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Residual mean first-passage time for jump processes: theory and applications to Lévy flights and fractional Brownian motion

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Abstract
We derive a functional equation for the mean first-passage time (MFPT) of a generic self-similar Markovian continuous process to a target in a one-dimensional domain and obtain its exact solution. We show that the obtained expression of the MFPT for continuous processes is actually different from the large system size limit of the MFPT for discrete jump processes allowing leapovers. In the case considered here, the asymptotic MFPT admits non-vanishing corrections, which we call *residual MFPT*. The case of Lévy flights with diverging variance of jump lengths is investigated in detail, in particular, with respect to the associated leapover behavior. We also show numerically that our results apply with good accuracy to fractional Brownian motion, despite its non-Markovian nature.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The first-passage time (FPT) of a random walker to a target point is an important concept for the modeling and interpretation of stochastic processes [1, 2]. This interest in the concept of FPTs is motivated by the crucial role played by FPTs in various contexts, including diffusion limited chemical reactions [3–5], the spreading of diseases [6], or target search processes [7–10]. A general formalism for the calculation of the mean first-passage time (MFPT) of a scale-invariant random process $\mathbf{r}_t$ in a confined domain of volume V has recently been derived in the large V limit in [11, 12], and the full distribution of the FPT has been obtained [13]. These results highlight the asymptotic dependence of the MFPT $\langle \mathbf{T} \rangle$ and its higher order moments on both the source-to-target distance r and the confinement volume in the case of scale-invariant processes, which can be characterized by the walk dimension d_w (defined by $\langle \mathbf{r}_t^2 \rangle \propto t^{2/d_w}$) and the fractal dimension d_f of the support of the random process [14]. In particular, in the case of compact (i.e., recurrent) processes, for which $d_w > d_f$, it was shown that

$$\lim_{V\to\infty} \frac{\langle \mathbf{T} \rangle}{V} = Cr^{d_w - d_f}, \tag{1}$$

where only the constant C depends on the process. For a Brownian walker the first passage at a given point x, which hereafter denotes the first *arrival at exactly* x, is equivalent to the first *crossing* of the value x. This is not generally true. For instance, in the case of Lévy flights with a scale-free distribution of jump lengths [15–17], pronounced leapovers across the threshold value occur. Thus, the first passage at the point x becomes considerably less likely than the first crossing of the value x [18] (see also [19] for the case of one-sided Lévy flights). For Markovian Lévy flights, the first crossing falls into the class of processes governed by the Sparre Andersen universality [20].

Discrete time Markovian jump processes are defined by an elementary jump distribution $w(\mathbf{r})$, which, at each discrete time step n, renders the probability that the random walker makes a jump of length $\mathbf{r}$, which we here assume to be discrete. For a generic distribution w, the searcher is in principle allowed to jump across the target, and performs what we define here as a leapover, as opposed to the case of nearest neighbor random walks. In the case of Euclidean spaces, symmetric jump processes are subject to the generalized central limit theorem [21, 22] and have a well-defined continuous limit which is scale invariant. More explicitly, let $P(\mathbf{r}, n)$ denote the discrete time and space propagator of the process in infinite space, starting from $\mathbf{r} = 0$ at time $n = 0$. Then we know that for the rescaled quantity

$$p_\epsilon(\mathbf{x} = \mathbf{r}\epsilon, t = n\epsilon^{d_w}) \equiv \frac{1}{\epsilon} P(\mathbf{r}, n), \tag{2}$$

the convergence to

$$\lim_{\epsilon\to 0} p_\epsilon(\mathbf{x} = \mathbf{r}\epsilon, t = n\epsilon^{d_w}) = p(\mathbf{x}, t) \equiv t^{-d_f/d_w} g(\mathbf{x}/t^{1/d_w}) \tag{3}$$

is fulfilled in the continuum limit $\epsilon \to 0$ with $\mathbf{x}$ and t fixed by virtue of the central limit theorem. Here g is a scaling function. If the jump distribution $w(\mathbf{r})$ has a second moment $\langle \mathbf{r}^2 \rangle$, the limit process is a Brownian motion with $d_w = 2$ and g is Gaussian; otherwise the limit process is of Lévy stable type with $0 < d_w < 2$, and g is a Lévy stable law of index d_w. In this continuous limit the asymptotic theory applies [11], for compact processes yielding the exact asymptotic form (1), where the constant C can be explicitly determined as a function of g. These results show in particular that the MFPT in the continuous limit becomes *independent* of the existence of leapovers.

In terms of the variables $\mathbf{r}$ and n of the discrete jump process, the continuum limit is equivalent to taking both $\mathbf{r}$ and n large, with $\mathbf{r}^{d_w}/n$ fixed. Hence, for discrete jump processes, equation (1) produces actually only the leading term of a large r expansion, and one should write more precisely

$$\lim_{V\to\infty} \frac{\langle \mathbf{T} \rangle}{V} = Br^{d_w - d_f} + o(r^{d_w - d_f}). \tag{4}$$

We show in this paper that the subleading term of this expansion actually strongly depends on the existence of leapovers and may yield non-vanishing corrections to the rescaled MFPT. This *residual MFPT* (not to be confused with the residual distribution that appears in the context of renewal processes) can have important consequences in the context of both search processes and numerical simulations of FPTs of random walks.

As a specific important example we discuss extensively the effect of leapovers on the MFPT in the context of one-dimensional (1D) Markov jump processes. By means of a functional equation, we first derive an exact expression of the MFPT for continuous time and space scale-invariant Markov processes valid for any starting position of the walker and confining domain size. Next, using the method of pseudo Green functions, we present an exact expression of the MFPT for arbitrary discrete time 1D Markov jump processes, which was previously derived in [1, 23]. We show that in the large volume limit, the leading term of the MFPT is the expected continuous limit of equation (1), and we calculate exactly the subleading term of this expansion. We show that this correction is indeed crucial in the case of random walks with leapovers, since it does not vanish in the limit $L \to \infty$ and $r \to 0$.

We consider a walker performing random independent jumps in a confined 1D system of size L (with periodic boundary conditions) and address the question of determining its MFPT $\langle \mathbf{T}_{TS} \rangle \equiv \langle \mathbf{T}(r, L) \rangle$ to a given target site T as a function of its starting site S, where r stands for the source-to-target distance $|ST|$. To proceed, we denote by w_{ji} the jump probability from discrete site i to j, where w_{ji} is assumed to be symmetric ($w_{ji} = w_{ij}$) and translation-invariant (w_{ji} is a function $|i - j|$ only). It is easily seen that the confined problem with periodic boundary conditions is equivalent to an infinite line with regularly spaced targets at positions kL with $k \in \mathbb{Z}$, a property which will be used below.

2. Continuous time and space scale-invariant jump processes

In this section, we derive an exact expression for the MFPT of a 1D scale-invariant Markov jump process in the limit of continuous space and time. We start from the definition in discrete time and space given above, and pass to the following classical backward equation for the MFPT [2]:

$$\sum_{i=-\infty}^{\infty} \langle \mathbf{T}_{Ti} \rangle (w_{iS} - \delta_{iS}) \equiv \Delta_S \langle \mathbf{T}_{TS} \rangle = -1, \tag{5}$$

completed by the condition $\langle \mathbf{T}(r = kL, L) \rangle = 0$ for all $k \in \mathbb{Z}$. It is easily seen that the following form of the MFPT satisfies both equation (5) and the boundary conditions above:

$$\langle \mathbf{T}(r, L) \rangle = \frac{\langle \mathbf{T}(r, 2L) \rangle + \langle \mathbf{T}(r + L, 2L) \rangle - \langle \mathbf{T}(L, 2L) \rangle}{2}. \tag{6}$$

Note that by definition, $\langle \mathbf{T}(r, L) \rangle$ is L-periodic. This provides a functional equation, which can be solved as follows. We assume that the jump process has a well-defined, self-similar continuous limit, characterized by a walk dimension d_w. We then define the continuous limit of the MFPT as

$$\theta(y, l) = \lim_{\epsilon \to 0} \epsilon^{d_w} \langle \mathbf{T}(r = y/\epsilon, L = l/\epsilon) \rangle, \tag{7}$$

where the starting position y and the system size l are fixed. In particular, we assume that the process is compact ($d_w > d_f = 1$), such that in the continuous limit the MFPT to a point-like target is finite. In this limit self-similarity implies

$$\theta(y, l) = l^{d_w} \theta(x = y/l, 1), \tag{8}$$

and therefore

$$\theta(x, 1) = 2^{d_w - 1} \left(\theta\left(\frac{x}{2}, 1\right) + \theta\left(\frac{x+1}{2}, 1\right) - \theta\left(\frac{1}{2}, 1\right) \right), \tag{9}$$

so that we now have to solve the following functional equation:

$$f(x) = 2^{d_w - 1} \left(f\left(\frac{x}{2}\right) + f\left(\frac{x+1}{2}\right) - f\left(\frac{1}{2}\right) \right). \tag{10}$$

We know that $f(x) = f(1-x)$ by symmetry and that $f(0) = f(1) = 0$. Differentiation of this equation yields

$$f'(x) = 2^{d_w-2}\left(f'\left(\frac{x}{2}\right) + f'\left(\frac{x+1}{2}\right)\right), \tag{11}$$

together with the symmetry condition $f'(x) = -f'(1-x)$. It can be checked directly that equation (11) is solved by the Hurwitz zeta function $\zeta(2-d_w, x)$, the latter being defined by the series

$$\zeta(s,q) = \sum_{n=0}^{\infty} \frac{1}{(q+n)^s}. \tag{12}$$

Note that $\zeta(2-d_w, 1-x)$ is also a solution. In order to satisfy the symmetry condition, a solution of equation (11) satisfying $f'(x) = -f'(1-x)$ is $\zeta(2-d_w, x) - \zeta(2-d_w, 1-x)$. A solution of the original equation (10) satisfying $f(0) = 0$ is then

$$f(x) = \int_0^x (\zeta(2-d_w, y) - \zeta(2-d_w, 1-y))\,\mathrm{d}y. \tag{13}$$

Furthermore, using the fact that the Hurwitz zeta function satisfies the relation

$$\frac{\partial\zeta(s,x)}{\partial x} = -s\zeta(s+1, x), \tag{14}$$

one can simplify equation (13) and write

$$f(x) = \frac{1}{d_w-1}(\zeta(1-d_w, x) + \zeta(1-d_w, 1-x) - \zeta(1-d_w, 0) - \zeta(1-d_w, 1)). \tag{15}$$

The MFPT eventually becomes

$$\theta(y,l) = AL^{d_w}\left(\zeta\left(1-d_w, \frac{y}{l}\right) + \zeta\left(1-d_w, 1-\frac{y}{l}\right) - \zeta(1-d_w, 0) - \zeta(1-d_w, 1)\right), \tag{16}$$

where A is a multiplicative constant which remains undetermined at this stage. For $d_w = 2$ (Brownian case), we retrieve the classical expression, using $\zeta(-n, x) = -B_{n+1}(x)/(n+1)$, where B_n are the Bernoulli polynomials ($B_2(x) = x^2 - x + 1/6$):

$$\begin{aligned} f(x) &= \zeta(-1, x) + \zeta(-1, 1-x) - \zeta(-1, 0) - \zeta(-1, 1) \\ &= -\tfrac{1}{2}(B_2(x) + B_2(1-x) - B_2(0) - B_2(1)) \\ &= x(1-x). \end{aligned}$$

Comparison of this expression to the well-known result $\theta(y,l) = y(l-y)$ yields $A = 1$ in this Brownian case, with $D = 1/2$.

In the general case $d_w \neq 2$, A can be calculated by using the exact asymptotic result in the large l limit of equation (1) (see [11] for details). For $y \ll l$, the asymptotic behavior of equation (16) readily produces

$$\lim_{l\to\infty} \frac{\theta(y,l)}{l} = Ay^{d_w-1}. \tag{17}$$

Comparison with the general result of [11] then delivers

$$A = \int_0^\infty \frac{\mathrm{d}u}{u^{d_f/d_w}} g^*(u^{-1/d_w}), \tag{18}$$

where the infinite space propagator of the process $p(r,t)$ satisfies

$$p(r,t) = t^{-1/d_w} g(r/t^{1/d_w}), \tag{19}$$

and $g^*(u) = g(0) - g(u)$ tends to 0 when $u \to 0$.

Because of the generalized central limit theorem invoked in the introduction, a generic continuous time self-similar Markov process with $d_w \neq 2$ is a Lévy process, whose infinite space propagator reads

$$p(r,t) = \frac{1}{\pi}\int_0^\infty \cos(rx)\,\mathrm{e}^{-t(cx)^{d_w}}\,\mathrm{d}x, \tag{20}$$

where c is a scaling parameter. We subsequently deduce

$$g(u) = \frac{1}{\pi}\int_0^\infty \frac{1}{u}\cos(v)\,\mathrm{e}^{-(\frac{cv}{u})^{d_w}}\,\mathrm{d}v, \tag{21}$$

and

$$g^*(u) = \frac{1}{\pi}\int_0^\infty \frac{1}{u}\,(1-\cos(v))\,\mathrm{e}^{-(\frac{cv}{u})^{d_w}}\,\mathrm{d}v. \tag{22}$$

The constant A can then be explicitly calculated and reads

$$\begin{aligned} A &= \int_0^\infty \frac{\mathrm{d}u}{\pi u^{1/d_w}}\int_0^\infty u^{1/d_w}\,(1-\cos(v))\,\mathrm{e}^{-(cv)^{d_w}u}\,\mathrm{d}v \\ &= \int_0^\infty \frac{1-\cos(v)}{\pi(cv)^{d_w}}\,\mathrm{d}v \\ A &= \frac{d_w}{2c^{d_w}\Gamma(1+d_w)\cos\left(\frac{(2-d_w)\pi}{2}\right)}. \end{aligned} \tag{23}$$

Equations (16) and (23) provide an explicit and exact expression of the MFPT for all r and L, valid for any continuous time and space scale-invariant Markov process.

In order to check equation (16), we simulated Lévy flights with various values of d_w. A Lévy flight is here modeled as a discrete-time random walk, where each step size is a random integer x, distributed according to the distribution

$$w(x=n) = \frac{1}{2\zeta(1+d_w)|n|^{1+d_w}}, \tag{24}$$

with $w(x=0) = 0$. The random walk takes place on a 1D lattice of size N, in discrete time, and with periodic boundary conditions. The target is located at the site of origin $0 \equiv N$. This process converges in the continuous limit defined in the introduction to a Lévy process, whose infinite space propagator is given by equation (20) with

$$c^{d_w} = \frac{\pi}{2d_w\sin\left(\frac{\pi d_w}{2}\right)\Gamma(d_w)\zeta(1+d_w)}. \tag{25}$$

We compared the exact expression (16) obtained in the continuous limit with our discrete simulation. Figures 1 and 2 show that as the lattice size N grows, the simulated discrete MFPT approaches the exact continuous limit, for different values of d_w (for each d_w, the multiplicative constant A is computed using (23)). Note the very slow convergence to the exact solution in the continuous limit. We show below that leapovers lead to non-vanishing corrections of the MFPT to this continuous limit in the large system size limit, which we define as the residual MFPT.

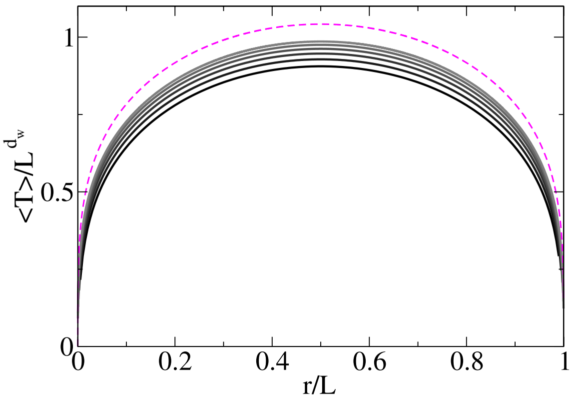

Figure 1. MFPT for a Lévy flight, for several sizes of the 1D lattice (200, 400, 800, 1600, 3200 and 6400 sites, from black (bottom) to light gray (top) as the size grows) compared to the theoretical expression (16) (magenta dotted line, the A constant being given by equation (23)), and for $d_w = 1.25$.

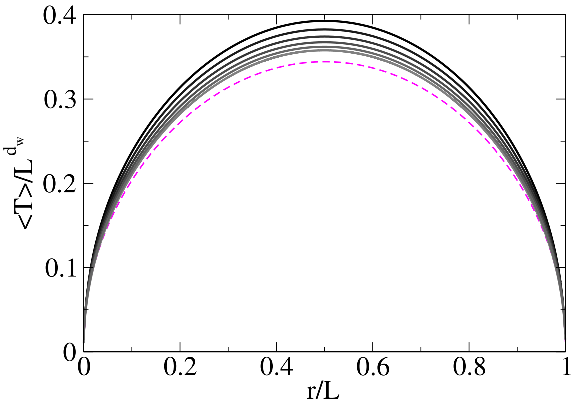

Figure 2. MFPT for a Lévy flight, for several sizes of the 1D lattice (200, 400, 800, 1600, 3200 and 6400 sites, from black (top) to light gray (bottom) as the size grows) compared to the theoretical expression of equation (16) (magenta dotted line, the A constant being given by equation (23)), and for $d_w = 1.5$.

3. Discrete time and space jump processes

To investigate the convergence of the discrete process to its continuous limit, we compute analytically the MFPT for a generic discrete time and space Markov jump process, regarding jump processes with and without second moments. We use the formalism developed by Montroll [23] (see also Hughes [1]). First, we define the structure function $\lambda(k)$, the Fourier transform of the jump distribution (24):

$$\lambda(k) = \sum_{n=-\infty}^{\infty} w(x=n)\,\mathrm{e}^{\mathrm{i}nk}. \tag{26}$$

Denoting by $\tilde{P}_t(k)$ the Fourier transform of the propagator at discrete time t in infinite space, we obtain $\tilde{P}_t(k) = \lambda(k)^t$. The infinite space Green's function then reads

$$G_{ji} = \sum_{t=0}^{\infty} P(j,t|i,0) = \sum_{t=0}^{\infty} \frac{1}{\pi}\int_0^{\pi} \cos(k|i-j|)\lambda(k)^t\,\mathrm{d}k$$
$$= \frac{1}{\pi}\int_0^{\pi} \frac{\cos(k|i-j|)}{1-\lambda(k)}\mathrm{d}k. \tag{27}$$

Recalling that there exists a set Σ of targets located at sites nL ($n \in \mathbb{Z}$) it is useful to define

$$G_{\Sigma r} = \sum_{n=-\infty}^{\infty} \frac{1}{\pi}\int_0^{\pi} \frac{\cos(k(r+nL))}{1-\lambda(k)}\mathrm{d}k \tag{28}$$

$$= \frac{1}{L}\sum_{m=1}^{L-1} \frac{\cos\left(\frac{2\pi mr}{L}\right)}{1-\lambda\left(\frac{2\pi m}{L}\right)}. \tag{29}$$

It can then be checked directly that the expression

$$\langle \mathbf{T}(r,L)\rangle = L(G_{\Sigma\Sigma} - G_{\Sigma r}) = \sum_{m=1}^{L-1} \frac{1-\cos\left(\frac{2\pi mr}{L}\right)}{1-\lambda\left(\frac{2\pi m}{L}\right)} \tag{30}$$

represents an exact solution for the MFPT of a 1D discrete time and discrete space symmetric random walk, since it satisfies both equation (5) and the boundary condition $\langle \mathbf{T}(r = nL, L)\rangle = 0$ for all $n \in \mathbb{Z}$. In what follows we distinguish (i) the continuous limit $\theta(y,l)$ of this exact expression, defined by equation (7), and (ii) the scaled MFPT in the large L limit, which reads according to equation (30)

$$\lim_{L\to\infty} \frac{\langle \mathbf{T}(r,L)\rangle}{L} \equiv \tau(r) = \frac{1}{\pi}\int_0^{\pi} \frac{1-\cos(kr)}{1-\lambda(k)}\mathrm{d}k. \tag{31}$$

While it is clear that the continuous limit $\theta(y,l)$ must yield the exact result of equation (16) derived independently above, we will show below that the scaled MFPT $\tau(r)$ can differ from this continuous limit as soon as the jump distribution allows leapovers. The residual MFPT corresponds to the non-vanishing, subleading term of $\tau(r)$ in the large r regime, which can be obtained by considering the $k \to 0$ behavior of $\lambda(k)$. We consider different examples below, corresponding to jump distributions with and without a second moment.

3.1. *Residual MFPT for jump distributions with a second moment*

We first consider a random walk whose jump distribution possesses a second moment. As a concrete example we employ the exponential law defined by

$$P(n) = \frac{(\mathrm{e}^{\beta}-1)}{2}\,\mathrm{e}^{-\beta|n|} \tag{32}$$

for $n \geqslant 1$ and $P(0) = 0$, where β is a scaling parameter. The second moment of this jump distribution becomes

$$\langle n^2\rangle = \sum_{n=-\infty}^{\infty} n^2 P(n) = \frac{\mathrm{e}^{\beta}(1+\mathrm{e}^{\beta})}{(\mathrm{e}^{\beta}-1)^2}, \tag{33}$$

so that the continuous limit of this jump process, according to equation (3), is a Brownian motion with diffusion coefficient $D = \langle n^2\rangle/2$, and therefore $d_w = 2$. In this continuous limit one obtains straightforwardly the following form of the MFPT:

$$\theta(y,l) = \lim_{\epsilon\to 0} \epsilon^{d_w}\langle \mathbf{T}(r = y/\epsilon, L = l/\epsilon)\rangle = \frac{(\mathrm{e}^{\beta}-1)^2}{\mathrm{e}^{\beta}(1+\mathrm{e}^{\beta})} y(l-y). \tag{34}$$

We now apply the formalism of the previous section and first compute the structure function $\lambda(k)$, obtaining

$$\lambda(k) = \sum_{n=-\infty}^{\infty} P(x=n)\,\mathrm{e}^{\mathrm{i}nk} = (\mathrm{e}^{\beta}-1)\sum_{n=1}^{\infty}\cos(nk)\,\mathrm{e}^{-\beta n}$$
$$= (\mathrm{e}^{\beta}-1)\frac{\mathrm{e}^{\beta}\cos(k)-1}{(\mathrm{e}^{\beta}\cos(k)-1)^2+(\mathrm{e}^{\beta}\sin(k))^2}. \tag{35}$$

An exact expression of the MFPT is then given by (30), for which we find for $r \neq nL$

$$\langle \mathbf{T}(r,L)\rangle = \sum_{m=1}^{L-1}\frac{1-\cos\left(\frac{2\pi m r}{L}\right)}{1-\lambda\left(\frac{2\pi m}{L}\right)}$$
$$= \frac{1}{\mathrm{e}^{\beta}(\mathrm{e}^{\beta}+1)}\sum_{m=1}^{L-1}\frac{1-\cos\left(\frac{2\pi m r}{L}\right)}{1-\cos\left(\frac{2\pi m}{L}\right)}\times\left((\mathrm{e}^{\beta}-1)^2+2\,\mathrm{e}^{\beta}\left(1-\cos\left(\frac{2\pi m}{L}\right)\right)\right)$$
$$= \frac{(\mathrm{e}^{\beta}-1)^2}{\mathrm{e}^{\beta}(\mathrm{e}^{\beta}+1)}r(L-r)+\frac{2\,\mathrm{e}^{\beta}}{\mathrm{e}^{\beta}(\mathrm{e}^{\beta}+1)}L. \tag{36}$$

While this result has the expected continuous limit (34), it reveals a significant difference from the scaled MFPT, containing a non-vanishing residual, subleading correction. More precisely we find that

$$\lim_{L\to\infty}\frac{\langle \mathbf{T}(r,L)\rangle}{L} = \tau(r) = \frac{(\mathrm{e}^{\beta}-1)^2}{\mathrm{e}^{\beta}(\mathrm{e}^{\beta}+1)}r + \frac{2\mathrm{e}^{\beta}}{\mathrm{e}^{\beta}(\mathrm{e}^{\beta}+1)}, \tag{37}$$

where we define the non-vanishing subleading term $2\mathrm{e}^{\beta}/(\mathrm{e}^{\beta}(\mathrm{e}^{\beta}+1))$ as the residual MFPT.

Actually, the residual MFPT for a generic jump distribution with the second moment can be fully derived. We write the small k expansion of the structure function as $\lambda(k) \sim 1 - Dk^2$, where the diffusion coefficient is given by $D = \langle n^2\rangle/2$ as above. Then one has

$$\tau(r) = \frac{1}{\pi}\int_0^{\pi}\frac{1-\cos(kr)}{Dk^2}\mathrm{d}k + B + o(1)$$
$$= \frac{r}{2D} + B + o(1), \tag{38}$$

where the residual MFPT is given by

$$B = \frac{1}{\pi}\int_0^{\pi}\left(\frac{1}{1-\lambda(k)}-\frac{1}{Dk^2}\right)\mathrm{d}k - \frac{1}{D\pi^2}. \tag{39}$$

This reveals the crucial difference between the large system size limit on the one hand and the continuous space and time limit for MFPTs of jump processes on the other. Our above analysis (see equation (39)) suggests that a residual MFPT exists in the large system size limit as soon as leapovers are allowed. In particular, the residual MFPT depends on the full jump distribution and not only on its second moment. For example, the case of a nearest neighbor random walk, for which $\lambda(k) = \cos(k)$, yields a vanishing residual MFPT, as can be checked from equation (39).

3.2. Residual MFPT for Lévy flights

We now turn to jump distributions with an infinite second moment. The continuous limit of such jump processes is a Lévy flight by virtue of the generalized central limit theorem. We start with the example of symmetric discrete space Lévy flights defined by the distribution (24), for which one has

$$\lambda(k) = \sum_{n=-\infty}^{\infty} w(x=n)\,\mathrm{e}^{\mathrm{i}nk} = \frac{1}{\zeta(d_w+1)} \sum_{n=1}^{\infty} \frac{\cos(nk)}{n^{d_w+1}}. \tag{40}$$

We first note that using this expression in the exact result (30) yields in the continuous limit the result (16) and (23), as expected. We consider below the large L limit of the MFPT and will therefore make use of the following small k expansion [1]:

$$\lambda(k) = 1 - \alpha_1 k^{d_w} + \alpha_2 k^2 + \mathcal{O}(k^4), \tag{41}$$

where

$$\alpha_1 = \frac{\pi}{2\zeta(d_w+1)\Gamma(d_w+1)\sin\left(\frac{\pi d_w}{2}\right)}, \tag{42}$$

and

$$\alpha_2 = \frac{\zeta(2-d_w)\Gamma(2-d_w)}{\zeta(1+d_w)(2\pi)^{2-d_w}} \cos\left(\frac{\pi d_w}{2}\right). \tag{43}$$

We then compute the following large r expansion of the scaled MFPT:

$$\tau(r) = \frac{1}{\pi}\int_0^{\pi} \frac{1-\cos(kr)}{\alpha_1 k^{d_w}}\,\mathrm{d}k + \mathcal{O}(r^{2d_w-3}). \tag{44}$$

For any value of $d_w \in]1, 2[$, we obtain the following expression of the leading term:

$$\begin{aligned}\tau(r) &\simeq \frac{r^{d_w-1}}{\alpha_1\pi}\int_0^{\infty} \frac{1-\cos(u)}{u^{d_w}}\,\mathrm{d}k \\ &\simeq \frac{d_w r^{d_w-1}}{2\alpha_1\Gamma(1+d_w)\cos\left(\frac{\pi(2-d_w)}{2}\right)}.\end{aligned} \tag{45}$$

We therefore obtain exactly the result (1) derived in the continuous limit, with the multiplicative constant given by (23). In particular, the leading term of the MFPT does not depend on the exact form of the discrete time propagator, but only on its continuous limit.

To assess the subleading term, we have to distinguish between the cases $d_w > 3/2$ and $d_w \leqslant 3/2$. For the latter case, we obtain a correction term to the scaled MFPT behaving as $\mathcal{O}(1)$,

$$\tau(r) = \frac{d_w}{2\alpha_1\Gamma(1+d_w)\cos\left(\frac{\pi(2-d_w)}{2}\right)} r^{d_w-1} + B + o(1), \tag{46}$$

where the subleading term B, defining the residual MFPT, is a constant, that does not vanish in the limit $L \to \infty$,

$$B = \frac{1}{\pi}\int_0^{\pi} \frac{1}{1-\lambda(k)} - \frac{1}{\alpha_1 k^{d_w}}\,\mathrm{d}k - \frac{1}{\alpha_1(d_w-1)\pi^{d_w}}. \tag{47}$$

The residual MFPT B depends on the full k expansion of $\lambda(k)$, and thus on the precise form of the propagator. If the leading term is the same for all jump processes sharing the same limiting propagator, the residual term depends on the shape of the jump distribution, as was found in the case of jump processes with a finite second moment. The validity of expansion (46) is verified numerically in figure 3.

For the case $d_w > 3/2$, the third term in the k expansion of $\lambda(k)$ has to be taken into account. We now need to compute a second subleading term in the large r expansion,

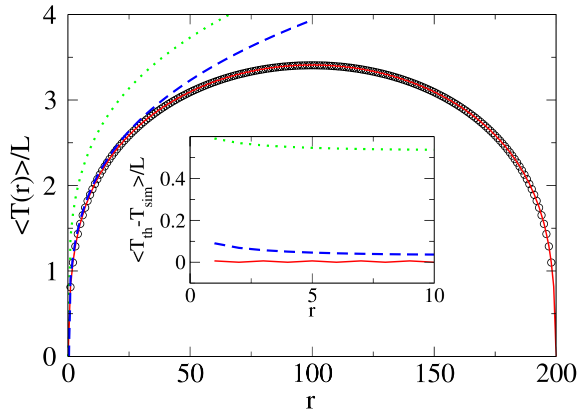

Figure 3. MFPT for a Lévy flight on a 1D lattice of size 200, for $d_w = 1.25$, in discrete time (black circles) compared to the theoretical expression of equation (30) (red line), to the rough approximation of (45) (green dotted line) and to the approximation (46) (blue dashed line). The inset shows the difference between the three theoretical expressions (T_{th}) and the simulation (T_{sim}).

$$\tau(r) = \frac{1}{\pi}\int_0^\pi \frac{1-\cos(kr)}{\alpha_1 k^{d_w}}\mathrm{d}k + \frac{1}{\pi}\int_0^\pi \frac{1-\cos(kr)}{\frac{\alpha_1^2}{\alpha_2}k^{2d_w-2}}\mathrm{d}k + B + o(1) \tag{48}$$

$$= \frac{d_w}{2\alpha_1\pi\Gamma(1+d_w)\cos\left(\frac{\pi(2-d_w)}{2}\right)}r^{d_w-1} + \frac{(2d_w-2)\alpha_2}{2\alpha_1^2\Gamma(2d_w-1)\cos(\pi d_w)}r^{2d_w-3} + B + o(1). \tag{49}$$

Importantly, this expansion yields again a residual term B, which does not vanish for small r, and which depends on the full jump distribution:

$$B = \frac{1}{\pi}\int_0^\pi\left(\frac{1}{1-\lambda(k)} - \frac{1}{\alpha_1 k^{d_w}} - \frac{\alpha_2}{\alpha_1^2 k^{2d_w-2}}\right)\mathrm{d}k - \frac{1}{\alpha_1(d_w-1)\pi^{d_w}} - \frac{\alpha_2}{\alpha_1^2(2d_w-3)\pi^{2d_w-2}}. \tag{50}$$

The validity of expansion (49) is verified numerically in figure 4.

To emphasize how critically the residual MFPT depends on the jump distribution, we consider the example of a Lévy flight in discrete time, but now in continuous space. At each time step, the random walker makes a step distributed according to a symmetric Lévy stable distribution of index $\alpha = d_w$. The structure function $\lambda(k)$ is then directly the characteristic function of the Lévy distribution,

$$\lambda(k) = \exp(-|ck|^{d_w}) = 1 - (ck)^{d_w} - \frac{(ck)^{2d_w}}{2} + \mathcal{O}(k^{2d_w}). \tag{51}$$

The leading term of the MFPT is then the continuous limit obtained in equations (17) and (23), with $\alpha_1 = c^{d_w}$. However, the subleading term in this case is always a constant residual MFPT, whose value depends on the specific shape of the jump distribution. This means that the scaled MFPT admits different large r expansions for Riemann walks (distribution (24)) and continuous space Lévy flights, which depend on the full jump distribution and not only its asymptotics. Importantly, we found that in both cases there exists a non-vanishing residual correction to the MFPT. These results, together with the previous section, suggest that a non-vanishing residual MFPT exists as soon as the jump distribution allows leapovers.

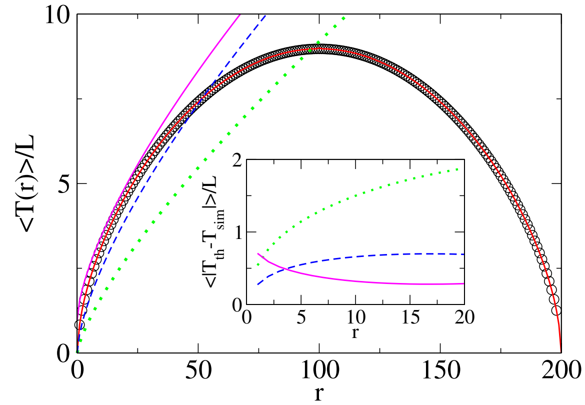

Figure 4. MFPT for a Lévy flight on a network of size 200, for $d_w = 1.75$, in discrete time (black circles) compared to the theoretical expression (30) (red line), to the rough approximation of (45) (green dotted line), and to the approximation (49) with the first subleading term (blue dashed line) and with two subleading terms (magenta plain line). The inset shows the difference between the last three theoretical expressions ($T_{\rm th}$) and the simulation ($T_{\rm sim}$).

4. Splitting probabilities

The above formalism can be extended to further first-passage observables, including observables involving several targets, following the method developed in [24]. As an illustrative example we consider the case of splitting probabilities. More precisely, we assume that the jump process takes place on a ring of length $2L$, with a target T_1 at position $r = 0$ and a target T_2 at position $r = L$. Note that in the case of processes with leapovers, first-passage problems involving $N > 2$ targets do not reduce to problems with two targets. We denote by P_1 the probability that the walker hits T_1 before ever reaching T_2. It is known that P_1 can be exactly expressed in terms of MFPTs as follows [25]:

$$P_1(r, L) = \frac{\langle \mathbf{T}(r + L, 2L)\rangle - \langle \mathbf{T}(r, 2L)\rangle + \langle \mathbf{T}(L, 2L)\rangle}{2\langle \mathbf{T}(L, 2L)\rangle}. \tag{52}$$

Indeed, it can be easily seen that this form satisfies the boundary conditions $P_1(0, L) = 1$ and $P_1(L, L) = 0$, as well as the backward equation $\Delta_r P_1(r, L) = 0$. The exact form of the MFPT derived in equation (30) therefore provides straightforwardly an exact expression of the splitting probabilities. In particular, it admits a simple closed form in the continuous limit, which reads

$$P_1\left(x = \frac{r}{L}\right) = \frac{1}{2}\frac{\zeta\left(1 - d_w, \frac{1+x}{2}\right) + \zeta\left(1 - d_w, \frac{1-x}{2}\right) - \zeta\left(1 - d_w, \frac{x}{2}\right) - \zeta\left(1 - d_w, 1 - \frac{x}{2}\right)}{2\zeta\left(1 - d_w, \frac{1}{2}\right) - \zeta(1 - d_w, 0) - \zeta(1 - d_w, 1)} + \frac{1}{2}. \tag{53}$$

For $d_w = 2$ (Brownian case), we retrieve the classical expression using $\zeta(-n, x) = -B_{n+1}(x)/(n + 1)$, where B_n are the Bernoulli polynomials ($B_2(x) = x^2 - x + 1/6$),

$$\begin{aligned} P_1(x) &= \frac{B_2\left(\frac{x}{2}\right) + B_2\left(1 - \frac{x}{2}\right) - B_2\left(\frac{1+x}{2}\right) - B_2\left(\frac{1-x}{2}\right)}{2B_2(0) + 2B_2(1) - 4B_2\left(\frac{1}{2}\right)} + \frac{1}{2} \\ &= 1 - x. \end{aligned}$$

In the generic case $d_w \neq 2$, equation (53) provides an exact expression for the splitting probability of a 1D Lévy process. We compare this exact solution in the continuous limit

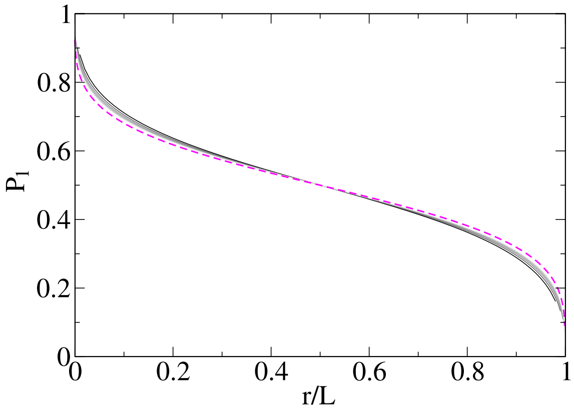

Figure 5. Splitting probability for Lévy flights, for several sizes of the discrete network (200, 400, 800, 1600, 3200 and 6400 sites, from black to light gray as the size grows) compared to the theoretical expression of equation (53) (magenta dotted line), and for $d_w = 1.25$.

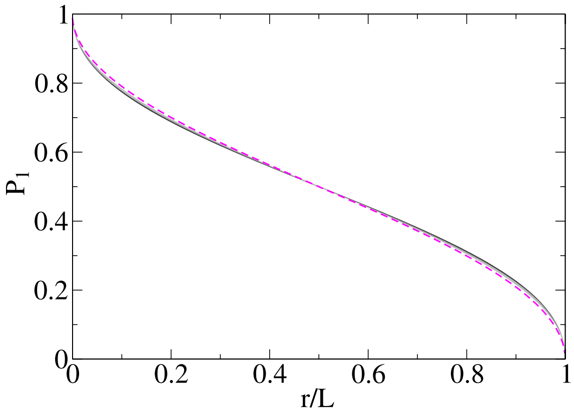

Figure 6. Splitting probability for Lévy flights, for several size of the discrete network (200, 400, 800, 1600, 3200 and 6400 sites, from black to light gray as the size grows) compared to the theoretical expression of equation (53) (magenta dotted line), and for $d_w = 1.5$.

(53) with numerical simulations of Lévy flights. The results are shown in figures 5, 6, and 7, indicating a rather slow convergence to the continuous limit as the system size grows. Clearly, the residual MFPT analyzed in previous sections yields a non-vanishing correction to the splitting probabilities in the large system size limit. Figure 7 shows that taking into account the residual MFPT in the evaluation of the MFPTs entering equation (52), significantly improves the results for finite size L in the regimes of small r and small $L-r$. These results can be straightforwardly generalized to a larger number of targets using the formalism developed in [24].

5. MFPT for fractional Brownian motion

Expressions (16) and (53) are valid for any continuous, compact, self-similar and Markovian 1D random walk. Fractional Brownian motion (FBM) shares all these properties except for

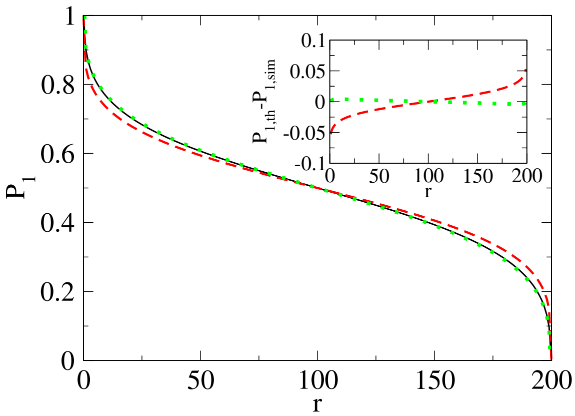

Figure 7. Splitting probability for Lévy flights on a network of size 200, for $d_w = 1.25$, in discrete time (black line), compared to the theoretical expression (53) (red dashed line), and to the exact expression (52) where the first subleading term of the MFPT of equation (47) is taken into account (green dotted line). The inset shows the difference between the two theoretical expressions ($P_{1,\text{th}}$) and the simulation ($P_{1,\text{sim}}$).

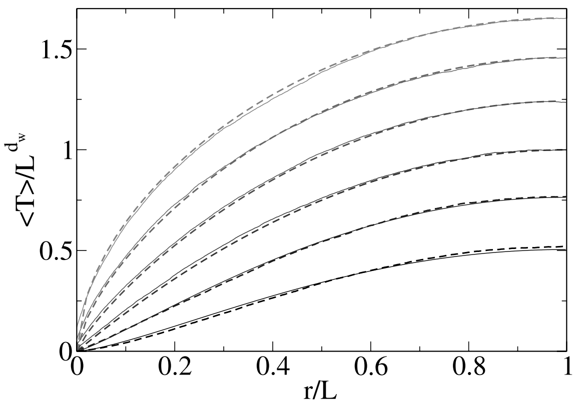

Figure 8. MFPT for an FBM, for several values of the Hurst exponent $H = 1/d_w$ (0.40, 0.45, 0.50, 0.55, 0.60 and 0.65, from black (bottom) to light gray (top) as H grows). The continuous lines represent the simulations results, and the dashed lines the theoretical expressions following equation (16), where A is a fitting parameter.

the Markov condition. FBM is defined as a continuous-time Gaussian process with zero mean and stationary increments. More specifically, FBM is defined through the Langevin equation

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = \xi(t) \tag{54}$$

for the position $x(t)$, which is driven by the stationary, fractional Gaussian noise $\xi(t)$ with $\langle \xi(t) \rangle = 0$ and the long-ranged noise correlation [26]

$$\langle \xi(t_1)\xi(t_2) \rangle = 2H(2H-1)|t_1 - t_2|^{2H-2} + 4H|t_1 - t_2|^{2H-1}\delta(t_1 - t_2), \tag{55}$$

where we chose a unity diffusion constant. This process has the following covariance:

$$\langle x(t)x(s) \rangle = \tfrac{1}{2}(|t|^{2H} + |s|^{2H} - |t-s|^{2H}). \tag{56}$$

For subdiffusive processes ($H < 1/2$), the underlying fractional Gaussian noise (55) is anticorrelated, while it is positively correlated in the superdiffusive case ($1/2 < H < 1$).

To test numerically the applicability of our above results to non-Markovian processes, we performed simulations of FBM and compared the MFPT to a target for this process with expression (16). The results shown in figure 8 demonstrate that expression (16) with free parameter A provides a surprisingly good approximation of the MFPT for FBM, even though this process is highly non-Markovian (see also the discussion in [27]). These numerical findings suggest that memory effects do not play an overly crucial role in the determination of MFPTs for FBM, and that the range of applications of the approach developed herein in practice extends to examples of non-Markovian processes.

6. Conclusion and summary

To conclude, we obtained a functional equation for the MFPT of a generic self-similar Markovian continuous process to a target in a 1D domain and derived its exact solution. We showed that such a continuous limit of the MFPT is actually different from the large system size limit for discrete jump processes allowing leapovers. In the leapover case, the large system size limit of the MFPT involves non-vanishing corrections, which we call residual MFPT. This residual time can have important consequences in the context of both search processes and numerical simulations of first-passage times of random walks. We have investigated in detail the case of Lévy flights and validated our results by numerical simulations. We also demonstrated numerically that our results apply with surprising accuracy to FBM, despite its non-Markovian nature.

Acknowledgments

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References

[1] Hughes B 1995 *Random Walks and Random Environments* (New York: Oxford University Press)
[2] Redner S 2001 *A Guide to First-Passage Processes* (Cambridge: Cambridge University Press)
[3] Rice S A 1985 *Diffusion-Limited Reactions* vol 25 (Amsterdam: Elsevier)
[4] Hänggi P, Talkner P and Borkovec M 1990 *Rev. Mod. Phys.* **62** 251–341
[5] Bénichou O, Loverdo C, Moreau M and Voituriez R 2008 *Phys. Chem. Chem. Phys.* **10** 7059
[6] Lloyd A L and May R M 2001 *Science* **292** 1316
[7] Benichou O, Coppey M, Moreau M, Suet P-H and Voituriez R 2005 *Phys. Rev. Lett.* **94** 198101
[8] Benichou O, Loverdo C, Moreau M and Voituriez R 2006 *Phys. Rev.* E **74** 020102
[9] Shlesinger M F 2006 *Nature* **443** 281
[10] Lomholt M A, Tal K, Metzler R and Joseph K 2008 *Proc. Natl Acad. Sci.* **105** 11055
[11] Condamin S *et al* 2007 *Nature* **450** 77
Benichou O, Meyer B, Tejedor V and Voituriez R 2008 *Phys. Rev. Lett.* **101** 130601
Benichou O and Voituriez R 2008 *Phys. Rev. Lett.* **100** 168105
[12] Tejedor V, Bénichou O and Voituriez R 2009 *Phys. Rev.* E **80** 065104
[13] Bénichou O, Chevalier C, Klafter J, Meyer B and Voituriez R 2010 *Nat. Chem.* **2** 472
[14] Ben-Avraham D and Havlin S 2000 *Diffusion and Reactions in Fractals and Disordered Systems* (Cambridge: Cambridge University Press)
[15] Bouchaud J-P and Georges A 1990 *Phys. Rep.* **195** 127
[16] Metzler R and Klafter J 2000 *Phys. Rep.* **339** 1
[17] Metzler R and Klafter J 2004 *J. Phys. A: Math. Gen.* **37** R161
[18] Chechkin A V, Metzler R, Gonchar V Y, Klafter J and Tanatarov L V 2003 *J. Phys. A: Math. Gen.* **36** L537

[19] Eliazar I and Klafter J 2003 *Physica* A **330** 8
[20] Koren T, Lomholt M A, Chechkin A V, Klafter J and Metzler R 2007 *Phys. Rev. Lett.* **99** 160602
[21] Pólya G 1920 *Mathematische Zeitschrift* **8** 171
[22] Gnedenko B V and Kolmogorov A N 1954 *Limit Distributions for Sums of Independent Random Variables* (Reading, MA: Addison-Wesley)
[23] Montroll E W and Weiss G H 1965 *J. Math. Phys.* **6** 167
[24] Chevalier C, Benichou O, Meyer B and Voituriez R 2011 *J. Phys. A: Math. Theor.* **44** 025002
[25] Condamin S, Benichou O and Moreau M 2007 *Phys. Rev. E* **75** 021111
[26] Mandelbrot B B and Ness J W V 1968 *SIAM Rev.* **10** 422
[27] Sliusarenko O Y, Gonchar V Y, Chechkin A V, Sokolov I M and Metzler R 2010 *Phys. Rev.* E **81** 041119