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Superdiffusive Klein-Kramers equation: Normal and anomalous time evolution and Lévy walk moments

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Abstract. – We introduce a fractional Klein-Kramers equation which describes sub-ballistic superdiffusion in phase space in the presence of a position-dependent external force field. This equation defines lower-order moments of Lévy walks which take place in the presence of an external force field and in phase space. In the velocity coordinate, the probability density relaxes in Mittag-Leffler fashion towards the Maxwell distribution whereas in the position coordinate, no stationary solution exists and the temporal evolution of moments exhibits a competition between Brownian and anomalous contributions.

Classically, Brownian stochastic transport processes are described by the deterministic Fokker-Planck equation which controls the temporal approach to the Gibbs-Boltzmann equilibrium [1,2]. In the force-free case Brownian transport is characterised through the Gaussian probability density function (pdf) and the linear time dependence $\langle x^2(t)\rangle = 2Kt$ of the mean-squared displacement in the force-free diffusion limit, its universality being guaranteed by the central-limit theorem [2,3]. In a broad variety of systems, however, it has been found that correlations in space or time give birth to *anomalous* transport whose pdf is non-Gaussian and/or whose mean-squared displacement is non-linear in time [3]. These systems include charge carrier transport in amorphous semiconductors [4], tracer dispersion in convection rolls and rotating flows [5,6], capillary surface waves [7], the motion of bacteria and the flight of an albatross [8], intracellular transport [9], transport in micelles [10], 2D dusty plasmas [11], the dynamics in (bio)polymeric systems [12], and the NMR diffusometry in porous glasses and percolation clusters [13], among others.

The systems we are interested in fall into the broad class whose *force-free* diffusion behaviour is characterised through the power law form $\langle x^2(t)\rangle \propto t^{\varkappa}$, which separates into subdiffusion ($0 < \varkappa < 1$) and superdiffusion ($\varkappa > 1$). The continuous time random walk (CTRW) model has proved to be a well-suited framework which accounts for such anomalous diffusion for the entire spectrum of $\varkappa$ [14]. Especially in the sub-ballistic superdiffusive domain $1 < \varkappa < 2$, *Lévy walks* which couple long flight times with a time cost have been a successful tool [15, 16], *e.g.*, in fluid dynamics [6, 17]. The space-time coupling of Lévy walks leads to finite moments and they are therefore fundamentally different from Lévy flights which exhibit a diverging variance [18].

In the presence of external force fields, the CTRW approach is less flexible. It has been realised that fractional equations constitute a tailor-made framework to formulate the underlying dynamics equations in coordinate and phase space; see, for instance, [18–23] and references therein. In the subdiffusive domain $0 < \varkappa < 1$, fractional Fokker-Planck equations (FFPE) were introduced and investigated in considerable detail by several authors (*e.g.*, [19, 23–25], among others). These equations can be microscopically derived, and on the phenomenological level they appear as linear response theories for systems with long power law memory [25]. The approach based on a univariate fractional Fokker-Planck equation is not well suited for the description of superdiffusion, since it may fail to guarantee the non-negative probabilities in the presence of external forces, due to an inappropriate ensemble averaging procedure neglecting strong correlations between positions and velocities. In the following, we pursue an approach embedded in phase space.

Classically, Brownian stochastic transport processes in the phase space spanned by velocity v and position coordinate x are described by the deterministic Klein-Kramers equation (KKE). In the low and high friction limits, the KKE reduces to the Rayleigh equation which describes the relaxation of the velocity pdf towards the Maxwell distribution, and the Fokker-Planck-Smoluchowski equation controlling the temporal approach of the Gibbs-Boltzmann equilibrium, respectively [2, 26]. In the subdiffusive domain $0 < \varkappa < 1$, a fractional KKE was derived from the Chapman-Kolmogorov equation [27]. The question for a similar consistent generalisation to systems in the regime $1 < \varkappa < 2$ is still open. In this note, we propose the fractional KKE

$$\frac{\partial P}{\partial t} = \left(-\frac{\partial}{\partial x}v - {}_0D_t^{1-\alpha}\varrho_\alpha\left[-\gamma\frac{\partial}{\partial v}v + \frac{F(x)}{m}\frac{\partial}{\partial v} - \kappa\frac{\partial^2}{\partial v^2}\right]\right)P(x,v,t),\ 0<\alpha<1 \qquad (1)$$

for the description of sub-ballistic superdiffusive anomalous transport. In particular, eq. (1) describes the lower-order moments of Lévy walk processes in phase space and in the presence of the external force $F(x)$, see below. In eq. (1), $P(x,v,t)\mathrm{d}x\mathrm{d}v$ is the joint probability to find the test particle of mass m with coordinate $x,\ldots,x+\mathrm{d}x$ and velocity $v,\ldots,v+\mathrm{d}v$ at time t. γ denotes the friction constant which quantifies the effective dissipative interaction with the environment, κ is the velocity diffusion constant and $F(x) = -\mathrm{d}\Phi(x)/\mathrm{d}x$ is an external force field. The factor ϱ_α has dimension $[\varrho_\alpha] = \mathrm{s}^{-\alpha}$ and is a function of some time scale τ characteristic for the waiting-time process and of an interaction time scale τ^* [27]. In the limit $\alpha = 1$, eq. (1) corresponds to the standard KKE whereas for $0 < \alpha < 1$, the process contains a scale-free memory of the power law type entering through the fractional Riemann-Liouville operator ${}_0D_t^{1-\alpha} \equiv \partial/\partial t\big({}_0D_t^{-\alpha}\big)$ with [28, 29]

$${}_0D_t^{-\alpha}W(v,t) \equiv \frac{1}{\Gamma(\alpha)}\int_0^t \mathrm{d}t' W(v,t')(t-t')^{\alpha-1}. \qquad (2)$$

The operator ${}_0D_t^{-\alpha}$ possesses the important property $\int_0^\infty e^{-ut}\,{}_0D_t^{-\alpha}f(t) = u^{-\alpha}f(u)$ under Laplace transformation.

With respect to its position coordinate x, eq. (1) is a Liouville-type equation which gives rise to the relation $\frac{\mathrm{d}}{\mathrm{d}t}\langle\langle x(t)\rangle\rangle = \langle\langle v(t)\rangle\rangle$ between the velocity- and position-averaged random variables x and v; by this, the KKE (1) differs fundamentally from the subdiffusive model in ref. [27]. The action of the friction, force and velocity diffusion in eq. (1) enters through the non-local memory relation brought about by the fractional operator; *i.e.*, the local fluctuations of velocity which follow from a Fokker-Planck–like equation in the Brownian case are now described by a fractional Fokker-Planck equation. The connection to the position coordinate is assumed to be given through the classical drift term $-\partial vP/\partial x$. From these basic physical assumptions, the fractional KKE (1) emerges.

Let us explore the behaviour predicted by eq. (1) in more detail. By integration over the spatial coordinate x, the fractional equation for the velocity pdf $P(v,t)$

$$\frac{\partial P}{\partial t} = {}_0D_t^{1-\alpha}\varrho_\alpha \left(\gamma\frac{\partial}{\partial v}v - \frac{F(x)}{\gamma m}\frac{\partial}{\partial v} + \kappa\frac{\partial^2}{\partial v^2}\right)P(v,t) \tag{3}$$

obtains which reduces to its Brownian counterpart in the limit $\alpha = 1$.

In the force-free limit, eq. (3) corresponds to the fractional Rayleigh equation discussed in refs. [27,30]. The relaxation of velocity moments can be inferred directly from eq. (3) in the force-free case. Accordingly, the fractional relaxation equation [18,31]

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\langle v(t)\rangle = -\gamma_\alpha\, {}_0D_t^{1-\alpha}\langle v(t)\rangle \tag{4}$$

emerges, where $\gamma_\alpha \equiv \varrho_\alpha\gamma$. For $v_0 = v(0)$, its solution

$$\langle v(t)\rangle = v_0 E_\alpha\left(-\gamma_\alpha t^\alpha\right) \tag{5}$$

features the Mittag-Leffler function $E_\alpha\left(-\gamma_\alpha t^\alpha\right) \equiv \sum_{n=0}^{\infty}\left(-\gamma_\alpha t^\alpha\right)^n/\Gamma(1+\alpha n)$ which is monotonically decaying and which interpolates between the initial stretched exponential behaviour $E_\alpha\left(-\gamma_\alpha t^\alpha\right) \sim \exp\left[-\gamma_\alpha t^\alpha/\Gamma(1+\alpha)\right]$ and the final inverse power law pattern $E_\alpha\left(-\gamma_\alpha t^\alpha\right) \sim \left(\gamma_\alpha t^\alpha\Gamma(1-\alpha)\right)^{-1}$ [32]. Thus, the mean relaxation time diverges. The second moment

$$\langle v^2(t)\rangle = \kappa/\gamma + (v_0^2 - \kappa/\gamma)E_\alpha\left(-2\gamma_\alpha t^\alpha\right) \tag{6}$$

relaxes in Mittag-Leffler fashion towards the equilibrium value κ/γ, and the pdf $P(v,t)$ equilibrates towards a Gaussian. In this respect our model differs considerably from the fractional KKEs proposed in refs. [20–22] in which the superdiffusive process is due to the Lévy-distributed fluctuations in velocity. In thermodynamical systems, by comparison, the velocity pdf follows the Maxwell distribution $P(v) = (2\pi k_\mathrm{B}T/m)^{-1/2}\exp\left[-mv^2/[2k_\mathrm{B}T]\right]$, the exact stationary solution of eq. (3), so that we find the Einstein relation $\kappa = k_\mathrm{B}T\gamma/m$ [18,19]. The velocity-velocity correlation function associated with eq. (3) is

$$\langle v(0)v(t)\rangle = v_0^2 E_\alpha\left(-\gamma_\alpha t^\alpha\right) \sim v_0^2\left(\gamma_\alpha t^\alpha\right)^{-1}, \tag{7}$$

whose long-time behaviour is equivalent to the CTRW-Lévy walk result where the $t^{-\alpha}$-scaling follows from the behaviour of the cumulative waiting-time distribution. The difference between the two processes corresponds to the fact that the distribution of the velocities in a genuine Lévy walk is bimodal, while in our case it is Gaussian (Maxwell).

This observation corresponds to the physical model underlying eq. (1): in the velocity space, we assume that the particle undergoes collisions, *i.e.*, random velocity changes, such that successive collisions are separated by time spans governed through the long-tailed waiting-time pdf $\psi(\mathfrak{t}) \sim A_\alpha(\mathfrak{t}/\tau)^{-1-\alpha}$, whose characteristic time $\mathfrak{T} = \int_0^\infty \mathfrak{t}\psi(\mathfrak{t})\mathrm{d}\mathfrak{t}$ diverges. In this case, the velocity-velocity correlation function is proportional to the probability that no scattering took place before time t, and thus $\langle v(0)v(t)\rangle = v_0^2\int_t^\infty \psi(\mathfrak{t})\mathrm{d}\mathfrak{t} \propto v_0^2(t/\tau)^{-\alpha}$. The characteristic behaviour of this model is that it includes arbitrarily long sojourns but leads to finite moments of any order and an exponentially decaying pdf P. We note that due to these properties the fractional KKE (1) is an approximation to genuine Lévy walks which offers the distinct possibility to study the effects of an external force field on the behaviour of lower-order moments of a Lévy walk. This statement becomes more transparent in the position space behaviour predicted by eq. (1).

The velocity average of the fractional KKE (1) can be performed by integration over $\int \mathrm{d}v$ and $\int v\mathrm{d}v$, and combination of the two resulting equations. With $\langle v^2\rangle = k_\mathrm{B}T/m$, this procedure yields the fractional telegrapher's type equation

$$\frac{1}{\gamma_\alpha}\frac{\partial^2 P}{\partial t^2} + {}_0D_t^{2-\alpha}P = \left(-{}_0D_t^{1-\alpha}\frac{\partial}{\partial x}\frac{F(x)}{\gamma m} + K\frac{\partial^2}{\partial x^2}\right)P(x,t)\,, \tag{8}$$

with $K \equiv k_\mathrm{B}T/(m\gamma_\alpha)$, which exhibits a transition from a short-time ballistic behaviour with $\langle x^2(t)\rangle \sim (K\gamma)t^2$ in the force-free case, to the long-time or high-friction limit governed through the fractional Fokker-Planck-Smoluchowski equation

$$\frac{\partial P}{\partial t} = \left(-\frac{\partial}{\partial x}\frac{F(x)}{\gamma m} + {}_0D_t^{\alpha-1}K\frac{\partial^2}{\partial x^2}\right)P(x,t). \tag{9}$$

Here, the difference to the fractional Fokker-Planck equation for subdiffusive processes derived in ref. [23] lies in the temporally local connection between the drift term and the time derivative of P.

The mean-squared displacement corresponding to eq. (9) with $F(x) = 0$ is given through

$$\langle x^2(t)\rangle = 2Kt^{2-\alpha}/\Gamma(3-\alpha) \tag{10}$$

which describes sub-ballistic superdiffusion in analogy to Lévy walks [14]. It is in the presence of an external force that the fractional KKE (1) reveals interesting dynamical patterns. To this end, consider the fractional Fokker-Planck equation (9) for non-trivial types of the external force $F(x)$. Accordingly, the first moment is given by $\frac{\mathrm{d}}{\mathrm{d}t}\langle x(t)\rangle = \langle F(x)\rangle/(m\gamma)$ which can be solved for constant or linear forces. In particular, for the constant drift $F(x) = Vm\gamma$, the first moment becomes

$$\langle x(t)\rangle = Vt\,, \tag{11}$$

which corresponds to the traditional drift behaviour [2]. The second moment

$$\langle x^2(t)\rangle = V^2t^2 + 2Kt^{2-\alpha}/\Gamma(3-\alpha) \tag{12}$$

combines this drift with the sub-ballistic behaviour $\propto t^{2-\alpha}$ such that the variance $\langle \Delta x(t)^2\rangle \equiv (\langle x^2(t)\rangle - \langle x(t)\rangle^2)$ is given by eq. (10). This behaviour is analogous to the Galilei-invariant diffusion-advection model derived in ref. [33] for the subdiffusive case. In our case, the analytical solution is given by the free (superdiffusive) solution explored in detail in ref. [34], taken at the translated coordinate $x - Vt$. Here, the two-hump solution travels with velocity V and is symmetric to the point $X(t) = Vt$. It should be noted that due to the behaviour of the first and second moments, a connection of the form $\langle x(t)\rangle_V \propto V\langle x^2(t)\rangle_0$ (see, *e.g.*, refs. [18,19]) between the first moment in the presence of the constant drift V to the second moment in absence of this drift, does not exist, in contrast to the subdiffusive case [23]. Similarly, for the Ornstein-Uhlenbeck potential $\Phi(x) = \frac{1}{2}m\omega^2x^2$ which exerts the linear restoring force $F(x) = m\omega^2 x$, the first moment shows the exponential relaxation

$$\langle x(t)\rangle = x_0 e^{-\omega^2 t/\gamma}\,, \tag{13}$$

which contrasts the Mittag-Leffler patterns recovered in the subdiffusive model in ref. [27]. The second moment has the Laplace transform $\langle x^2(u)\rangle = (x_0^2 + 2Ku^{\alpha-2})/(u + 2\omega^2/\gamma)$ whose inversion leads to

$$\langle x^2(t)\rangle = x_0^2 e^{-2\omega^2 t/\gamma} + \frac{2Kt^{2-\alpha}}{\Gamma(3-\alpha)}\,{}_1F_1\left(1; 3-\alpha; -\frac{2\omega^2}{\gamma}t\right), \tag{14}$$

which combines the exponential relaxation of the initial condition x_0^2, which was already found for the first moment, with the confluent hypergeometric function ${}_1F_1$. Note that the second term in eq. (14) is equal to the expression $2Kt^{2-\alpha}E_{1,3-\alpha}\left(-2\omega^2 t/\gamma\right) = 2Kt^{2-\alpha}\cdot \sum_{n=0}^{\infty}\left(-2\omega^2 t/\gamma\right)/\Gamma(3-\alpha+n)$ in which we used the generalised Mittag-Leffler function $E_{1,3-\alpha}$ [32]. The variance is consequently given in terms of

$$\Delta x(t)^2 = 2Kt^{2-\alpha}E_{1,3-\alpha}\left(-2\omega^2 t/\gamma\right), \tag{15}$$

which interpolates between the freely diffusive behaviour (10) for short times, and the long-time power law pattern

$$\Delta x(t)^2 \sim \frac{K\gamma}{\omega^2}\frac{t^{1-\alpha}}{\Gamma(2-\alpha)}. \tag{16}$$

Accordingly, the mean-squared displacement $\Delta x(t)^2$ *increases* in the course of time even for long times, despite the restoring Ornstein-Uhlenbeck force. It is straightforward to show in general that the solution of the fractional Fokker-Planck-Smoluchowski equation (9) does not have a stationary solution. This is intuitively expected from a Lévy walk whose main characteristic is the continuous approximation to a Lévy stable distribution: only at infinite time, the Lévy walk has possibly accessed the entire space. Before, there are always large enough fluctuations by which additional regions can be explored, even against a confining potential. This typical Lévy walk property is associated with the sharp fronts given by the finite maximum velocity [14–16]. In our model, these fronts are blurred such that the position pdf falls off compressed Gaussian fashion for large $|x|$, but features distinct countermoving *humps*. This bimodal character was explored in detail in the enhanced diffusion approach reported in ref. [34] which corresponds to the force-free limit of eq. (9). Up to second order in the position coordinate, and to arbitrary order in the velocity coordinate, the FKKE (1) therefore describes the exact moments of a forced Lévy walk in phase space. The very combination of pseudo-Markoffian and anomalous properties in the moments calculated above demonstrate the *a priori* surprising richness of this process type which has not been realised before.

Formally, the fractional KKE (1) corresponds to the "Lévy rambling" model developed in ref. [27] but with the force entering symmetrically to friction and diffusion (*i.e.*, $\langle v\rangle = -\eta v\tau^* + F(x)\tau^*/m$ in eq. (62) of ref. [27]). In that sense, eq. (1) corresponds to an approximation to the Lévy walk model in which the particle undergoes continuous motion between scattering events which change the velocity coordinate. Friction and force remain events which enter through an effective time scale τ^*, *i.e.*, they correspond to point-like interactions in the long-time limit $t \gg \max\{\tau, \tau^*\}$. This gives rise to the fact that the spatial distribution does not reach an equilibrium state, or, in other words, that space and time do not decouple in the underlying eqs. (1) and (9) so that the variables x and t cannot be separated, also a typical property of CTRW-Lévy walks. Consequently, the identity $K \equiv k_B T/(m\gamma_\alpha)$ inherent in eq. (9) does not represent a generalised Einstein relation, as it is a non-equilibrium property.

How does our FKKE (1) compare to the previously proposed FKKE for superdiffusion from ref. [30]? Both models produce the same Mittag-Leffler relaxation towards the Maxwell distribution in v-space, and have identical form in the force-free case. However, it is the distinct behaviour in x-space in the presence of a non-trivial force which sets our new model equation apart from the previous approach: here, the behaviour in position space is a pronounced non-equilibrium process. Thus, the slow but incessant evolution of the position space distribution defined by eqs. (1) and (9) reflecting the non-equilibrium character of Lévy walks opens up new vistas in the modelling of complex dynamical processes in external fields.

We have introduced a new fractional approach to the phase space description of superdiffusive sub-ballistic transport processes. The obtained fractional KKE leads to the Mittag-Leffler relaxation of the velocity distribution towards the classical Maxwell-Boltzmann equilibrium. In contrast, the long-time or high-friction limit of the spatial distribution does not possess a stationary solution. The process is characterised by a combination of the classical time evolution found for the first moment, such as the exponential relaxation of the initial condition in the presence of a linear force field, with a time dependence which is governed by the fractional order α, *i.e.*, the "memory strength". The fractional KKE fulfils a generalised Einstein relation in velocity space. In coordinate space, no analogous generalisation of the Einstein relation exists. These properties set the present approach apart from previous fractional models. We expect that the present study contributes to a better understanding of superdiffusive transport and instigates future research on the role of "equilibrium" in anomalous transport processes.

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