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Lévy meets Boltzmann: strange initial conditions for Brownian and fractional Fokker–Planck equations

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Abstract

We study normal and anomalous diffusion processes with initial conditions of the broad Lévy type, i.e., with such initial conditions which, per se, exhibit a diverging variance. In the force-free case, the behaviour of the associated probability density function features distinct shoulders which can be related to the probability current flowing away from the origin. In the presence of an external potential which eventually leads to the emergence of a non-trivial, normalisable equilibrium probability density function, the initially diverging variance becomes finite. In particular, the effects of strange initial conditions for the harmonic Ornstein–Uhlenbeck potential are explored to some detail. Methods to quantify the dynamics related to such kinds of processes are investigated. © 2001 Elsevier Science B.V. All rights reserved.

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Anomalous transport studies, generically, are concerned with dynamic stochastic processes in systems which are inherently disordered in some sense and which give rise to long-range spatial or temporal correlations [1–3]. Characteristically, anomalous transport processes no longer fall into the basin of attraction of the central limit theorem which gives rise to the Gaussian character of normal diffusion processes [4,5], but they are often associated with Lévy stable laws which govern either the jump lengths or the waiting times of the process. Anomalous transport processes of this type are therefore connected with the generalised central limit theorem which in turn leads to the existence of a well-defined and unique probability density function (pdf) $W(x,t)$ [1,6,7].

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Two extreme limits can be distinguished. On the one hand, there are processes whose internal clock measures the so-called "fractal time" giving rise to temporal correlations expressed through a system memory which controls the particular temporal approach to thermal equilibrium. On the other hand, Lévy flights are distinguished by the occurrence of long jumps permitted with a comparably high probability following from Lévy stable jump length distributions. In the latter case, one observes the divergence of the mean squared displacement, $\langle x^2(t)\rangle = \int_{-\infty}^{\infty} x^2 W(x,t)\,\mathrm{d}x$ [1,4,5]. In other words, in a Lévy flight the possibility of extremely long jumps causes the pdf to fall off in the power-law fashion $W(x,t) \sim t/|x|^{1+\mu}$ with $0 < \mu < 2$ such that $\langle x^2(t)\rangle \to \infty$ [8–11].

Here, we study the complementary problem, namely a transport process whose propagator, i.e., the pdf for δ-initial condition, possesses converging spatial moments of any order, and supplement it with an *initial condition which has long tails* such that the variance of this initial distribution diverges. Such situations may occur when a system initially performs a Lévy flight for a certain time, and subsequently turns over to a Brownian or subdiffusive regime due to some change in the external parameters. In such a case, the initial condition for the secondary process whose clock starts at time T will be a Lévy stable distribution, i.e., the solution of the fractional diffusion equation for Lévy flights for a given time T. This strange initial condition scenario might be relevant to certain situations in groundwater contaminant spreading where initially pollutants are broadly distributed and then they penetrate through the soil. In this latter case, the associated horizontal stochastic process is to be considered force-free if the soil is homogeneous, or funnelled towards some main outflow channel in the aquifer geometry [12]. Similar constellations might be encountered in single molecule experiments [13] where such a turnover could be triggered in the energy diffusion. One could possibly speculate whether it might also occur in bacterial motion [14] or the famed albatross flight [15,16] when a sparse food distribution is replaced by ample prey.

To be more specific, we investigate solutions of the fractional Fokker–Planck equation [17–21]

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

with $0 < \alpha \leqslant 1$, for the Lévy type initial condition

$$W_0(x) = L_\rho(x/\ell)\,, \tag{2}$$

which is characterised by the asymptotic power-law behaviour

$$W_0(x) \sim \frac{\ell^\rho}{|x|^{1+\rho}}\,. \tag{3}$$

We define $W_0(x) \equiv \lim_{t\to 0^+} W(x,t)$. Eq. (1) describes anomalous diffusion in the external force field $F(x) = -V'(x)$ which relaxes towards the classical Boltzmann equilibrium $W_{\mathrm{st}}(x) = \mathscr{N}\exp(-V(x)/[k_{\mathrm{B}}T])$ [17–21]. This relaxation is dominated by the *Mittag–Leffler pattern* which issues a turnover from an initial stretched exponential decay to a final inverse power-law pattern [17]. In the limiting case $\alpha = 1$, Eq. (1) is the traditional Fokker–Planck–Smoluchowski equation with *exponential* mode relaxation.

In Eq. (2), L_ρ denotes the symmetric Lévy stable law defined in terms of the characteristic function [7]

$$\varphi(k) \equiv \int_{-\infty}^{\infty} e^{ikx} L_\rho(x/\ell) = e^{-(\ell|k|)^\rho} \tag{4}$$

from which one easily infers that the variance or mean squared displacement diverges and that the initial condition is normalised, $\varphi(0) = 1$. The parameter ℓ defines an internal length scale such that for $|x| \gg \ell$, the power-law dependence (3) holds.

In the force-free limit and for the sharp initial condition $W_0(x) = \delta(x)$, the anomalous character displayed by Eq. (1) leads to the non-linear form

$$\langle x^2(t)\rangle = 2K_\alpha t^\alpha/\Gamma(1+\alpha) \tag{5}$$

of the mean squared displacement [2]. In this force-free limit, the fractional Fokker–Planck equation describes subdiffusion ($0 < \alpha < 1$) [17–21]. The fractional Riemann–Liouville operator ${}_0D_t^{1-\alpha} \equiv (d/dt){}_0D_t^{-\alpha}$ in Eq. (1) is defined in terms of the convolution [15]

$${}_0D_t^{-\alpha} f(t) \equiv \frac{1}{\Gamma(\alpha)} \int_0^t \frac{f(t')}{(t-t')^{1-\alpha}} \tag{6}$$

so that one obtains the convenient relation $\mathscr{L}\{{}_0D_t^{-\alpha} f(t)\} = u^{-\alpha} f(u)$ for the Laplace transformation of ${}_0D_t^{-\alpha}$. Note that due to definition (6), the fractional Riemann–Liouville operator describes systems which are prepared at time $t = 0$, and thus it explicitly considers initial values [22]. Note also that the generalised friction and diffusion constants appearing in Eq. (1) are of dimensions $[\eta_\alpha] = s^{\alpha-2}$ and $[K_\alpha] = cm^2\, s^{-\alpha}$, and they are connected through the generalised Einstein–Stokes relation $K_\alpha = k_B T/(m\eta_\alpha)$ [17,18,23–25]. In the following, we use the normalised variables such that $K_\alpha = 1$, $\eta_\alpha = 1$, and $\ell = 1$.

Suppose that the Green's function for the fractional Fokker–Planck equation (1), i.e., the solution for the initial condition $W_0(x) = \delta(x - x_0)$ is $G(x, x_0, t)$. Then, the solution for any initial condition $W_0(x)$ is given via the integral

$$W(x,t) = \int_{-\infty}^{\infty} G(x, x_0, t) W_0(x_0)\, dx_0 . \tag{7}$$

With the Green's function G, we investigate Eq. (1) with the strange initial condition (2) for the force-free diffusion case, and for the Ornstein–Uhlenbeck process. If the external potential field is constant, i.e., $V'(x) = 0$ vanishes, the propagator is homogeneous in x and can be written as $G(x, x_0, t) = G(x - x_0, t)$. In this case of free diffusion, the Fourier transform of the pdf $W(x,t)$ splits up into the product

$$W(k,t) = G(k,t) W_0(k) \tag{8}$$

and consequently, we find $\langle x^2(t)\rangle \to \infty$ for all times t. That is, for $t < \infty$, the divergence is due to the influence of the strange initial condition, and for $t = \infty$ the trivial Boltzmann equilibrium, i.e., the equidistribution, is reached. Conversely, if $V(x)$

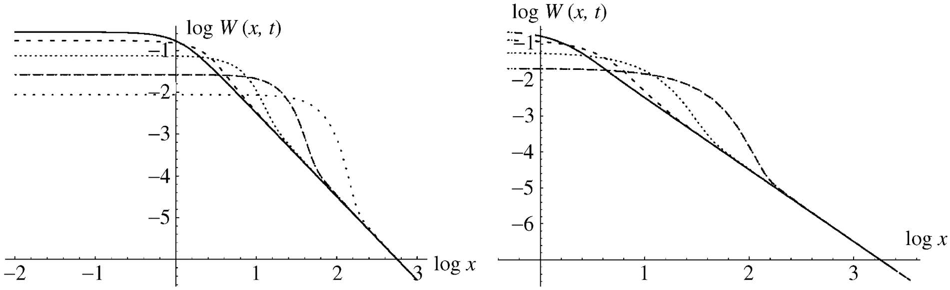

Fig. 1. Force-free diffusion with strange initial condition of the Cauchy type, $\log_{10}$–$\log_{10}$ scale: (left) Brownian case; (right) subdiffusive case with $\alpha=\frac{1}{2}$. For increasing time, a distinct shoulder propagates towards increasing x and thereby eats up the power law. Dimensionless times: $t=0.1,1,10,100,1000$ (left); $0.1,10,1000,10^5$ (right).

is confining such that eventually the system relaxes towards the Gibbs–Boltzmann equilibrium $W_{\rm st}(x)\equiv\lim_{t\to\infty}W(x,t)=\mathcal{N}\exp(-V(x)/(k_BT))$, the Green's function loses its memory of the initial condition, $\lim_{t\to\infty}G(x,x_0,t)=G_{\rm st}(x)$. Thus,

$$\begin{aligned} W_{\rm st}(x) &= \int_{-\infty}^{\infty} G_{\rm st}(x)W_0(x)\,\mathrm{d}x_0 \\ &= G_{\rm st}(x)=\mathcal{N}\mathrm{e}^{-V(x)/(k_BT)} \end{aligned} \tag{9}$$

by means of the normalisation $\int_{-\infty}^{\infty}W_0(x)\,\mathrm{d}x=1$. In this case, the mean squared displacement finally reaches the stationary, thermal value $x_{\rm th}\equiv\int_{-\infty}^{\infty}x^2W_{\rm st}(x)\,\mathrm{d}x$, and is *finite*, also see below. Let us now investigate the behaviour of the pdf for the strange initial condition (2) in more detail. As in most of what follows we are limited to numerical calculations, we choose the particular Cauchy (Lorentz) distribution

$$W_0(x)=\frac{1}{\pi}\frac{1}{1+x^2}\leftrightarrow\varphi(k)=\exp(-|k|) \tag{10}$$

as a prototype strange initial condition which allows to evaluate the associated integrals within the memory range.

For a constant external potential, the initial condition enters through convolution fashion, leading to the product form (8). In this case, one finds the analytic expression for the Cauchy case (10)

$$W(x,t)=\frac{\mathrm{e}^{-(x+\mathrm{i})^2/(4t)}}{4\sqrt{\pi t}}\left\{1+\mathrm{e}^{ix/t}\,\mathrm{erfc}\left(\frac{1+\mathrm{i}x}{2\sqrt{t}}\right)+i\,\mathrm{erfi}\left(\frac{x+\mathrm{i}}{2\sqrt{t}}\right)\right\}\,, \tag{11}$$

which is real valued, as it should.

In Fig. 1, we show the pdf $W(x,t)$, Eq. (11), for successive times. Accordingly, the large $|x|$ behaviour

$$W(x,t)\sim t|x|^{-2} \tag{12}$$

is found. Clearly, the direction of the net flow is away from the symmetry centre $x=0$, and distinct shoulders successively eat up the power-law tail reminiscent of the initial Cauchy distribution. Thus, for any finite time t, there exists a leftover region

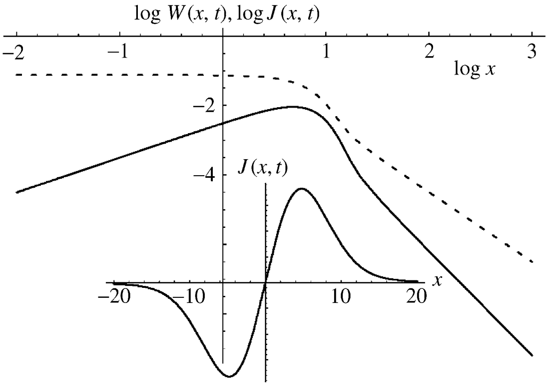

Fig. 2. Force-free diffusion with strange initial condition of the Cauchy type, $t = 10$. Probability current (full line) and pdf (dashed) in $\log_{10}$–$\log_{10}$ scale. Inset: linear plot of the flux J.

still exhibiting the strange initial condition. Let us quantify the probability spread in the course of time in terms of the probability current (flux) of the Green's function G:

$$\jmath(x,t) \equiv -\frac{\partial G(x,x_0,t)}{\partial x}\,, \tag{13}$$

which in the force-free case is given through the uneven expression $\jmath(x,x_0,t) = (4\sqrt{\pi}t^{3/2})^{-1}(x-x_0)\exp(-(x-x_0)^2/(4t))$ so that the overall flux corresponding to the strange initial condition $W_0(x)$ is found to be

$$J(x,t) = \int_{-\infty}^{\infty} \mathrm{d}x_0\, W_0(x_0)\jmath(x,x_0,t)\,. \tag{14}$$

The result is plotted in Fig. 2 and illustrates that the probability current in the presence of the strange initial condition is still peaked off-centre, and the maximum current is close to the location of the shoulders in the pdf $W(x,t)$.

In the parabolic Ornstein–Uhlenbeck potential $V(x) = x^2/2$, the pdf *initially* exhibits stable character, as well; close to the symmetry centre $x = 0$, the behaviour is similar to the spreading shoulders in the force-free case, see Figs. 3 and 4. However, for increasing time, the pdf becomes more confined (dashed line in Fig. 3) until it reaches the Gaussian–Boltzmann form. In particular, the stable character becomes also eaten up from its tails where the restoring force exerted through the parabolic potential increasingly pushes the random walker back towards the origin. This is displayed in Figs. 3 and 4 for both the Brownian and the anomalous case.

The initially broadly spread probability becomes increasingly concentrated around the origin. This can be quantified through the finite interval mean squared displacement

$$\langle x^2(t)\rangle_a \equiv \int_{-a}^{a} W(x,t)x^2\,\mathrm{d}x\,. \tag{15}$$

For the Ornstein–Uhlenbeck potential, and for any other confining external field, we expect the finite interval mean squared displacement to exhibit a *decrease* from $t = 0$ to the stationary state. This is, of course, due to the restoring force which leads to the

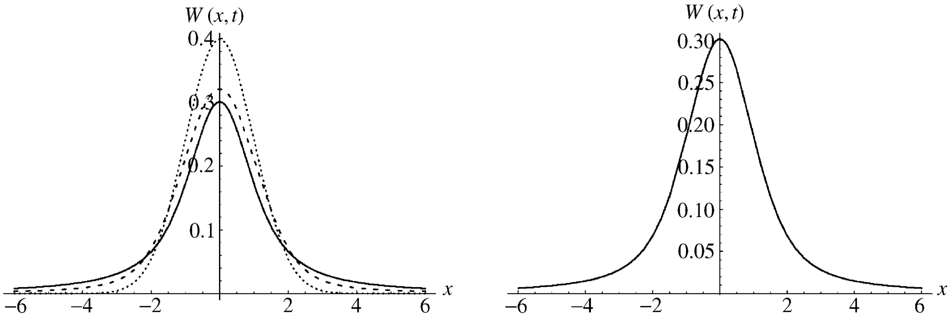

Fig. 3. Pdf $W(x,t)$ for the Ornstein–Uhlenbeck case, and for $\rho = 1$. Note that for increasing time, the maximum grows, corresponding to the net influx of probability from the shrinking tails: (left) Brownian case for dimensionless times $t = 0.1$ (full line), 1 (dashed), 10 (dotted); (right) fractional case, $t = 0.1$. In the linear plot scale, no difference to the Brownian case is perceptible. In Fig. 4, the Brownian case is plotted on a log–log scale, for comparison.

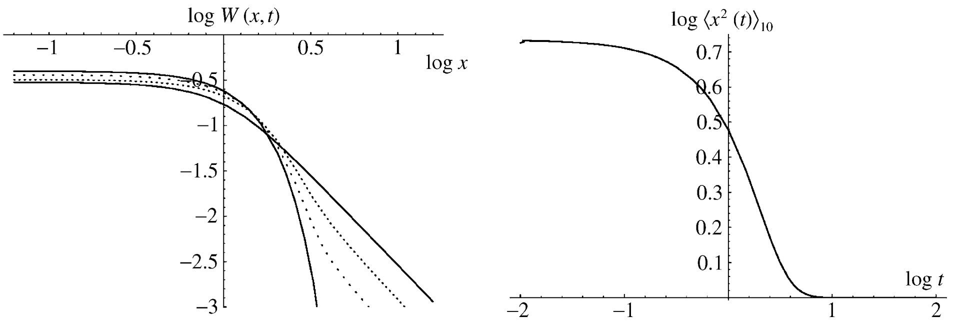

Fig. 4. $\log_{10}$–$\log_{10}$ representation corresponding to Fig. 3: (left) dimensionless times $t = 0.1$ (full line, rightmost for long times), 1 (dotted), 2 (light-dotted), and 10 (full line, leftmost for long times). The latest time already matches the stationary Gibbs–Boltzmann form, within the plot range; (right) finite interval mean squared displacement (15) with $a = 10$ for the Ornstein–Uhlenbeck process with strange initial conditions, showing the decrease towards the stationary value (in our units, $\log\langle x^2(t)\rangle \to 0$, for $t \to \infty$).

confinement of the broad initial distribution. In Fig. 4, we demonstrate this behaviour for the Brownian Ornstein–Uhlenbeck case; compare the sharp initial value scenario discussed in Ref. [17].

To conclude, we have considered the case when an initial condition with infinite variance is assumed for a dynamical process which itself possesses a propagator with converging moments of any order. *When Lévy meets Boltzmann*, it is the latter which eventually wins out and leads to the confinement of the pdf, i.e., its relaxation towards thermodynamic equilibrium. As generally observed for non-sharp initial conditions or in the presence of boundaries, the pdf for the Brownian and the fractional cases look similar, it is only the temporal approach towards this stationary solution which significantly differs.

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