight character of  $M \propto -|k|^\mu$ ,

we arrive at the FFPE (5). We now derive the kernel connected with the assumptions (13, 18) and (8) from an extended random walk scheme which we establish below. Although our derivations are more general, we will employ the typical notions from continuous time random walk theory [9, 10, 32], these being the waiting time probability density function  $w(t)$  from which the waiting time is drawn which elapses between one jump and the next, as well as the jump length pdf  $\lambda(x)$  through which a value is assigned to the jump length or transfer distance  $|x - x'|$  covered by a jump event from the departure site  $x'$  to the arrival site  $x$ .

### 3 From jump statistics to Fokker-Planck operators

Both standard diffusion and fractional diffusion equations, as well as their equivalent representation in continuous time random walk theory, are intimately related to the homogeneity in space, which manifests itself in the transport kernel obeying the functional form  $\mathfrak{K}(x, x'; t - t') = \mathfrak{K}(x - x'; t - t')$ . In general, an external field will break this homogeneity. To take this effect into consideration, we start off from a discrete and local random walk process for which we introduce continuum limits in time and space. The new scheme addresses simultaneously the introduction of a continuous time leading to memory effects, as well as the continuum limit in space, accounting for non-local transfer statistics.

#### 3.1 The derivation of the Fokker-Planck equation

Let us at first consider the derivation of the standard FPE (3) from the discrete local master equation [10]

$$W_j(t + \Delta t) = A_{j-1} W_{j-1}(t) + B_{j+1} W_{j+1}(t), \quad (19)$$

where the index  $j$  denotes the position, and the transfer coefficients  $A_{j-1}$  and  $B_{j+1}$  are the probabilities to jump from site  $j - 1$  [ $j + 1$ ] to site  $j$ , respectively. These coefficients fulfil the normalisation condition  $A_j + B_j = 1$ . From Taylor expansions in  $\Delta t$  and  $\Delta x$  according to

$$W_j(t + \Delta t) \sim W_j(t) + \Delta t \frac{\partial W_j(t)}{\partial t} \quad (20)$$

$$A_{j-1} W_{j-1}(t) \sim A(x) W(x, t) - \Delta x \frac{\partial A(x) W(x, t)}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 A(x) W(x, t)}{\partial x^2} \quad (21)$$

one recovers in the continuum limit the FPE (2a) with the FP-operator (2b), where the coefficients are given by

$$\frac{\Phi'(x)}{m\eta} \equiv \lim_{\Delta x \rightarrow 0, \Delta t \rightarrow 0} \frac{\Delta x}{\Delta t} [B(x) - A(x)] \quad (22a)$$

$$K \equiv \lim_{\Delta x \rightarrow 0, \Delta t \rightarrow 0} \frac{(\Delta x)^2}{2\Delta t}. \quad (22b)$$

Thereby, we assume that the lattice spacing  $\Delta x$  and the time increment  $\Delta t$  are becoming small quantities going to zero such that the limit  $\lim_{\Delta x \rightarrow 0, \Delta t \rightarrow 0} (\Delta x)^2 / \Delta t$  is finite. Furthermore, we assume  $A(x) + B(x) = 1$ . Note that the limit in equation (22a) exists as  $A(x - \Delta x) - B(x + \Delta x) = O(\Delta x)$  under the assumption that the inhomogeneity in jumping left or right follows the Boltzmann distribution for the potential  $\Phi(x)$ . We now consider the non-local analogue of the master equation (19), and its continuum limit.

### 3.2 Non-local jump statistics – Continuous space

Equation (19) for discrete but non-local jumps takes on the form

$$W_j(t + \Delta t) = \sum_{n=1}^{\infty} A_{j,n} W_{j-n}(t) + \sum_{n=1}^{\infty} B_{j,n} W_{j+n}(t), \quad (23)$$

so that jumps from all other sites  $j \mp n$  to the site  $j$  are possible. The transition matrix elements underlie the normalisation condition  $\sum_{n=1}^{\infty} (A_{j,n} + B_{j,n}) = 1$  accounting for the long-range jumps. For the continuum limit of equation (23), we note that the Taylor expansion in orders of  $\Delta x$  no longer converges. To find an alternative procedure to take the continuum limit, we employ the idea of a direction-dependent, but still site-independent jump length distribution  $\lambda^{\pm}(x) = \lambda^+(x)\Theta(x) + \lambda^-(x)\Theta(-x)$ , introduced in reference [22] to study anomalous diffusion in a constant force field, where  $\Theta(x)$  denotes Heaviside's jump function. Thus, if  $\lambda^+(x) \neq \lambda^-(x)$ , the jump is biased, *i.e.*, there is a preference for either direction.

An explicitly space-dependent force  $F(x)$  acting upon the system, the symmetry of the homogeneous random walk concept is broken, and each jump is characterised by a *local* preference of a certain direction in space: as the external field is space-dependent, the jump length pdf shows a direction-preference depending on the position of the departure position  $x'$ . We assume a site-dependent transfer distribution of the form

$$\Lambda(x, x') \equiv \lambda(x - x') \left( A(x')\Theta(x - x') + B(x')\Theta(x' - x) \right), \quad (24)$$

*i.e.*, we assume the statistical independence of the local asymmetry due to the external field which is expressed through the coefficients  $A(x')$  and  $B(x')$ , from the jump length pdf  $\lambda(x)$  which accounts for the transfer distance between departure and arrival site. That means that we assume the functional form  $\Lambda(x, x') = \Lambda(x - x' | x')$  for the transfer function  $\Lambda(x, x')$  on which we impose the normalisation condition

$$\int_{-\infty}^{\infty} d\delta \Lambda(x, \delta) = 1 \quad (25)$$

which is equivalent to requiring  $A(x) + B(x) = 1$ . Then, the continuum version of equation (23) is given through

$$W(x, t + \Delta t) = \int_{-\infty}^{\infty} dx' \Lambda(x, x') W(x', t). \quad (26)$$

In Fourier space, the corresponding equation reads

$$W(k, t + \Delta t) = \lambda_{\mathcal{C}}(k) W(k, t) + i\lambda_{\mathcal{S}}(k) \left\{ [A(k) - B(k)] * W(k, t) \right\} \quad (27)$$

where the Fourier convolution denoted by  $*$  is to be taken within the braces  $\{\cdot\}$  [33]. The indices  $\mathcal{C}$  and  $\mathcal{S}$  denote the Fourier cosine and sine transformation according to the definitions

$$f_{\mathcal{C}} \equiv 2 \int_0^{\infty} dx f(x) \cos(x), \quad f_{\mathcal{S}} \equiv 2 \int_0^{\infty} dx f(x) \sin(x) \quad (28)$$

where we introduce the factor 2 for sake of the normalisation (25) of the transfer function  $\Lambda(x, x')$ .

### 3.3 Memory effects – Continuous time

To include also the memory effects governed by the waiting time pdf  $w(t)$  which account for a distribution of waiting times, we consider the continuous time master equation for a discrete space [9, 10, 32]:

$$W_j(t) = \int_0^t d\tau \left( A_{j-1} W_{j-1}(\tau) + B_{j+1} W_{j+1}(\tau) \right) w(t - \tau) + \Psi(t) \delta_{j,m} \quad (29)$$

with the initial concentration  $W_j(0) = \delta_{j,m}$  at the site  $m$ , where  $\delta_{j,m}$  denotes the Kronecker symbol. The explicit occurrence of the initial value is due to the possibility of staying at the initial site according to the cumulative probability

$$\Psi(t) = 1 - \int_0^t dt' w(t'). \quad (30)$$

Proceeding along the same steps as introduced in Section 3.2, the continuous space version of equation (29) is given through

$$W(x, t) = \int_{-\infty}^{\infty} dx' \int_0^t d\tau w(t - \tau) \Lambda(x' | x - x') W(x', \tau) + \Psi(t) W_0(x), \quad (31)$$

which can be rewritten in Fourier-Laplace space in the form

$$uW(k, u) - W_0(k) = uw(u) \left\{ \Lambda(k) * W(k, u) \right\} - w(u) W_0(k), \quad (32)$$

from which it is easy to verify that equation (31) is equivalent to the GME (1) with the kernel

$$\mathfrak{K}(x, x'; u) = \frac{u\Lambda(x, x') - \delta(x)}{1 - w(u)} w(u). \quad (33)$$

Equation (31), or the GME (1) with the kernel (33) are general expressions which have been derived from the generalised, non-homogeneous random walk scheme. In the following subsections, we show how the FFPE (5) emerges from this concept.

### 3.4 Subdiffusion in an external field

Subdiffusion is described by the combination of a broad waiting time distribution of the one-sided Lévy type  $w(t) = L_\gamma^+$  whose asymptotic behaviour follows

$$w(t) \sim \tau^\gamma / t^{1+\gamma}, \quad 0 < \gamma < 1, \quad (34)$$

and whose long-time limit reads [4]

$$w(u) \sim 1 - (u\tau)^\gamma \quad (35)$$

in Laplace space, with a narrow (for instance, Gaussian) jump length distribution leading to

$$\lambda_C \sim 1 - \sigma^2 |k|^2 \quad (36)$$

and

$$\lambda_S(k) \sim \sigma k, \quad (37)$$

compare Section 5, equation (61a) *et seq.*, so that we obtain from equation (32), in the diffusion limit ( $k \rightarrow 0$ ,  $u \rightarrow 0$ ) and after some manipulations, the algebraic relation

$$W(k, u) - \frac{W_0(k)}{u} = u^{-\gamma} L_{\text{FP}}(k) W(k, u), \quad (38)$$

with the Fourier space equivalent of the FP-operator from equation (2b),  $L_{\text{FP}}(k)$ . Fourier-Laplace inversion leads to the FFPE

$$W(x, t) - W_0(x) = {}_0D_t^{-\gamma} L_{\text{FP}} W(x, t). \quad (39)$$

In the last step, we employed the property

$$\mathcal{L}\left\{{}_0D_t^{-\gamma} W(x, t)\right\} = u^{-\gamma} W(x, u) \quad (40)$$

of the Riemann-Liouville operator defined in equation (10). Applying the differential operator  $\frac{\partial}{\partial t}$  on equation (39), we retrieve the FFPE

$$\frac{\partial W}{\partial t} = {}_0D_t^{1-\gamma} L_{\text{FP}} W(x, t) \quad (41a)$$

with the FP-operator

$$L_{\text{FP}} = \left( \frac{\partial}{\partial x} \frac{\Phi'(x)}{m\eta_\gamma} + \frac{\partial^2}{\partial x^2} K_\gamma \right) \quad (41b)$$

and the coefficients [34]

$$\frac{\Phi'(x)}{m\eta_\gamma} \equiv \frac{\sigma}{\tau^\gamma} [B(x) - A(x)] \quad (42a)$$

$$K_\gamma \equiv \frac{\sigma^2}{\tau^\gamma}. \quad (42b)$$

### 3.5 Interplay between fractal time and Lévy flights in an external field

In Section 3.4 we showed the generalisation of the FPE (3) to subdiffusion. We now show how Lévy-type jump length statistics come into play. Therefore (compare Sect. 5), we assume a broad jump length statistics of the form  $\lambda_C(k) \sim 1 - \sigma^\mu |k|^\mu$  and  $\lambda_S(k) \sim \frac{2}{\mu} \sigma k$  with the Lévy index  $\mu \in (1, 2]$ . Combining these transfer statistics with the results (32) *et seq.*, we arrive at the FFPE (5), involving the coefficients

$$\frac{\Phi'(x)}{m\eta_\gamma} \equiv \frac{2\sigma}{\mu\tau^\gamma} [B(x) - A(x)] \quad (43a)$$

$$K_\gamma^\mu \equiv \frac{\sigma^\mu}{\tau^\gamma}. \quad (43b)$$

The FFPE (5) is the general version of an FFPE which can be derived from our modified CTRW scheme in the long time limit. Note that whereas the diffusion term now includes the Riesz-Weyl operator  ${}_{-\infty}D_x^\mu$  generalising the second-order derivative, the first order derivative in the drift term is not changed, see Section 5. Note that for  $\mu < 2$ , the mean squared displacement diverges. This is unphysical for a massive particle in direct space, it might however be meaningful for certain processes such as diffusion in energy space, as encountered in the modelling of single molecule spectroscopy.

## 4 Physical properties and solutions of fractional Fokker-Planck equations

### 4.1 Subdiffusion in an external field: Fractional Fokker-Planck equation close to thermal equilibrium

Let us consider the (normalised) FFPE (41a) which describes subdiffusion in the external potential field  $\Phi(x)$ . It can be shown that equation (41a) relaxes towards the Boltzmann equilibrium

$$W_{\text{st}}(x) \propto \exp\left(-\frac{\Phi(x)}{k_B T}\right) \quad (44)$$

where  $k_B T$  denotes the Boltzmann temperature and  $W_{\text{st}} \equiv \lim_{t \rightarrow \infty} W(x, t)$  is the stationary solution fulfilling the classical stationarity condition  $\frac{\partial W}{\partial t} \stackrel{!}{=} 0$ . In thermal equilibrium, one can derive the generalised Einstein-Stokes relation [23, 35, 40]

$$K_\gamma = \frac{k_B T}{m\eta_\gamma} \quad (45)$$

for the generalised diffusion and friction constants,  $K_\gamma$  and  $\eta_\gamma$ . One can show further that equation (41a) fulfils the second Einstein relation for the constant force  $F$  [23],

$$\langle x(t) \rangle_F = \frac{1}{2} \frac{F \langle x^2(t) \rangle_0}{k_B T}, \quad (46)$$

connecting the first moment in presence of the force with the second moment in absence of  $F$ :

$$\langle x^2(t) \rangle_0 = \frac{2K_\gamma}{\Gamma(1+\gamma)} t^\gamma. \quad (47)$$

#### 4.2 Lévy flights and subdiffusion in competition

The general FFPE (5) which we derived from our random walk formalism, involves a fractional operator in both space and time. The time-fractional Riemann-Liouville operator  ${}_0D_t^{1-\gamma}$  accounts for the non-Markovian nature of the transport process, whereas the space-fractional Riesz derivative  ${}_{-\infty}D_x^\mu$  emanates due to the assumption of long-range jumps typical for Lévy flights. Equation (5) can be solved by the separation ansatz [3]

$$W_n(x, t) = T_n(t)\varphi_n(x) \quad (48)$$

for a given mode  $n$  corresponding to the eigenvalue  $\lambda_{n,\gamma}$ . A single mode then relaxes according to the Mittag-Leffler pattern of the temporal eigensolution

$$T_n(t) = E_\gamma(-\lambda_{n,\gamma}t^\gamma) \equiv \sum_{l=0}^{\infty} \frac{(-\lambda_{n,\gamma}t^\gamma)^l}{\Gamma(1+\gamma l)} \quad (49)$$

which has the power-law asymptotic behaviour  $T_n(t) \sim 1/[t^\gamma \lambda_{n,\gamma} \Gamma(1-\gamma)]$ . For  $\gamma = 1$ ,  $E_1(-\lambda_{n,1}t) = \exp(-\lambda_{n,1}t)$ , and we recover the exponential relaxation of the modes typical for the Brownian FPE (3).

The spatial eigensolution for a given mode is governed by the ordinary (fractional) differential eigenequation

$$L_{\text{FFP}}\varphi_n(x) = -\lambda_{n,\gamma}\varphi_n(x). \quad (50)$$

Thus, for the stationary solution of a Lévy flight in the harmonic potential  $\Phi(x) = \frac{1}{2}\omega^2x^2$ , we find the Lévy stable law [19]

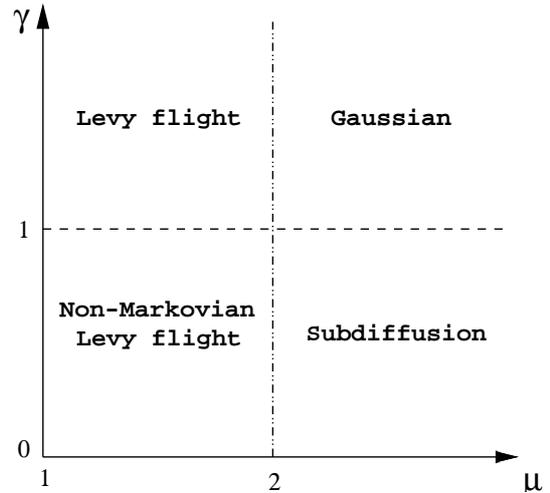
$$W_{\text{st}}(k) = \exp\left(-\frac{\eta_1 m K_1^\mu |k|^\mu}{\omega^2 \mu}\right) \quad (51)$$

in Fourier space, with the corresponding asymptotic behaviour

$$W_{\text{st}}(x) \sim \frac{\eta_1 m K_1^\mu}{\omega^2 \mu |x|^{1+\mu}}. \quad (52)$$

Thus, for  $\mu < 2$ , the FFPE (5) describes systems off thermal equilibrium, and the spatial solution for a given mode  $n$  is governed by a stable law, whereas its relaxation follows the non-exponential, slow Mittag-Leffler pattern. Consequently, for  $\mu < 2$  in equation (5), no generalisation of the Einstein relations like equations (45) and (46) can be found, furthermore the mean square displacement diverges:

$$\langle x^2(t) \rangle = \infty, \quad (53)$$



**Fig. 1.** “Phase diagram” of the diffusion properties of the fractional Fokker-Planck equation (5). The parameter space is spanned by the waiting time index  $\gamma$  and the Lévy index  $\mu$  of the jump length distribution. If  $\gamma > 1$ , a characteristic waiting time  $T$  exists, and the resulting motion locks on the Poissonian limit. In the same way, for  $\mu > 2$ , the jump length variance  $\Sigma^2$  exists, see reference [18]. Compare also to Table 1.

a typical feature of Lévy flights [2–4,9,32]. Only lower-order fractional moments  $\langle |x|^\beta(t) \rangle$  with  $\beta < \mu$  can be calculated [4,19]. For the force-free case, these are

$$\langle |x|^\beta(t) \rangle \propto t^{\beta\gamma/\mu} \quad (54)$$

which can be obtained through a cutoff-parameter [2,17–19] which is equivalent to the calculation of the time-broadening of a given percentage of the total probability [19], or through scaling relations [17,18]. We summarise the diffusion properties in the “phase diagram” drawn in Figure 1.

The properties of the FFPE (5) in respect to the existence or divergence of the characteristic waiting time

$$T \equiv \int_0^\infty dt w(t)t \quad (55)$$

or the jump length variance

$$\Sigma^2 \equiv \int_{-\infty}^\infty dx \lambda(x)x^2 \quad (56)$$

are summarised in Table 1.

#### 4.3 Comparison to results in literature

The general result of our derivation, the FFPE (5), is equivalent to several FFPEs discussed in literature. For  $\mu = 2$ , it was used for the description of subdiffusive systems close to thermal equilibrium in reference [23]. For the Markovian case  $\gamma = 1$  the Lévy flight in different potential types was solved and discussed in reference [19].

**Table 1.** Summary of the physical properties of the fractional Fokker-Planck equation (5), characterised through the existence/divergence of the characteristic waiting time  $T$  and the jump length variance  $\Sigma^2$ .

	$\Sigma^2 < \infty$	$\Sigma^2 = \infty$
$T < \infty$	$\langle x^2(t) \rangle = 2K_1 t$ $K_1 = \frac{k_B T}{m\eta_1}$ $T_n(t) = e^{-\lambda_n t}$	$\langle  x ^\beta(t) \rangle \propto t^{\beta/\mu}, \beta < \mu$ $\cdot / \cdot$ $T_n(t) = e^{-\lambda_n t}$
$T = \infty$	$\langle x^2(t) \rangle = \frac{2K_\gamma}{\Gamma(1+\gamma)} t^\gamma$ $K_\gamma = \frac{k_B T}{m\eta_\gamma}$ $T_n(t) = E_\gamma(-\lambda_n t^\gamma)$	$\langle  x ^\beta(t) \rangle \propto t^{\beta\gamma/\mu}, \beta < \mu$ $\cdot / \cdot$ $T_n(t) = E_\gamma(-\lambda_n t^\gamma)$

The Riemann-Liouville operator  ${}_0D_t^{1-\gamma}$  describes physical systems which were prepared at  $t_0 = 0$ . On the other hand, systems are often prepared at a very remote time, so that one can assume  $t_0 = -\infty$ . Then the Riemann-Liouville operator is replaced by the so-called Weyl fractional operator  ${}_{-\infty}D_t^{1-\gamma}$ , compare [28]. In this case, the FFPE (5) is equivalent to the equations derived in references [17, 18] from a generalised Langevin equation approach. The FFPE proposed by Zaslavsky and coworkers [21] is of a different type which is briefly discussed in the following Section 5.

It is interesting to note that a Fourier space equation which is equivalent to equation (5) for  $\gamma = 1$  was derived in reference [36].

## 5 Generalised Kramers-Moyal expansion

The FPE (3) is a special case of the Kramers-Moyal (KM) expansion which foost on an expansion of the distribution function

$$P(x, t + \tau | x', t) = \int dy \delta(y - x) P(y, t + \tau | x', t) \quad (57)$$

where  $P$  denotes the transition probability from  $x'$  to  $x$  during time  $\tau$ . With the formal expansion

$$\delta(y - x) = \sum_{n=0}^{\infty} \frac{(y - x)^n}{n!} \left( -\frac{\partial}{\partial x} \right)^n \delta(x' - x) \quad (58)$$

one can derive the KM-expansion [11, 12]

$$\frac{\partial W}{\partial t} = \sum_{n=1}^{\infty} \left( -\frac{\partial}{\partial x} \right)^n D^{(n)}(x) W(x, t). \quad (59)$$

$D^{(1)}(x)$  and  $D^{(2)}(x)$  are the drift and diffusion coefficients, respectively. The sum in equation (59), according to the Pawula theorem, stops either after the first or the second term, or it includes an infinite number of terms [37]. For a Gaussian,  $\delta$ -correlated noise in the underlying Langevin equation, all terms of order 3 and higher vanish; consequently in this case, the KM-expansion is equivalent to the

FPE [11]. For the following, note that the KM-expansion can be obtained from the master equation (19) by taking along all orders in the Taylor expansions (20) and (21).

Here we want to investigate the analogue to the KM-expansion (59) in our generalised random walk model. Therefore, we first calculate the higher order expansion terms for the cosine and sine transforms of the jump length distributions  $\lambda$  from which we will infer the generalised KM-expansion. To this end, we start off from the symmetric and centred stable law  $p(x) = L_\mu(x)$  of Lévy index  $\mu \in (1, 2]$ , the characteristic function of which is given by [4]

$$p(k) = e^{-\sigma^\mu |k|^\mu}. \quad (60)$$

In  $x$  space, an exact representation can be given in terms of Fox's  $H$ -functions [38]:

$$p(x) = \frac{1}{\sqrt{4\pi\mu^2\sigma^2}} H_{1,2}^{1,1} \left[ \frac{|x|}{2\sigma} \left| \begin{matrix} \left(1 - \frac{1}{\mu}, \frac{1}{\mu}\right) \\ \left(0, \frac{1}{2}\right); \left(\frac{1}{2}, \frac{1}{2}\right) \end{matrix} \right. \right] \quad (61a)$$

$$= \frac{1}{\sqrt{\pi\mu^2\sigma^2}} \sum_{n=0}^{\infty} \frac{\Gamma([1+2n]/\mu)}{\Gamma(1/2+n)} \frac{(-1)^n}{n!} \left( \frac{|x|}{2\sigma} \right)^{2n} \quad (61b)$$

$$= \sum_{n=1}^{\infty} (-1)^{1+n} \frac{\Gamma(1+\mu n)}{n!} \sin\left(\frac{n\pi\mu}{2}\right) \left( \frac{2\sigma}{|x|} \right)^{1+\mu n} \quad (61c)$$

where the series expansions are valid for small  $|x|$  and large  $|x|$ , respectively. In the limit  $\mu \rightarrow 2$ , the usual Gaussian is recovered:  $p(x) = \frac{1}{\sqrt{4\pi\sigma^2}} \exp\left(-\frac{x^2}{4\sigma^2}\right)$ , as it should [4, 38].

For the calculations, according to equation (27), we need the one-sided Fourier cosine and sine transforms of the function  $p(x)$ . The cosine transform is given by

$$p_C(k) = e^{-\sigma^\mu |k|^\mu} \quad (62a)$$

$$\sim 1 - \sigma^\mu |k|^\mu + \frac{1}{2} \sigma^{2\mu} |k|^{2\mu} + \dots \quad (62b)$$

The sine transform results in [38, 39]

$$p_S(k) = \frac{2}{\mu} H_{2,3}^{2,1} \left[ \sigma^2 |k|^2 \left| \begin{matrix} \left(\frac{1}{2}, 1\right) \\ \left(\frac{1}{2}, 1\right), \left(0, \frac{2}{\mu}\right); (0, 1) \end{matrix} \right. \right] \quad (63a)$$

$$= 2\sigma k \sum_{n=1}^{\infty} \frac{(-1)^{n+1} \sin\left(\frac{\mu n \pi}{2}\right)}{2n! \sin\left(\frac{\pi}{2}[1+\mu n]\right)} (\sigma |k|)^{\mu n}$$

$$- 2\sigma k \sum_{n=0}^{\infty} \frac{\Gamma\left(-\frac{2n+1}{\mu}\right)}{\pi\mu} (\sigma |k|)^{2n}. \quad (63b)$$

For  $\mu = 2$ , the coefficients of the first sum vanish identically to zero, and only the uneven terms in powers of  $|k|$  of the second sum remain, adding up to the standard KM-expansion, together with the even terms from  $p_C$ .

In the general case  $0 < \mu < 2$ , if

$$\lambda_C(k) \equiv p_C(k), \quad \lambda_S(k) \equiv p_S(k). \quad (64)$$

denote the Fourier sine and cosine transforms of the jump length pdf, one obtains the generalisation of the KM-expansion from the fractional kinetic equation (compare Eq. (27))

$$\frac{\partial W}{\partial t} = {}_0D_t^{1-\gamma} \left( \lambda_C(k)W(k, t) + i\lambda_S(k) \left\{ [A(k) - B(k)] * W(k, t) \right\} \right) \quad (65)$$

where the Fourier convolution, denoted by the asterisk, is to be taken within the braces  $\{\cdot\}$  only. The result is the generalised KM-expansion

$$\begin{aligned} \frac{\partial W}{\partial t} = & {}_0D_t^{1-\gamma} \left[ \sum_{n=1}^{\infty} -{}_{\infty}D_x^{n\mu} D^{(n)}(x) \right. \\ & + \sum_{n=1}^{\infty} (-1)^n \frac{\partial}{\partial x} -{}_{\infty}D_x^{n\mu} \bar{D}^{(n)}(x) \\ & \left. + \sum_{n=0}^{\infty} (-1)^{1+n} \left( \frac{\partial}{\partial x} \right)^{1+2n} \tilde{D}^{(n)}(x) \right] W(x, t) \quad (66) \end{aligned}$$

with the coefficients

$$D^{(n)}(x) = \frac{\sigma^{n\mu}}{\tau^\gamma} [A(x) + B(x)] \quad (67a)$$

$$\begin{aligned} \bar{D}^{(n)}(x) = & \left( 1 - \delta_{2,\mu} \right) \frac{\sigma^{1+n\mu}}{\tau^\gamma} \\ & \times [A(x) - B(x)] \frac{\sin\left(\frac{n\mu\pi}{2}\right)}{2n! \sin\left(\frac{\pi}{2}[1+n\mu]\right)} \quad (67b) \end{aligned}$$

$$\tilde{D}^{(n)}(x) = \frac{\sigma^{1+2n}}{\tau^\gamma} [A(x) - B(x)] \frac{\Gamma\left(-\frac{1+2n}{\mu}\right)}{\pi\mu} \quad (67c)$$

where we made use of the Kronecker symbol  $\delta_{2,\mu}$ , and redefined the Riesz-Weyl fractional operator such that no imaginary coefficients occur, compare references [28, 31]. Overall, the pdf  $W(x, t)$  as defined through the generalised KM-expansion (66) is *real valued* as can be checked by explicitly inserting the defining integrals for the occurring Riesz-Weyl fractional derivatives, following Oldham and Spanier [28] and Samko *et al.* [31].

Note that in the full KM-expansion (66) no limit has to be taken, as the full Taylor expansion has to be included through the consideration of all terms in the series expansions (62b) and (63b). This fact leads to an understanding of the Pawula theorem: if not terminated after the second lowest derivative  $-{}_{\infty}D_x^\mu$ , it is impossible to properly define the limits, as only two small parameters exist which account for well-defined limits for  $(\Delta x)^2/\Delta t$ , or  $\sigma^\mu/\tau^\gamma$ .

Let us now discuss the generalised KM-expansion in more detail. At first it is apparent that both integer order and fractional order derivatives occur in equation (66). If the constraint  $A(x) + B(x) = 1$  is imposed, the KM-coefficients  $D^{(n)}$  will be constants, the lowest corresponding to the generalised diffusion constant  $K_\gamma^\mu$ . Higher order

diffusive terms all contain a multiple of the fractional operator order  $\mu$ . At the same time, the drift terms are characterised through the difference  $A(x) - B(x) \propto -\Phi'(x)$ . These terms come in both integer order and fractional order derivatives. However, and this is a crucial point, the lowest order derivative of these terms for any index  $\mu \geq 1$ , *i.e.*, the drift term, is *always* given through  $\propto \partial/\partial x \Phi'(x)W$ . Consequently, in the Markovian case  $\gamma = 1$ , the typical response of the stochastic system to a linear force  $f_0$  in terms of the linearly growing drift

$$\langle x(t) \rangle = f_0 t \quad (68)$$

is *preserved*<sup>1</sup>. For  $\gamma < 1$ , this relation is modified to  $\langle x(t) \rangle = f_{0,\gamma} t^\gamma$ , where  $[f_{0,\gamma}] = \text{sec}^{-\gamma}$ .

If we do not impose the constraint  $A(x) + B(x) = 1$ , the coefficients  $D^{(n)}$  will be position dependent, *i.e.*, the corresponding FFPE is the fractional extension of equation (3). Also, the normalisation condition of the transfer function has to be replaced by:  $\int d\delta \int dx \Lambda(x, \delta) / \int dx [A(x) + B(x)]$ . It is still clear that the coefficients  $D^{(n)}$  describe the diffusive part of the transport process, as they involve the *sum* of the asymmetry functions  $A(x)$  and  $B(x)$ . Thus, for  $0 < \mu < 1$ , the situation occurs that the diffusion term  $\propto -{}_{\infty}D_x^\mu D^{(1)}W$  is of lower order than the drift term  $\propto \partial/\partial x \Phi'(x)W$ . However, the drift is still the lowest order term containing the external potential, *i.e.*, the difference of the asymmetry functions. Also in this case, the drift character is thus securely connected to the first order derivative  $\partial/\partial x$ . Note that for  $\mu = 1$ , *i.e.*, the Cauchy propagator in the force-free case, both drift and diffusion term are of the same order.

The fundamental result of our extended Kramers-Moyal expansion (66) is accordingly that the lowest order force term involves an *integer-order* derivative  $\frac{\partial}{\partial x}$ . This is in accordance to the derivation of Fogedby [17, 18], compare also reference [19]. Quintessentially, it mirrors the *additivity* of the overall drift and the diffusive contribution. In the non-Markovian case, this additivity is underlined by the fact that both drift and diffusion terms are under the fractional time operator which can be understood from the derivation of these equations from the fundamental Chapman-Kolmogorov equation in phase space, see reference [40].

The observation for the drift preservation is different from the alternative derivation by Zaslavsky *et al.* [21] in the context of Hamiltonian chaotic systems, who assume an expansion of the form  $P(x, y; t + \tau) = \delta(x - y) + A(y; \tau)\delta^{(\alpha)}(x - y) + \frac{1}{2}B(y; \tau)\delta^{(2\alpha)}(x - y) \dots$ ,  $0 < \alpha \leq 1$ , a generalisation of equation (58) which leads to an FFPE of the form  $\frac{\partial^\beta W(x, t)}{\partial t^\beta} = \frac{\partial^\alpha}{\partial (-x)^\alpha} [\mathcal{A}W(x, t)] + \frac{\partial^{2\alpha}}{\partial (-x)^{2\alpha}} [\mathcal{B}W(x, t)]$  where the generalised drift term contains an  $\alpha$ th order derivative. (Note that the fractional operators  $\frac{\partial^\beta}{\partial t^\beta}$  and  $\frac{\partial^\alpha}{\partial (-x)^\alpha}$  are defined in a slightly different way to our definition of the Riemann-Liouville and Riesz

<sup>1</sup> Note that for  $0 < \mu \leq 1$ , the first moment  $\langle x(t) \rangle$  exists whereas the mean of the absolute value of  $x$ ,  $\langle |x(t)| \rangle$ , diverges.

fractional operators, which is irrelevant for the comparison.) This is a fundamentally different result and might be understood in the light of the recent derivation of an FFPE from a broadly distributed subordination process in reference [41].

## 6 Conclusions

Fokker-Planck equations belong to the fundamental equations in the physics of stochastic processes. We have demonstrated how apparently different approaches for the description of anomalous diffusion, with or without an external potential field, can be understood from a generalised master equation. To account for the broken symmetry of homogeneity, paramount for the standard CTRW scheme, we introduced a site-dependent jump length distribution. Fractional operators in space and time were shown to arise from slowly decaying transfer kernels. More specific, a diverging characteristic waiting time  $T$  leads to a fractional operator  ${}_0D_t^{1-\gamma}$ , whereas a diverging jump length variance  $\Sigma^2$  gives rise to the fractional Riesz-Weyl operator  ${}_{-\infty}D_x^\mu$  in space. By this representation through the fractional operators, it is clear, that the FFPEs are convolution integral equations.

We derived the generalised Kramers-Moyal expansion for processes that involve Lévy stable jump length distributions leading to  $\Sigma^2 \rightarrow \infty$ . In this case, it was shown that the KM-expansion leads to mixed integer and fractional orders in the belonging spatial derivatives, but that the drift term is always associated with a first order derivative. Accordingly, the classical definition of a drift also applies to Lévy flight systems. From the associated random walk approach it is obvious that an analogous version of the Pawula theorem holds for these kind of processes.

It should finally be stressed once more that the generalised FPEs we derived in this work are *linear* fractional differential equations. Thus, the result from our probabilistic approach is fundamentally different from the non-linear generalisations of the FPE found in the theory of generalised thermostatistics, see for example references [42]. The equilibrium distributions reached by the processes associated with the FFPEs discussed herein, are of the Boltzmann type in the case  $\mu = 2$ , only. For Lévy flights, it has been shown that the stationary distribution reached is Lévy stable, and thus far off the Boltzmann equilibrium state, see the discussions in references [19, 23]. This sets the presented approach apart from the one pursued in the recent reference [41].

Discussions with Yossi Klafter, Eli Barkai and Peter Wolynes are gratefully acknowledged. Financial support from the TMR programme of the European Commission (SISITOMAS), the German-Israeli foundation (GIF), the Alexander von Humboldt Stiftung, Bonn am Rhein, the Minerva foundation, and the Deutsche Forschungsgemeinschaft are acknowledged as well.

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