International Journal of Modern Physics B, Vol. 15, No. 17 (2001) 2351–2358

ACCELERATING THROUGH A POTENTIAL LANDSCAPE: A FRACTIONAL DYNAMICS APPROACH TO ENHANCED MOTION IN AN EXTERNAL FORCE FIELD?

RALF METZLER*

Department of Physics, Massachusetts Institute of Technology,
77 Massachusetts Avenue, Room 12-109, Cambridge, Massachusettes 02139, USA

Received 21 May 2001

We address the question of describing enhanced transport in an external force field close to thermal equilibrium, within the framework of fractional dynamics. We demonstrate that in the overdamped regime inconsistencies arise, in the existence of negative regions of the propagator. Despite of this observation, we claim that this approach might be useful for the long time description of such systems.

PACS number(s): 05.40.-a, 05.60.-k, 02.50.Ga

The temporal evolution of a Brownian particle under the influence of an external force is usually described in terms of the deterministic Klein–Kramers equation in phase space, and through its underdamped and overdamped limits, the Rayleigh and Fokker–Planck equations which control the system equilibration towards the Maxwell and Gibbs–Boltzmann equilibriums in velocity and position space, respectively.[1] In the force free diffusion limit, the mean squared displacement is given by the central limit form $\langle x^2(t)\rangle \sim 2Kt$.

Conversely, there exists a diversity of systems which exhibit the power-law behavior[2]

$$\langle x^2(t)\rangle \sim 2K_\gamma^* t^\gamma\,, \qquad \gamma \neq 1 \tag{1}$$

of the mean squared displacement in the force free diffusion limit where the generalized diffusion constant K_γ^* has dimension $[K_\gamma^*] = \mathrm{cm}^2\ \mathrm{sec}^{-\gamma}$.

Anomalous transport processes characterized through Eq. (1) have been studied extensively in the slow ($0 < \gamma < 1$), and in the enhanced ($1 < \gamma$) domains through a number of models,[3] among others. Here we concentrate on the fractional dynamics approach to enhanced transport processes in the presence of an external force field. This research was instigated by the success of the fractional dynamics description of slow systems which has been highlighted as a made-to-measure approach that

*E-mail: metz@mit.edu; URL: www.mit.edu/˜metz/

generalizes the set of the above deterministic equations to fractional order, featuring a nonlocal approach with a slowly decaying self-similar memory.[5–8] Moreover, it has been shown that fractional equations can be solved with the methods known from the analogous Brownian equations.[4]

For the description of enhanced, sub-ballistic processes, Barkai and Silbey proposed the fractional Klein–Kramers equation[9]

$$\frac{\partial W}{\partial t} + v\frac{\partial W}{\partial x} + \frac{F(x)}{m}\frac{\partial W}{\partial v} = {}_0D_t^{1-\alpha}\eta^* L(v)W(x,v,t) \tag{2}$$

for the probability density function (PDF) $W(x,v,t)$, with the Klein–Kramers operator $L(v) \equiv (\frac{\partial}{\partial v}v + \frac{k_\mathrm{B}T}{m}\frac{\partial^2}{\partial v^2})$. Equation (2) features the generalized friction constant η^* of dimension $[\eta^*] = \sec^\alpha$, and puts the drift into a temporally local relation to the time derivative $\frac{\partial}{\partial t}W$. The latter contrasts the slow dynamics approach pursued in Ref. 8. A unifying approach to fractional Klein–Kramers and the related equations has been carried out on the basis of the generalized Chapman–Kolmogoroff equation in Ref. 10. The fractional Riemann–Liouville operator ${}_0D_t^{1-\alpha} \equiv \frac{\partial}{\partial t}{}_0D_t^{-\alpha}$ occurring in Eq. (2) is defined through the convolution[11]

$${}_0D_t^{-\alpha}W(x,v,t) \equiv \frac{1}{\Gamma(\alpha)}\int_0^t dt' \frac{W(x,v,t')}{(t-t')^{1-\alpha}}\,, \tag{3}$$

according to which Eq. (2) possesses a slowly decaying memory, defined through the scale-free power-law kernel $\propto t^{\alpha-1}$. In the Brownian limit $\alpha \to 1$, the fractional Klein–Kramers equation (2) reduces to the standard Klein–Kramers equation.

In the force-free limit, integration of Eq. (2) over the position coordinate leads to the fractional Rayleigh equation $\frac{\partial}{\partial t}W = {}_0D_t^{1-\alpha}\eta^* L(v)W(v,t)$ that governs the equilibration of the velocity PDF $W(v,t)$.[8–10] In this equation, the equilibration of single modes and velocity moments is governed through the Mittag–Leffler function

$$E_\alpha(-(t/\tau)^\alpha) \equiv \sum_{n=0}^{\infty}\frac{(-(t/\tau)^\alpha)^n}{\Gamma(1+\alpha n)} \tag{4}$$

that replaces the exponential pattern encountered in the traditional Brownian limit, for which we find the reduction $\lim_{\alpha\to 1} E_\alpha(-(t/\tau)^\alpha) = \exp(-t/\tau)$. For $0 < \alpha < 1$, $E_\alpha(-\eta^* t^\alpha)$ interpolates strictly monotonically between the initial stretched exponential behavior $E_\alpha(-\eta^* t^\alpha) \sim \exp(-\eta^* t^\alpha/\Gamma(1+\alpha))$ and the long time power-law pattern $E_\alpha(-\eta^* t^\alpha) \sim (\eta^*\Gamma(1-\alpha)t^\alpha)^{-1}$. Accordingly, the fractional result $W_\alpha(v,t)$ can be expressed in terms of its Brownian counterpart, $W_1(v,t)$ through the scaling relation $W_\alpha(v,u) = \frac{\eta^*}{\eta}u^{\alpha-1}W_1(v,\frac{\eta^*}{\eta}u^\alpha)$ in Laplace space $W(v,u) \equiv \int_0^\infty dt W(v,t)e^{-ut}$.[7,8]

In the overdamped, *force free* limit it was already proved by Schneider and Wyss that the solution of the corresponding *fractional wave equation* is a proper PDF. This solution was investigated in more detail in Ref. 13 where it was demonstrated that the PDF exhibits counter-moving humps with a simultaneous antipersistent depletion of the origin, compare also Ref. 14.

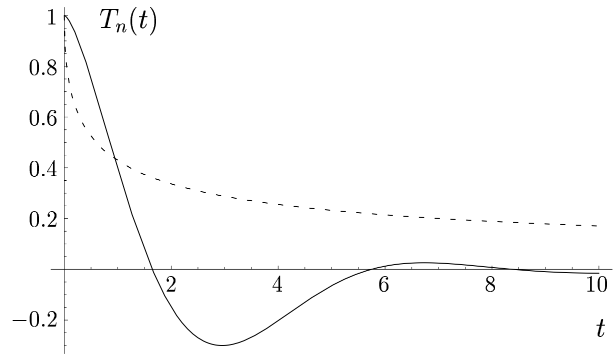

Fig. 1. Fokker–Planck mode relaxation $E_{3/2}(-\lambda_n t^{3/2})$ which exhibits oscillations superimposed to the relaxation (full line), in comparison to the corresponding Rayleigh mode relaxation $E_{1/2}$ $(-\eta^* t^{1/2})$ which is strictly monotonic.

Let us now turn towards the *forced* overdamped regime. The corresponding kinetic equation is obtained via integration of the fractional Klein–Kramers equation (2) over velocity, $\int_{-\infty}^{\infty} dv \cdot$, and of v times Eq. (2) over velocity, $\int_{-\infty}^{\infty} v dv \cdot$.[15] This method produces two independent equations whose combination leads to the fractional telegrapher's type equation

$$\frac{1}{\eta^*} {}_0D_t^{2+\alpha} W + \frac{\partial^2 W}{\partial t^2} = {}_0D_t^{\alpha} L(x) W(x,t) \tag{5}$$

the high-friction limit of which is the superdiffusive fractional Fokker–Planck equation

$$\frac{\partial^2 W}{\partial t^2} = {}_0D_t^{\alpha} L(x) W(x,t) \tag{6}$$

with the Fokker–Planck operator $L(x) \equiv -\frac{\partial}{\partial x} \frac{F(x)}{m\eta^*} + K_\alpha \frac{\partial^2}{\partial x^2}$. In the force-free limit, this equation reduces to the above-mentioned fractional wave equation,[5,13] and the mean squared displacement for $W_0(x) = \delta(x)$ is accordingly given by Eq. (1) with $\gamma = 2 - \alpha$ and $K_\alpha^* \equiv K_\alpha / \Gamma(3-\alpha)$. By comparison with Eq. (2), one obtains the generalized Einstein–Stokes relation $K_\alpha = k_{\mathrm{B}} T / (m\eta^*)$ which has been derived analogously in the subdiffusive case.[7,8]

For the determination of the mode relaxation of the fractional Fokker–Planck equation (6), we introduce the separation ansatz $W(x,t) = \varphi(x) T(t)$, to find

$$T_n(t) = E_{2-\alpha}(-\lambda_n t^{2-\alpha}) \tag{7}$$

for the temporal eigenfunction belonging to the eigenvalue λ_n. The dependence on the Mittag–Leffler function of index $2-\alpha$ is *a priori* remarkable as it is different from the mode relaxation of the corresponding fractional Rayleigh equation, proportional to $E_\alpha(-\tilde{\lambda}_n t^\alpha)$. As $1 < 2 - \alpha < 2$, the Mittag–Leffler function in Eq. (7) is no longer a monotonic function. Instead, Eq. (7) exhibits damped oscillations, as displayed in Fig. 1, in comparison to the strictly monotonic Rayleigh mode relaxation. The physical reason for this oscillatory behavior is buried in the existence of the moving humps.[13]

Equation (6) can be rewritten in the integral form

$$W(x,t) - W_0(x) = {}_0D_t^{\alpha-2} L(x) W(x,t) \tag{8}$$

where we chose the vanishing initial field velocity $W_{t,0}(x) \equiv \lim_{t\to 0+} (\frac{\partial}{\partial t} W(x,t))_{t=0} = 0$ for norm conservation. Note firstly that for times $t > 0$, such a field velocity $W_t(x,t) \neq 0$ exists which enters Eq. (8) in the form $-tW_t(x,t)$ which gives rise to the moving humps. Secondly, note that the convolution kernel of the fractional operator ${}_0D_t^{\alpha-2}$ has a finite characteristic time, indicating that the initial condition does not exhibit the same persistence as in the slow case. In contrast, the distribution is depleted around the initial value, this antipersistence being balanced by two counter-moving humps which become asymmetric in the presence of the external force field $F(x)$, see below.

For the further discussion of Eq. (6), we investigate the enhanced version of the Ornstein–Uhlenbeck process, i.e. enhanced motion in the external harmonic potential $V(x) = \frac{1}{2} m\omega^2 x^2$ which corresponds to the restoring linear force $F(x) = -m\omega^2 x$. With the method of separation of variables, we obtain the series solution[7]

$$W(x,t) = \sqrt{\frac{m\omega^2}{2\pi k_{\mathrm{B}} T}} \sum_0^\infty \frac{1}{2^n n!} E_{2-\alpha}(-nt^{2-\alpha}) H_n\left(\frac{x_0}{\sqrt{2}}\right) H_n\left(\frac{x}{\sqrt{2}}\right) e^{-x^2/2} \tag{9}$$

for the initial condition $W_0(x) = \delta(x - x_0)$, in reduced coordinates. H_n denotes the Hermite polynomials. The convergence of the series (9) is rather poor. We have evaluated it with `Mathematica` and obtained the graphs displayed in Fig. 2. Whereas the wings of the curves are still somewhat short of convergence, the characteristic feature of the two asymmetric humps is numerically assured. It becomes even more distinct for an enhanced number of summation terms. Thus, the left hump sliding down into the potential well is larger than the counterwise hump moving uphill. Eventually, the whole curve equilibrates towards the Gaussian Gibbs–Boltzmann distribution. The most striking feature of the plots is, however, the existence of *negative regions*. Although their very shape is beyond the numerical convergence on our computing facilities,[20] their existence can be revealed analytically by calculating the moments of this process. In the course of time, the negative area spanned by the distribution becomes less, until a proper PDF emerges which eventually approaches the Gibbs–Boltzmann distribution.

This behavior is mirrored in the moments. Accordingly, the first moment for the enhanced Ornstein–Uhlenbeck process $\langle x(t)\rangle = x_0 E_{2-\alpha}(-\frac{\omega^2}{\eta^*} t^{2-\alpha})$ becomes negative for certain time intervals, but also the second moment

$$\langle x^2(t)\rangle = x_{th}^2 + (x_0^2 - x_{th}^2) E_{2-\alpha}\left(-2\frac{\omega^2}{\eta^*} t^{2-\alpha}\right), \quad x_{th}^2 = \frac{k_{\mathrm{B}} T}{m\omega^2} \tag{10}$$

exhibits negative parts if only x_0 is large enough, i.e. if either the initial condition is asymmetric enough, or the temperature activation $k_{\mathrm{B}}T$ is too low. The definition of

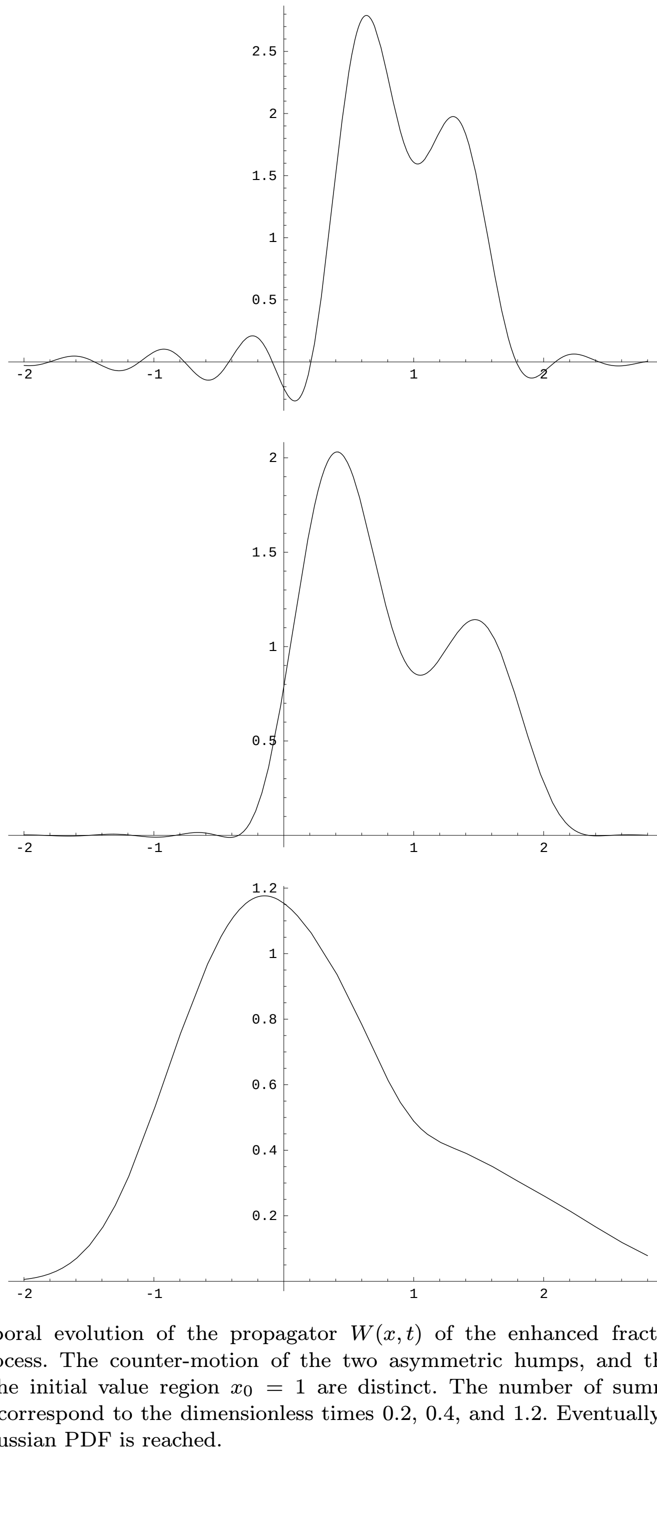

Fig. 2. Temporal evolution of the propagator $W(x,t)$ of the enhanced fractional Ornstein–Uhlenbeck process. The counter-motion of the two asymmetric humps, and the simultaneous depletion of the initial value region $x_0 = 1$ are distinct. The number of summation terms is 80. The plots correspond to the dimensionless times 0.2, 0.4, and 1.2. Eventually, the stationary symmetric Gaussian PDF is reached.

the second moment, $\langle x^2(t)\rangle \equiv \int_{-\infty}^{\infty} x^2 W(x,t)dx$, implies that the solution $W(x,t)$ of the fractional equation (6) indeed contains negative segments, i.e. $W(x,t)$ is *no proper PDF!* Conversely, for longer times, the second moment oscillates around the stationary value x_{th}^2 without further crossing the zero mark. Similarly, higher order moments $\langle x^{2n}\rangle$ involve the function $E_{2-\alpha}(-2n(\omega^2/\eta^*)t^{2-\alpha})$, i.e. they incorporate an increasingly larger relaxation rate and reach stationarity even earlier: *for long enough times the solution* $W(x,t)$ *becomes a proper PDF.*

However, as Risken elaborates on cases of the Kramers–Moyal expansion which is truncated after the $(n+2)$th term, $n = 1, 2, \ldots$ (Ref. 16, p. 71): "Though the transition probability must then have negative values at least for sufficiently small times, these negative values may be very small." And (*ibid.* p. 78): "an approximate distribution function need not be positive everywhere. As long as the negative values and the region where they occur are small this approximate distribution function may be very useful". Indeed, this also applies to our situation, as the solution of Eq. (6) for large enough times becomes a proper PDF approaching the Gibbs–Boltzmann distribution, and the numerical evaluation of the enhanced fractional Ornstein–Uhlenbeck process shows that the negative parts are rather small for "reasonable" combinations of asymmetric initial condition x_0 and activation $k_{\rm B}T$. Therefore we claim that for long enough times, the fractional dynamics framework for enhanced transport in an external force field renders reliable information and is thus meaningful, see also the forthcoming discussion in Ref. 19.

Let us examine the properties of Eq. (6) and its solution somewhat further. There exist two ways of connecting the enhanced solution $W_{2-\alpha}(x,t)$ from Eqs. (6) and (8) to Markovian equations. Firstly, we find the scaling relation

$$W_{2-\alpha}(u) = \sqrt{\frac{\eta^*}{\eta_2}}u^{-\alpha/2}W_2\left(\sqrt{\frac{\eta^*}{\eta_2}}u^{1-\alpha/2}\right) \tag{11}$$

between $W_{2-\alpha}$ and the solution of the forced wave equation $\frac{\partial^2}{\partial t^2}W = L(x)\, W(x,t)$ which can be alternatively expressed through the generalized Laplace transformation

$$W_{2-\alpha}(x,t) = \int_0^\infty ds E(s,t) W_2(x,s) \tag{12}$$

which is similar to the transformation introduced by Barkai and Silbey.[9] From Eq. (11) it follows that $E(s,u) = -[\partial/(1-\alpha/2)s\partial u]\exp(-s^* u^{1-\alpha/2})$, i.e. $E(s,u)$ is the characteristic function of the modified one-sided Lévy distribution $[(1-\alpha/2)s]^{-1}tL^+_{1-\alpha/2}(t/(s^*)^{1/(1-\alpha/2)})$.[17] By help of the Fox function, we can express the kernel E in the closed form ($s^* \equiv s\sqrt{K/K_{2-\alpha}}$)

$$E(s,t) = \frac{1}{s}H^{1,0}_{1,1}\left[s^* t^{\alpha/2-1}\left| \begin{matrix} \left(1, 1-\dfrac{\alpha}{2}\right) \\ (1,1) \end{matrix}\right.\right] \tag{13}$$

$$= \frac{1}{s}\sum_{n=0}^{\infty}\frac{(-1)^n (s^* t^{\alpha/2-1})^{1+n}}{n!\Gamma(1-2-\alpha/2(1+n))}\,. \tag{14}$$

Conversely, we obtain the down-grade transformation

$$W_n^{(1)}(x,t) = \int_0^\infty dsE^*(s,t)W_{2-\alpha}(x,s) \tag{15}$$

from the enhanced solution $W_{2-\alpha}$ to its Brownian Fokker–Planck counterpart W_1 where the kernel, defined through $E^*(s,u) = -\frac{\beta\partial}{s\partial u}\exp(-s^*u^{1/\beta})$, $s^* \equiv (\eta/\eta^*)^{1/\beta}s$, is given in terms of the Fox function[18]

$$E^*(s,t) = \frac{\beta}{s}H_{1,1}^{1,0}\left[\frac{(s^*)^\beta}{t}\middle|\begin{matrix}(1,1)\\(1-\beta,\beta)\end{matrix}\right] \tag{16}$$

$$= \frac{1}{s}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!\Gamma(1-\beta^{-1}-\beta^{-1}n)}\left(\frac{s^*}{t^{1/\beta}}\right)^{1+n} \tag{17}$$

and $\beta \equiv 2-\alpha$. Note that a map *from* the Brownian W_1 *to* the enhanced solution $W_{2-\alpha}$ is not connected with a one-sided Lévy stable law as $2-\alpha > 1$, nor does the corresponding Fox function exist.[17,18]

Concluding, we have investigated the possible extension of fractional dynamics to enhanced, sub-ballistic transport in the presence of an external force field. Although certain inconsistencies exist in respect of the distribution for shorter times, we believe that fractional dynamics can give valuable information for the description of sub-ballistic processes that eventually converge to the Gibbs–Boltzmann equilibrium form.

RM thanks Yossi Klafter, Eli Barkai and Igor Sokolov for discussions. Financial support from the Minerva foundation (Amos de Shalit programme) and the DFG within the Emmy Noether programme is gratefully acknowledged.

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20. Higher order nodes get slightly shifted by taking along higher order terms in the summation (9); however, the amplitude of either hump remains roughly unchanged, and therefore the existence of nodes is certain.