J. Phys. A: Math. Gen. 36 (2003) L537-L544

PII: S0305-4470(03)67248-3

LETTER TO THE EDITOR

First passage and arrival time densities for Lévy flights and the failure of the method of images

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Received 4 August 2003 Published 1 October 2003 Online at stacks.iop.org/JPhysA/36/L537

Abstract

We discuss the first passage time problem in the semi-infinite interval, for homogeneous stochastic Markov processes with Lévy stable jump length distributions $\lambda(x) \sim \ell^{\alpha}/|x|^{1+\alpha}$ ($|x| \gg \ell$), namely, Lévy flights (LFs). In particular, we demonstrate that the method of images leads to a result, which violates a theorem due to Sparre Andersen, according to which an arbitrary continuous and symmetric jump length distribution produces a first passage time density (FPTD) governed by the universal long-time decay $\sim t^{-3/2}$. Conversely, we show that for LFs the direct definition known from Gaussian processes in fact defines the probability density of first arrival, which for LFs differs from the FPTD. Our findings are corroborated by numerical results.

PACS numbers: 05.40.Fb, 02.50.Ey, 05.60.Cd, 05.10.Gg

Lévy flights (LFs) and Lévy walks (LWs) are the prime examples in the investigation of non-standard transport processes whose stationary solutions do not converge towards the Boltzmann form [1–4]. Being subject to the generalized central limit theorem [5, 6], LFs correspond to a Markov process in which extremely long excursions can occur with appreciable probability, whereas in LWs long excursions are penalized through a time cost introduced via a spatiotemporal coupling [7]. Applications of LFs and LWs range from the famed flight of an albatross [8], the spreading of spider-monkeys [9] or the grazing patterns of bacteria [10], over economical data [11] to molecular collisions [12] and plasmas [13]. Despite their wide usage, the detailed behaviour of even the simpler, uncoupled LF processes, on which we concentrate in the following, in external potentials and under non-trivial boundary conditions is still not fully explored. Thus, recently bifurcations have been discovered between multimodal states of the probability density function (PDF) of LFs in steeper than harmonic external fields, in whose presence also the variance becomes finite [14, 15], and rich band structures have been reported for LFs in periodic potentials [16].

Of particular interest in random processes is the first passage time density (FPTD) [17–20]. For LFs, the FPTD was determined through the method of images on a finite

domain in [21], and with similar methods in [22]. These methods lead to results for the FPTD in the semi-infinite domain, whose long-time behaviour explicitly depends on the Lévy index α . In contrast, a theorem due to Sparre Andersen proves that for any discrete-time random walk process starting at $x_0 \neq 0$ with each step chosen from a continuous, symmetric but otherwise arbitrary distribution, the FPTD asymptotically decays as $\sim n^{-3/2}$ with the number *n* of steps [20, 23, 24] being *fully independent* of the index of the LF, i.e., universal. In the case of a Markov process, the continuous time analogue of the Sparre Andersen result reads

$$p(t) \sim t^{-3/2}$$
. (1)

The analogous universality was proved by Frisch and Frisch for the special case in which an absorbing boundary is placed at the location of the starting point of the LF at t > 0 [25], and numerically corroborated by Zumofen and Klafter [26]. In the following, we demonstrate that the method of images is generally inconsistent with the universality of the FPTD, and therefore cannot be applied to solve FPTD problems for LFs. We also show that for LFs the FPTD differs from the PDF for first arrival.

Let us start by recalling that an unbiased LF can be defined through the space-fractional diffusion equation for the PDF W(x, t) [2, 27, 28]

$$\frac{\partial}{\partial t}W = D\frac{\partial^{\alpha}}{\partial |x|^{\alpha}}W(x,t) \qquad \therefore \int_{-\infty}^{\infty} e^{ikx} \frac{\partial^{\alpha}W}{\partial |x|^{\alpha}} dx \equiv -|k|^{\alpha}W(k,t) \qquad (2)$$

where we define the fractional derivative $\partial^{\alpha}/\partial |x|^{\alpha}$ by its Fourier transform. (Here and in the following, we restrict ourselves to $1 < \alpha < 2$.) In position space, the fractional derivative is defined in terms of the convolution (see [14] for the case $\alpha = 1$)

$$\frac{\partial^{\alpha}}{\partial |x|^{\alpha}} W(x,t) \equiv \frac{D}{\kappa} \frac{\partial^2}{\partial x^2} \int_{-\infty}^{\infty} \frac{W(x',t)}{|x-x'|^{\alpha-1}} \qquad \therefore \ \kappa \equiv 2\Gamma(2-\alpha) \left|\cos\frac{\pi\alpha}{2}\right|. \tag{3}$$

Equivalently, LFs can be described in terms of continuous time random walks with long-tailed jump length distributions $\lambda(x) \sim \ell^{\alpha}/|x|^{1+\alpha}$ [7, 29]. The associated PDF W(x, t) for natural boundary conditions $(\lim_{|x|\to\infty} W(x,t) = 0)$ with initial condition $\delta(x)$ is the Lévy stable law $W(x,t) = \int_{-\infty}^{\infty} \exp(-ikx - D|k|^{\alpha}t) dk/(2\pi)$ [5, 6]. In Fourier–Laplace space⁴, this PDF corresponds to $W(k,s) = (s + D|k|^{\alpha})^{-1}$. A characteristic of LFs is the divergence of the variance of both W(x,t) and $\lambda(x)$. Equipping equation (2) with a δ -sink of strength $p_{fa}(t)$, we obtain the diffusion–reaction equation for the non-normalized density function f(x, t),

$$\frac{\partial}{\partial t}f(x,t) = D\frac{\partial^{\alpha}}{\partial |x|^{\alpha}}f(x,t) - p_{\rm fa}(t)\delta(x) \tag{4}$$

from which by integration over the unrestricted space, we find the quantity

$$p_{\rm fa}(t) = -\frac{\rm d}{{\rm d}t} \int_{-\infty}^{\infty} f(x,t) \,{\rm d}x \tag{5}$$

i.e., $p_{fa}(t)$ is the negative time derivative of the survival probability. By definition of the sink term, $p_{fa}(t)$ is the PDF of *first arrival*: once a random walker arrives at the sink, it is annihilated. By solving equation (4) through standard methods (determining the homogeneous and inhomogeneous solutions), it is straightforward to calculate the solution f in terms of the propagator W of equation (2) with initial condition $f(x, 0) = \delta(x - x_0)$ yielding $f(k, u) = [e^{ikx_0} + p_{fa}(u)]/(s + D|k|^{\alpha})$, from which, in turn, we find that $p_{fa}(t)$ satisfies the chain rule $(p_{fa} \text{ implicitly depends on } x_0)$

$$W(-x_0, t) = \int_0^t p_{fa}(\tau) W(0, t - \tau) d\tau$$
(6)

⁴ We denote the Laplace and Fourier transforms through the explicit use of the image variables: $p(s) \equiv \int_0^\infty p(t) e^{-st} dt$ and $f(k, t) \equiv \int_{-\infty}^\infty f(x, t) e^{ikx} dx$.

which corresponds to the Laplace space relation $p_{fa}(s) = W(-x_0, s)/W(0, s)$. Equation (6) is well known and for any sufficiently well-behaved continuum, a diffusion process is commonly employed to define the FPTD [18, 20].

For Gaussian processes with propagator $W(x,t) = 1/\sqrt{4\pi Dt} \exp(-x^2/[4Dt])$, one obtains, by direct integration of the diffusion equation with appropriate boundary condition, the FPTD [20]

$$p(t) = x_0 (4\pi D t^3)^{-1/2} \exp\left(-x_0^2 / (4Dt)\right)$$
(7)

including the asymptotic behaviour $p(t) \sim t^{-3/2}$ for $t \gg x_0^2/(4D)$. In this Gaussian case, the quantity $p_{fa}(t)$ is equivalent to the FPTD. From a random walk perspective, this is due to the fact that individual steps are of the same increment, and the jump length statistics therefore ensures that the walker cannot hop across the sink in a long jump without actually hitting the sink and being absorbed. This behaviour becomes drastically different for Lévy jump length statistics: there, the particle can easily cross the sink in a long jump. Thus, before eventually being absorbed, it can pass by the sink location numerous times, and therefore the statistics of the first arrival will be different from that of the first passage. In fact, with $W(x, s) = (2\pi)^{-1} \int_{-\infty}^{\infty} e^{ikx} (s + D|k|^{\alpha})^{-1} dk$, we find

$$p_{\rm fa}(s) = 1 - \frac{\int_0^\infty (1 - \cos kx_0)/(s + Dk^{\alpha}) \,\mathrm{d}k}{\int_0^\infty 1/(s + Dk^{\alpha}) \,\mathrm{d}k} \tag{8}$$

by use of the de Moivre identity $\exp(iz) = \cos z + i \sin z$. With $\int_0^\infty (s + Dk^\alpha)^{-1} dk = \pi s^{1/\alpha - 1}/(\alpha D^{1/\alpha} \sin(\pi/\alpha))$ and

$$\int_0^\infty \frac{1 - \cos kx_0}{s + Dk^\alpha} \sim \frac{\Gamma(2 - \alpha)\sin(\pi(2 - \alpha)/2)x_0^{\alpha - 1}}{(\alpha - 1)D} \qquad s \to 0 \quad \alpha > 1$$

we obtain the limiting form

$$p_{\rm fa}(s) \sim 1 - x_0^{\alpha - 1} s^{1 - 1/\alpha} D^{-1 + 1/\alpha} \tilde{\Lambda}(\alpha)$$
 (9)

where $\tilde{\Lambda}(\alpha) = \alpha \Gamma(2-\alpha) \sin(\pi(2-\alpha)/2) \sin(\pi/\alpha)/(\alpha-1)$. We note that the same result is obtained by the exact expressions for $W(x_0, s)$ and W(0, s) in terms of Fox *H*-functions and systematic expansion [30]. The inverse Laplace transform of the small *s*-behaviour (9) can be obtained by completing (9) to an exponential, and then computing the Laplace inversion by the identification $e^z = H_{0,1}^{1,0}[z|(0, 1)]$ with the Fox *H*-function [30], for which the exact Laplace inversion can be performed [31]. Finally, a series expansion of this result leads to the long-*t* form

$$p_{\rm fa}(t) \sim C(\alpha) \frac{x_0^{\alpha - 1}}{D^{1 - 1/\alpha} t^{2 - 1/\alpha}}$$
 (10)

with $C(\alpha) = \alpha \Gamma(2-\alpha) \Gamma(2-1/\alpha) \sin(\pi [2-\alpha]/2) \sin^2(\pi/\alpha)/(\pi^2(\alpha-1))$. Clearly, in the Gaussian limit, the required asymptotic form $p(t) \sim x_0/\sqrt{4\pi Dt^3}$ for the FPTD is consistently recovered, whereas in the general case the result (10) is slower than in the universal FPTD behaviour in equation (1), as it should as the δ -trap used in equation (4) to define the first arrival for LFs is weaker than the absorbing wall used to properly define the FPTD. For LFs, the PDF for first arrival thus scales like (10) (i.e., it explicitly depends on the index α of the underlying Lévy process), and, as shown below, it *differs* from the corresponding FPTD.

Before calculating this FPTD, we first demonstrate the validity of equation (10) by means of a simulation the results of which are shown in figure 1. Random jumps with LF jump length statistics are performed, and a particle is removed when it hits a certain interval of width w around the sink; for our simulations we found an optimum value $w \approx 0.3$. As seen in figure 1

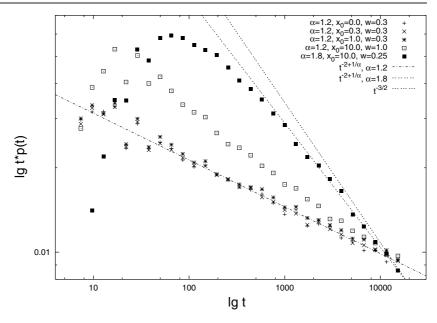


Figure 1. First arrival PDF for $\alpha = 1.2$ demonstrating the $t^{-2+1/\alpha}$ scaling, for optimal trap width w = 0.3. For comparison, we show the same scaling for $\alpha = 1.8$, and the power-law $t^{-3/2}$ corresponding to the FPTD. The behaviour for too large w = 1.0 shows a shift of the decay towards the -3/2 slope. Note that on the abscissa we plot $\lg tp(t)$. Note also that for the initial condition $x_0 = 0.0$, the trap becomes activated *after* the first step, consistent with [26].

(note that we plot $\lg tp(t)$!) and for analogous results not shown here, relation (10) is nicely fulfilled for all $1 < \alpha < 2$, whereas for larger w, the slope increases.

The proper dynamical formulation of an LF on the semi-infinite interval with an absorbing boundary condition at x = 0, and thereby the determination of the FPTD, has to make sure that in terms of the above random walk picture, jumps across the sink are forbidden. This can be consistently achieved by setting $f(x, t) \equiv 0$ on the left semi-axis, i.e., actually removing the particle when it crosses the point x = 0. This formally corresponds to the modified dynamical equation

$$\frac{\partial f(x,t)}{\partial t} = \frac{D}{\kappa} \frac{\partial^2}{\partial x^2} \int_0^\infty \frac{f(x',t)}{|x-x'|^{\alpha-1}} \, \mathrm{d}x' \equiv \frac{\partial^2}{\partial x^2} \mathcal{F}(x,t) \tag{11}$$

in which the fractional integral is truncated to the semi-infinite interval. After Laplace transformation and integrating over x twice, one obtains

$$\int_0^\infty K(x - x', s) f(x', s) \, \mathrm{d}x' = (x - x_0) \Theta(x - x_0) - xp(s) - \mathcal{F}(0, s) \tag{12}$$

where p(t) is the FPTD and the kernel $K(x, s) = sx\Theta(x) - (\kappa |x|^{\alpha-1})$. This equation is formally of the Wiener–Hopf type of the first kind [32]. After some manipulations similar to those applied in [26], we arrive at the asymptotic expression $p(s) \simeq 1 - Cs^{1/2}$, where C = const, in accordance with the universal behaviour (1) and with the findings in [26]. Thus, the dynamic equation (11) consistently phrases the FPTD problem for LFs. We note that due to the truncation of the fractional integral it was not possible to modify the wellestablished Grünwald–Letnikov scheme [33] to numerically solve equation (11) with enough computational efficiency to numerically obtain the direct solution for f(x, t). However, to

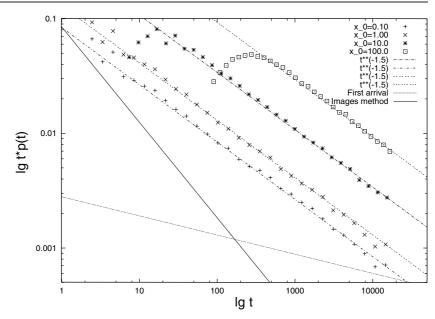


Figure 2. Numerical results for the FPTD process on the semi-infinite domain, for an LF with Lévy index $\alpha = 1.2$. Note that on the abscissa, we plot tp(t). For all initial conditions $x_0 = 0.10$, 1.00, 10.0 and 100.0 the universal slope -3/2 in the $\log_{10}-\log_{10}$ plot is nicely reproduced, and it is significantly apart from the two slopes predicted by the images method and the direct definition of the FPTD.

corroborate the validity of the Sparre Anderson universality, we perform a simulation of an LF in the presence of an absorbing wall, i.e., random jumps with LF jump length statistics are performed along the right semi-axis, and a particle is removed when it jumps across the origin to the left semi-axis. Results of such a detailed random walk study are displayed in figures 2 and 3. The expected universal $t^{-3/2}$ scaling is nicely obtained for various initial conditions and α . Clearly, the scaling for the first arrival and the image method-FPTD derived below are significantly different.

We now demonstrate that the method of images produces a result, which is consistent neither with the universal behaviour of the FPTD (1) nor with the behaviour of the PDF of first arrival (10). Given the initial condition $\delta(x - x_0)$, the solution $f_{im}(x, t)$ for the absorbing boundary value problem with the analogous Dirichlet condition $f_{im}(0, t) = 0$ according to the method of images is given via the difference [19, 20]

$$f_{\rm im}(x,t) = W(x - x_0, t) - W(x + x_0, t)$$
(13)

in terms of the free propagator W, i.e., a *negative* image solution originating at $-x_0$ balances the probability flux across the absorbing boundary. The corresponding pseudo-FPTD is then calculated in the same way as in equation (5). For the image solution in Fourier–Laplace space, we obtain

$$f_{\rm im}(k,s) = [2i\sin(kx_0)]/(s+D|k|^{\alpha})$$
(14)

for a process which starts at $x_0 > 0$ and takes place in the right half space. In Laplace space, the image method-FPTD becomes

$$p_{\rm im}(s) = 1 - s \int_0^\infty dx \int_{-\infty}^\infty \frac{dk}{2\pi} \, e^{-ikx} \frac{2i\sin kx_0}{s + D|k|^{\alpha}}.$$
 (15)

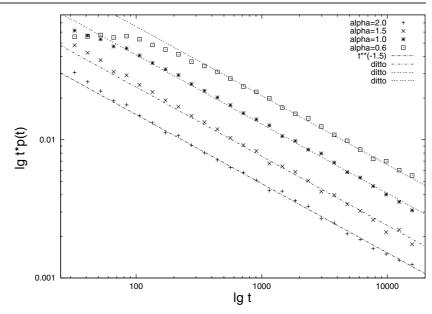


Figure 3. Same as in figure 2, for $\alpha = 2.0, 1.5, 1.0$ and 0.6, and for the initial condition $x_0 = 10.0$. Again, the universal $\sim t^{-3/2}$ behaviour is obtained.

After some transformations, we arrive at

$$p_{\rm im}(s) = 1 - 2/\pi \int_0^\infty \mathrm{d}\xi \sin(\xi s^{1/\alpha} x_0 / D^{1/\alpha}) / [\xi(1+\xi^\alpha)]. \tag{16}$$

In the limit of small *s*, this expression reduces to $p_{\rm im}(s) \sim 1 - \Lambda(\alpha)x_0D^{-1/\alpha}s^{1/\alpha}$, with $\Lambda(\alpha) = (2/\pi)\int_0^\infty (1 + \xi^{\alpha})^{-1} d\xi = 2/(\alpha \sin(\pi/\alpha))$. Following the same procedure as outlined above, we find the long-*t* form

$$p_{\rm im}(t) \sim 2\Gamma(1/\alpha) x_0 / (\pi \alpha D^{1/\alpha} t^{1+1/\alpha})$$
 (17)

for the image method-FPTD. In the Gaussian limit $\alpha = 2$, expression (17) produces $p_{im}(t) \sim x_0/\sqrt{4\pi Dt^3}$, in accordance with equation (7). Conversely, for general $1 < \alpha < 2$, $p_{im}(t)$ according to equation (17) would decay faster than $\sim t^{-3/2}$. The method of images breaks down for LFs due to their special non-local nature, displayed by the integrals in equations (2) and (3), and (11), namely having a long-tailed jump length distribution. This leads to leapovers beyond the absorbing boundary. The method of images is expected to work when the boundary is also a turning point of the trajectory, as actually happens for nearest neighbour random walks, or the Wiener process.

Qualitatively, the following argument may be brought forth in favour of the observed universality of the LF-FPTD: the long-time decay is expected to be governed by short-distance jump events, corresponding to the central region of very small jump lengths for the Lévy stable jump length distribution. But this region is, apart from a prefactor, indistinguishable from the Gaussian distribution, and therefore the long-time behaviour should in fact be the same for any continuous jump length distribution $\lambda(x)$. In fact, the universal law (1) can only be modified in the presence of non-Markov effects such as broad waiting time processes or spatiotemporally coupled walks [2, 7, 20, 34, 35]. In terms of the special case covered by the theorem of Frisch and Frisch [25], in which the absorbing boundary coincides with the initial condition, we can understand the general situation for finite $x_0 > 0$, as in the long-time limit, the distance x_0 becomes negligible in comparison to the diffusion length $\langle |x(t)| \rangle \sim t^{1/\alpha}$: therefore the asymptotic behaviour is necessarily governed by the same universality.

Concluding, we demonstrated that the method of images, which has been developed as a powerful tool in Gaussian diffusion also beyond the homogeneous case [19, 20] and in the presence of long-tailed waiting times [2, 34, 35], fails for LF processes, leading to a false result for the FPTD. Moreover, we showed that for such broad jump length statistics, the PDF of first arrival at a point differs from the FPTD. We also provided a framework in terms of a truncated fractional diffusion equation to solve the FPTD problem for an LF. This study is expected to significantly contribute to the understanding of the, at instances, non-trivial behaviour of LFs.

Acknowledgments

We are happy to acknowledge discussions with Igor Sokolov. We also acknowledge financial support through the INTAS project 00-0847 from the European Commission.

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