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UNIVERSAL CHARACTER OF ESCAPE KINETICS FROM FINITE INTERVALS*

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We study a motion of an anomalous random walker on finite intervals restricted by two absorbing boundaries. The competition between anomalously long jumps and long waiting times leads to a very general kind of behavior. Trapping events distributed according to the power-law distribution result in occurrence of the Mittag–Leffler decay pattern which in turn is responsible for universal asymptotic properties of escape kinetics. The presence of long jumps which can be distributed according to non-symmetric heavy tailed distributions does not affect asymptotic properties of the survival probability. Therefore, the probability of finding a random walker within a domain of motion decays asymptotically according to the universal pattern derived from the Mittag–Leffler function, which describes decay of single modes in subdiffusive dynamics.

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1. Introduction

In close to equilibrium situations interactions of a test particle with other particles, by means of the central limit theorem, can be approximated by the white Gaussian noise. In far-from-equilibrium realms, a stochastic process describing interactions of the test particle with the environment can be distributed according to some more general distributions. The application of the generalized central limit theorem leads to α-stable densities [1–3], which are still invariant under convolution, however they are of the heavy-tailed type.

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In porous or gel-like media a particle performing a random walk can be trapped, *i.e.* after each jump it waits for some (random) time before the next jump occurs. Traditionally, this approach is assumed in the continuous time random walk (CTRW) scenarios [4, 5]. In particular, when the jump length and the waiting time distributions have power-law asymptotics, *i.e.* $p(x) \propto |x|^{-(\alpha+1)}$ $(0<\alpha<2)$ and $p(t) \propto t^{-(\nu+1)}$ $(0<\nu<1)$, the concept of CTRW leads to the idea of the fractional dynamics [6–10]. In the very general case, when there is a competition between anomalously long waiting times and anomalously long jumps, the appropriate fractional diffusion equation, which describes asymptotic evolution of the probability density of finding a random walker at time t in the vicinity of point x, reads [7–9]

$$\frac{\partial p(x,t)}{\partial t} = {}_0D_t^{1-\nu}\left[\frac{\partial^\alpha}{\partial|x|^\alpha}\right] p(x,t)\,. \qquad (1)$$

In Eq. (1), $\partial^\alpha/\partial|x|^\alpha$ stands for the Riesz fractional (space) derivative which is defined via the Fourier transform $\mathcal{F}\left[\partial^\alpha f(x)/\partial|x|^\alpha\right] = -|k|^\alpha \mathcal{F}f(x)$, while ${}_0D_t^{1-\nu}$ denotes the Riemann–Liouville fractional (time) derivative ${}_0D_t^{1-\nu} = d/dt\ {}_0D_t^{-\nu}$ defined by the relation [7, 11] ${}_0D_t^{1-\nu} f(x,t) = 1/(\Gamma(\nu)) d/dt \times \int_0^t dt'\ f(x,t')/(t-t')^{1-\nu}$.

2. Model and results

We extend earlier studies [12–15] by investigating the influence of the competition between long waiting times and long jumps on the escape from finite intervals restricted by two absorbing boundaries. More precisely, we study the escape of a free particle from a finite interval in the situation when subdiffusion coexists with Lévy flights, see Eq. (1) and [16–18]. Initially, at time $t=0$ a test particle is located in the middle of the interval $[-L, L]$. We assume that jumps length are distributed according to general α-stable densities [1, 3, 19]. We compare two situations when jumps are distributed according to symmetric α-stable densities $(\beta = 0)$ with the situation when jumps' lengths are distributed according to skewed α-stable densities (as an exemplary value of the asymmetry parameter we use $\beta = 1$, see below).

For the subdiffusion parameter $\nu < 1$ (see Eq. (1)), the stochastic representation of Eq. (1) is provided by the subordination method [17, 20], *i.e.* the process inspected $X(t)$ is obtained as a function $X(t) = \tilde{X}(S_t)$ by using a stochastic clock S_t. The S_t is a ν-stable subordinator providing a link between the operational time s and the physical time t. The ν-stable subordinator is defined as $S_t = \inf\{s : U(s) > t\}$, where $U(s)$ stands for a strictly increasing ν-stable process whose distribution $L_{\nu,1}$ has the Laplace transform $\langle e^{-kU(s)}\rangle = e^{-sk^\nu}$. The parent process $\tilde{X}(s)$ is composed of independent increments of the α-stable motion described in the operational time s

$$d\tilde{X}(s) = dL_{\alpha,\beta}(s)\,. \qquad (2)$$

Increments of the α-stable process are distributed according to the probability density function whose characteristic function is ($\alpha \neq 1$)

$$\phi(k) = \langle \exp(ik\Delta L_{\alpha,\beta}) \rangle = \exp\left[-\Delta t \sigma^{\alpha} |k|^{\alpha} \left(1 - i\beta\, \mathrm{sgn} k \tan\frac{\pi\alpha}{2}\right)\right] . \quad (3)$$

For $\beta = 0$, the above setup provides a proper stochastic realization of the random process described by the fractional Fokker–Planck equation (1) [17, 20]. For $\beta \neq 0$, Eq. (2) gives a stochastic representation of the following fractional Fokker–Planck equation [21]

$$\frac{\partial p(x,t)}{\partial t} = {}_0D_t^{1-\nu}\left[\beta \tan\frac{\pi\alpha}{2}\frac{\partial}{\partial x}\frac{\partial^{\alpha-1}}{\partial |x|^{\alpha-1}} + \frac{\partial^{\alpha}}{\partial |x|^{\alpha}}\right] p(x,t) . \quad (4)$$

In order to quantify the process of the escape from finite intervals we use the first passage time density and the survival probability $S(t)$, which is the complementary cumulative distribution of the first passage time density $f(t)$. The first passage time density is related to the probability density $p(x,t)$, see Eqs. (1) and (4), by the relation

$$f(t) = -\frac{d}{dt}\int_{-L}^{L} p(x,t)dx = -\frac{d}{dt}S(t) , \quad (5)$$

where $S(t) = \int_{-L}^{L} p(x,t)dx$. The survival probability $S(t)$ represents the probability that at time t a test particle, which started its motion in the middle of the interval, has not been yet absorbed at the boundaries located at $\pm L$. We do not use the mean first passage time to characterize the escape kinetics because for $\nu < 1$, due to trapping events, this quantity diverges.

Properties of the first passage time distribution can be determined from Eqs. (1) and (5). Using the method of separation of variables, the solution $p(x,t)$ of Eq. (1) can be written [7] as a sum of eigenfunctions

$$p(x,t) = \sum_i c_i p_i(x,t) = \sum_i c_i T_i(t)\varphi_i(x) , \quad (6)$$

where $T_i(t)$ and $\varphi_i(x)$ fulfill

$$\frac{dT_i(t)}{dt} = -\lambda_{i,\nu}\, {}_0D_t^{1-\nu} T_i(t) , \quad (7)$$

$$\left[\beta \tan\frac{\pi\alpha}{2}\frac{\partial}{\partial x}\frac{\partial^{\alpha-1}}{\partial |x|^{\alpha-1}} + \frac{\partial^{\alpha}}{\partial |x|^{\alpha}}\right]\varphi_i(x) = -\lambda_{i,\nu}\varphi_i(x) . \quad (8)$$

The solution of Eq. (7) is given by the Mittag–Leffler function [11]

$$T_i(t) = E_\nu(-\lambda_{i,\nu}t^\nu) \equiv \sum_{j=0}^{\infty} \frac{(-\lambda_{i,\nu}t^\nu)^j}{\Gamma(1+\nu j)}\,, \tag{9}$$

which interpolates between the stretched exponential form for small values of the argument $E_\nu(-t^\nu) \propto \exp\left[-t^\nu/\Gamma(1+\nu)\right]$, while asymptotically for large arguments it behaves like $E_\nu(-t^\nu) \propto t^{-\nu}$, see [7]. In the limit of $\nu = 1$ the Mittag–Leffler function is equivalent to the exponential function. Finally, eigenvalues $\lambda_{i,\nu}$ are defined by boundary conditions to Eq. (8) and c_i are determined by the initial condition.

In order to estimate the survival probability, it is necessary to collect the sample of first passage times. Required first passage times are obtained by numerical simulation of the subordinated Langevin equation. The Langevin equation (2) is simulated until the first escape from the domain of motion, *i.e.* as long as $-L < x(s) < L$. After the escape from the interval the operational time s is converted into the physical time t by use of the inverse ν-stable subordinator S_t. For $\alpha < 2$, trajectories of the process $x(t)$ are discontinuous and boundary conditions become non-local [13,14]. Therefore, within simulations it is assumed that the entire semi lines $x \leqslant -L$ and $x \geqslant L$ are absorbing.

Figures 1 and 2 present survival probabilities for different values of the subdiffusion parameter ν: $\nu = 0.7$ (Fig. 1) and $\nu = 0.95$ (Fig. 2). In each figure various panels correspond to different values of the stability index α: $\alpha = 1.9$ (left-top panel), $\alpha = 1.5$ (right-top panel), $\alpha = 1.1$ (left-bottom panel) and $\alpha = 0.7$ (right-bottom panel). Within each panel various curves correspond to various values of the asymmetry parameter β: $\beta = 0$ — symmetric jump length distributions — '$\circ$' and $\beta = 1$ — asymmetric jump length distributions — '$+$'.

The asymptotic properties of the survival probability are determined by the Mittag–Leffler function, which asymptotically behaves like a power-law characterized by the exponent $-\nu$ $(0 < \nu < 1)$, *i.e.* $E_\nu(-t^\nu) \propto t^{-\nu}$. Therefore, for sufficiently large time the decay of the survival probability is of the power-law type with the exponent defined by the value of the subdiffusion parameter ν, see Figs. 1, 2 and [22]. The asymmetry of the jump length distribution changes the shape of survival probabilities, however it does not affect the asymptotic form of these distributions. Furthermore, for a large value of the stability index α, differences between survival probabilities are minimal. It is the consequence of the fact that for large values of the stability index α, the asymmetry does not affect the shape of the jump length distribution so drastically as for small values of the stability index α. For small values of the subdiffusion parameter ν, the asymptotic power-law decay

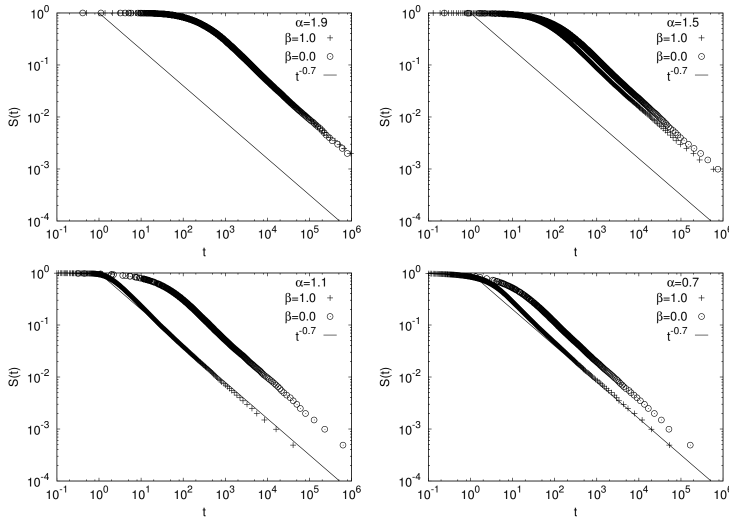

Fig. 1. Survival probability $S(t)$, *i.e.* the probability of finding a random walker within $[-L, L]$ interval at time t. The value of the subdiffusion parameter is set to $\nu = 0.7$. Different panels present results for various values of the stability index α: $\alpha = 1.9$ (left-top panel), $\alpha = 1.5$ (right-top panel), $\alpha = 1.1$ (left-bottom panel) and $\alpha = 0.7$ (right-bottom panel). Various curves correspond to different values of the asymmetry parameter β: '○' — $\beta = 0$ — symmetric jump length distributions and '+' — $\beta = 1$ — asymmetric jump length distributions.

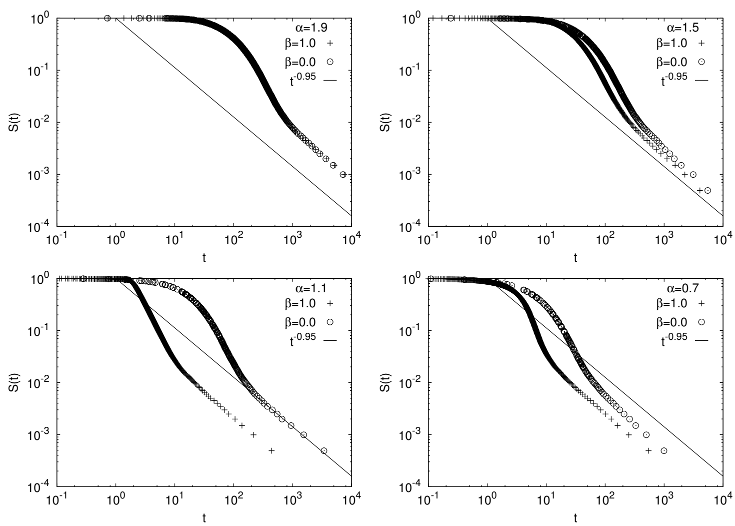

Fig. 2. The same as in Fig. 1 with $\nu = 0.95$: $\alpha = 1.9$ (left-top panel), $\alpha = 1.5$ (right-top panel), $\alpha = 1.1$ (left-bottom panel) and $\alpha = 0.7$ (right-bottom panel).

of survival probabilities is very well visible. With increasing value of the subdiffusion parameter ν, the power-law part of survival probabilities shifts toward larger times. Finally, for $\nu = 1$, the Markovian case is reconstructed and the survival probability $S(t)$ attains an exponential form.

Figures 3 and 4 present the location of the median ($q_{0.5}$) of the first passage time distributions and their width defined as the interquantile distance $q_{0.9} - q_{0.1}$, *i.e.* as the width of the interval containing 90% of collected first passage times. Due to (slow) power-law decay both the mean first passage time and variance of the first passage time diverge. In Figs. 3 and 4 lines are drawn to guide the eye only. In Fig. 3, the case of $\alpha = 1$ with $\beta = 1$, as leading to numerical instabilities, is excluded.

There is a significant difference between properties of the median location and the distribution width for asymmetric ($\beta = 1$, see top-panel of Fig. 3) and symmetric ($\beta = 0$, see bottom-panel of Fig. 3) jump length distributions. Symmetric jump length distributions result in a monotonic dependence of the median location and the distribution width as a function of the stability index α. On the contrary, asymmetric jump length distributions result in the non-monotonic dependence. The median location and the distribution width

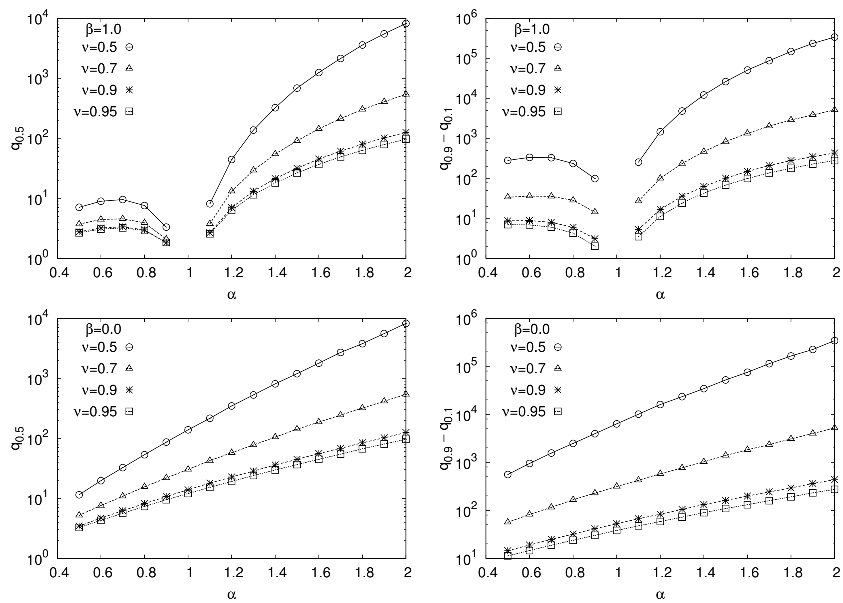

Fig. 3. Location of the median $q_{0.5}$ (left panel) and the distribution width $q_{0.9} - q_{0.1}$ (right panel) for asymmetric α-stable jump length distributions ($\beta = 1$, top panel) and symmetric α-stable jump length distributions ($\beta = 0$, bottom panel). Various curves correspond to different values of the subdiffusion parameter ν. Lines are drawn to guide the eye only.

as a function of the subdiffusion parameter ν, regardless of the value of the asymmetry parameter β, behave in a monotonic way. Consequently, with a decreasing value of the subdiffusion parameter, both the median and the distribution width increase, see Fig. 4. This reflects the fact that a decreasing value of the subdiffusion parameter slows down the escape process.

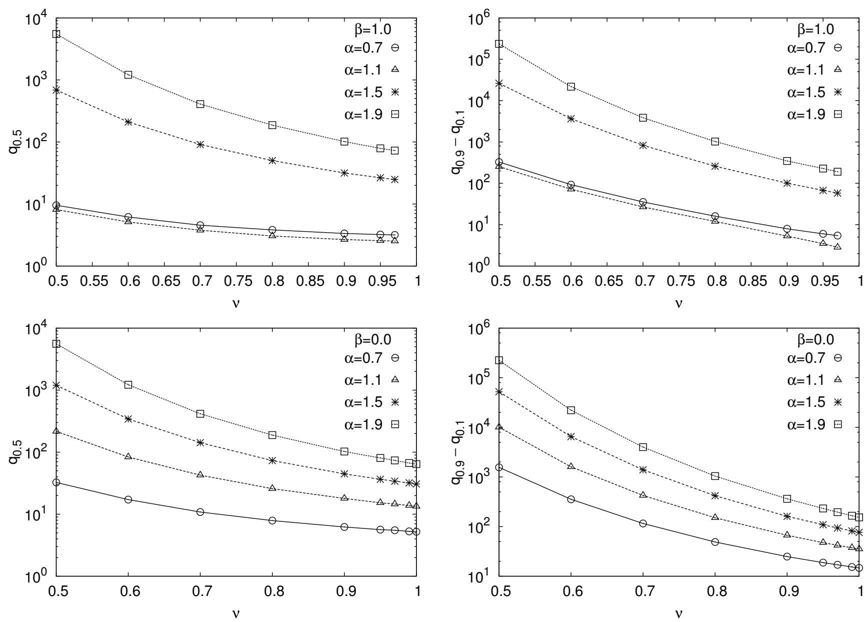

Fig. 4. Location of the median $q_{0.5}$ (left panel) and the distribution width $q_{0.9} - q_{0.1}$ (right panel) for asymmetric α-stable jump length distributions ($\beta = 1$, top panel) and symmetric α-stable jump length distributions ($\beta = 0$, bottom panel). Various curves correspond to different values of the stability index α. Lines are drawn to guide the eye only.

3. Summary and conclusions

Using analytical arguments derived from the properties of the Mittag–Leffler function we have demonstrated that for a system exhibiting competition between long jumps and long waiting times the asymptotic dependence of the survival probability is determined by the value of the subdiffusion parameter ν. Furthermore, numerical results constructed by the subordination method nicely confirmed analytical predictions. The observed decay patterns of the survival probability are very general for systems whose dynamics contains a subdiffusive component. The subdiffusive component is responsible for an introduction of the Mittag–Leffler decay pattern of single relaxation modes. The competition between subdiffusion (long waiting time) and Lévy flights (anomalously long jumps) does not affect the asymptotic form of the survival probability. Finally, the asymmetry of the jump length distribution can change the shape of the survival probability. Nevertheless, the asymptotics remains unaffected.

Computer simulations have been performed at the Institute of Physics, Jagellonian University and the Academic Computer Center, Cyfronet AGH.

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