On Distributions of Functionals of Anomalous Diffusion Paths

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Abstract Functionals of Brownian motion have diverse applications in physics, mathematics, and other fields. The probability density function (PDF) of Brownian functionals satisfies the Feynman-Kac formula, which is a Schrödinger equation in imaginary time. In recent years there is a growing interest in particular functionals of non-Brownian motion, or anomalous diffusion, but no equation existed for their PDF. Here, we derive a *fractional* generalization of the Feynman-Kac equation for functionals of anomalous paths based on sub-diffusive continuous-time random walk. We also derive a backward equation and a generalization to Lévy flights. Solutions are presented for a wide number of applications including the occupation time in half space and in an interval, the first passage time, the maximal displacement, and the hitting probability. We briefly discuss other fractional Schrödinger equations that recently appeared in the literature.

1 Introduction

A Brownian functional is defined as $A = \int_0^t U[x(\tau)]d\tau$, where $x(t)$ is a trajectory of a Brownian particle and $U(x)$ is a prescribed function [1]. Functionals of diffusive motion arise in numerous problems across a variety of scientific fields from condensed matter physics [2–4], to hydrodynamics [5], meteorology [6], and finance [7, 8]. The distribution of these functionals satisfies a Schrödinger-like equation, derived in 1949 by Kac inspired by Feynman's path integrals [9]. Denote by $G(x, A, t)$ the joint probability density function

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(PDF) of finding, at time t, the particle at x and the functional at A. The Feynman-Kac theory asserts that (for $U(x) > 0$) [1, 9]

$$\frac{\partial}{\partial t}G(x, p, t) = K\frac{\partial^2}{\partial x^2}G(x, p, t) - pU(x)G(x, p, t), \tag{1}$$

where the equation is in Laplace space, $A \to p$, and K is the diffusion coefficient.

The celebrated Feynman-Kac equation (1) describes functionals of normal Brownian motion. However, we know today that in a vast number of systems the underlying processes exhibit anomalous, non-Brownian sub-diffusion, as reflected by the nonlinear relation: $\langle x^2 \rangle \sim t^\alpha$, $0 < \alpha < 1$ [10–14]. While a few specific functionals of anomalous paths have been investigated [15, 16], a general theory is still missing.

Several functionals of anomalous diffusion are of interest. For example, the time spent by a particle in a given domain, or the occupation time, is given by the functional $A = \int_0^t U[x(\tau)]d\tau$, where $U(x) = 1$ in the domain and is zero otherwise [17–20]. Such a functional can be used in kinetic studies of chemical reactions that take place exclusively in the domain. Consider for example a particle diffusing in a medium containing an interval that is absorbing at rate R. The average survival probability of the particle is $\langle \exp(-RA) \rangle$ [21]. Two other related functionals are the occupation time in the positive half-space ($U(x) = \Theta(x)$) and the local time ($U(x) = \delta(x)$) [15, 16, 22–24].

Another interesting family of functionals arises in the study of NMR [25]. In a typical NMR experiment, the macroscopic measured signal can be written as $E = \langle e^{i\varphi} \rangle$ where $\varphi = \gamma \int_0^t B[x(\tau)]d\tau$ is the phase accumulated by each spin, γ is the gyromagnetic ratio, $B(x)$ is a spatially-inhomogeneous external magnetic field, and $x(\tau)$ is the trajectory of each particle. NMR therefore indirectly encodes information regarding the motion of the particles. Common choices of the magnetic field B are $B(x) = x$ and $B(x) = x^2$ [25]. For dispersive systems with inhomogeneous disorder where the motion of the particles is non-Brownian, the phase φ is a non-Brownian functional with $U(x) = x$ or $U(x) = x^2$.

In this paper, we develop a general theory of non-Brownian functionals. The process we consider as the mechanism that leads to non-Brownian transport is the sub-diffusive continuous-time random-walk (CTRW). This is an important and widely investigated process that is frequently used to describe the motion of particles in disordered systems [10–12, 26, 27]. In the scaling limit of this process, we derive the following *fractional* Feynman-Kac equation:

$$\frac{\partial}{\partial t}G(x, p, t) = K_\alpha\frac{\partial^2}{\partial x^2}\mathcal{D}_t^{1-\alpha}G(x, p, t) - pU(x)G(x, p, t), \tag{2}$$

where the symbol $\mathcal{D}_t^{1-\alpha}$ is Friedrich's *substantial fractional derivative* and is equal in Laplace space $t \to s$ to $[s + pU(x)]^{1-\alpha}$ [28]. In the rest of the paper, we derive (2) and its backward version and then investigate applications for specific functionals of interest. A brief report of part of the results has recently appeared in [29].

2 Derivation of the Equations

We use the continuous-time random-walk (CTRW) model as the underlying process leading to anomalous diffusion [10–12, 26, 27]. In CTRW, an infinite one-dimensional lattice with spacing a is assumed, and allowed jumps are to nearest neighbors only and with equal probability of jumping left or right. Waiting times between jump events are independent

identically distributed random variables with PDF $\psi(\tau)$, and the process starts with a particle at $x = x_0$. The particle waits at x_0 for time τ drawn from $\psi(\tau)$ and then jumps with probability $1/2$ to either $x_0 + a$ or $x_0 - a$, after which the process is renewed. We assume that no external forces are applied and that for long waiting times, $\psi(\tau) \sim B_\alpha \tau^{-(1+\alpha)}/|\Gamma(-\alpha)|$. For $0 < \alpha < 1$, the average waiting time is infinite and the process is sub-diffusive with $\langle x^2 \rangle = 2K_\alpha t^\alpha / \Gamma(1 + \alpha)$ ($K_\alpha = a^2/(2B_\alpha)$, units m^2/sec$^\alpha$) [30]. We look for the differential equation that describes the distribution of functionals in the scaling limit of this model.

2.1 Derivation of the Fractional Feynman-Kac Equation

Recall that the functional is defined as $A = \int_0^t U[x(\tau)]d\tau$ and that $G(x, A, t)$ is the joint PDF of x and A at time t. For the particle to be at (x, A) at time t, it must have been at $[x, A - \tau U(x)]$ at the time $t - \tau$ immediately after the last jump was made. Let $Q_n(x, A, t)dt$ be the probability of the particle to make its nth jump into (x, A) in the time interval $[t, t + dt]$. Thus,

$$G(x, A, t) = \int_0^t W(\tau) \sum_{n=0}^\infty Q_n[x, A - \tau U(x), t - \tau]d\tau, \tag{3}$$

where $W(\tau) = 1 - \int_0^\tau \psi(\tau')d\tau'$ is the probability for *not* moving in a time interval of length τ.

To arrive into (x, A) after $n + 1$ jumps, the particle must have arrived after n jumps into either $[x - a, A - \tau U(x - a)]$ or $[x + a, A - \tau U(x + a)]$, where τ the time between the jumps. Since the probabilities of jumping left and right are equal, we can write a recursion relation for Q_n:

$$Q_{n+1}(x, A, t) = \int_0^t \psi(\tau) \left\{ \frac{1}{2} Q_n[x + a, A - \tau U(x + a), t - \tau] \right.$$
$$\left. + \frac{1}{2} Q_n[x - a, A - \tau U(x - a), t - \tau] \right\} d\tau, \tag{4}$$

where $\psi(\tau)$ is the PDF of τ, the time between jumps. For $n = 0$ (no jumps were made), $Q_0 = \delta(x - x_0)\delta(A)\delta(t)$.

Assume that $U(x) \geq 0$ for all x and thus $A \geq 0$ (an assumption we will relax later). Let $Q_n(x, p, t)$ be the Laplace transform $A \to p$ of $Q_n(x, A, t)$—we use along this work the convention that the variables in parenthesis define the space we are working in. We note that

$$\int_0^\infty e^{-pA} Q_n[x, A - \tau U(x), t]dA = e^{-p\tau U(x)} \int_0^\infty e^{-pA'} Q_n(x, A', t)dA'$$
$$= e^{-p\tau U(x)} Q_n(x, p, t),$$

where we used the fact that $Q_n(x, A, t) = 0$ for $A < 0$. Thus, Laplace transforming $A \to p$ equation (4) we find

$$Q_{n+1}(x, p, t) = \frac{1}{2} \int_0^t \psi(\tau) e^{-p\tau U(x+a)} Q_n(x + a, p, t - \tau)d\tau$$
$$+ \frac{1}{2} \int_0^t \psi(\tau) e^{-p\tau U(x-a)} Q_n(x - a, p, t - \tau)d\tau. \tag{5}$$

Laplace transforming $t \to s$ equation (5) using the convolution theorem,

$$Q_{n+1}(x, p, s) = \frac{1}{2}\hat{\psi}[s + pU(x + a)]Q_n(x + a, p, s)$$

$$+ \frac{1}{2}\hat{\psi}[s + pU(x - a)]Q_n(x - a, p, s), \qquad (6)$$

where $\hat{\psi}(s)$ is the Laplace transform of the waiting time PDF. Fourier transforming $x \to k$ equation (6),

$$Q_{n+1}(k, p, s) = \cos(ka) \int_{-\infty}^{\infty} e^{ikx}\hat{\psi}[s + pU(x)]Q_n(x, p, s)dx.$$

Applying the Fourier transform identity $\mathcal{F}\{xf(x)\} = -i\frac{\partial}{\partial k}f(k)$,

$$Q_{n+1}(k, p, s) = \cos(ka)\hat{\psi}\left[s + pU\left(-i\frac{\partial}{\partial k}\right)\right]Q_n(k, p, s). \qquad (7)$$

Note that the order of the terms is important: $\hat{\psi}[s + pU(-i\frac{\partial}{\partial k})]$ does not commute with $\cos(ka)$. Summing (7) over all n, using the initial condition $Q_0(k, p, s) = e^{ikx_0}$, and rearranging, we obtain,

$$\sum_{n=0}^{\infty} Q_n(k, p, s) = \left\{1 - \cos(ka)\hat{\psi}\left[s + pU\left(-i\frac{\partial}{\partial k}\right)\right]\right\}^{-1} e^{ikx_0}. \qquad (8)$$

We next use our expression for $\sum_{n=0}^{\infty} Q_n$ to calculate $G(x, A, t)$. Transforming (3) $(x, A, t) \to (k, p, s)$,

$$G(k, p, s) = \frac{1 - \hat{\psi}\left[s + pU\left(-i\frac{\partial}{\partial k}\right)\right]}{s + pU\left(-i\frac{\partial}{\partial k}\right)} \sum_{n=0}^{\infty} Q_n(k, p, s), \qquad (9)$$

where we used $\hat{W}(s) = \int_0^{\infty} e^{-st}[1 - \int_0^t \psi(\tau)d\tau]dt = [1 - \hat{\psi}(s)]/s$. Substituting (8) into (9), we find the formal solution

$$G(k, p, s) = \frac{1 - \hat{\psi}\left[s + pU\left(-i\frac{\partial}{\partial k}\right)\right]}{s + pU\left(-i\frac{\partial}{\partial k}\right)}$$

$$\times \left\{1 - \cos(ka)\hat{\psi}\left[s + pU\left(-i\frac{\partial}{\partial k}\right)\right]\right\}^{-1} e^{ikx_0}. \qquad (10)$$

To derive a differential equation for $G(x, p, t)$, we recall the waiting time distribution is $\psi(t) \sim B_\alpha t^{-(1+\alpha)}/|\Gamma(-\alpha)|$ and write its Laplace transform $\hat{\psi}(s)$ for $s \to 0$ as [12]

$$\hat{\psi}(s) \sim 1 - B_\alpha s^\alpha; \quad 0 < \alpha < 1, \ s \to 0. \qquad (11)$$

Substituting (11) into (10), applying the small k expansion $\cos(ka) \sim 1 - k^2a^2/2$, and neglecting the high order terms, we have

$$G(k, p, s) = \left[s + pU\left(-i\frac{\partial}{\partial k}\right)\right]^{\alpha-1}\left\{K_\alpha k^2 + \left[s + pU\left(-i\frac{\partial}{\partial k}\right)\right]^\alpha\right\}^{-1} e^{ikx_0},$$

where we used the generalized diffusion coefficient $K_\alpha \equiv \lim_{a^2, B_\alpha \to 0} a^2/(2B_\alpha)$ [30]. By neglecting the high order terms in s and k we effectively reach the scaling limit of the lattice walk [31–33]. Rearranging the expression in the last equation we find

$$sG(k, p, s) - e^{ikx_0} = -K_\alpha k^2 \left[s + pU\left(-i\frac{\partial}{\partial k}\right) \right]^{1-\alpha} G(k, p, s)$$

$$- pU\left(-i\frac{\partial}{\partial k}\right) G(k, p, s).$$

Inverting $k \to x, s \to t$ we finally obtain our fractional Feynman-Kac equation

$$\frac{\partial}{\partial t}G(x, p, t) = K_\alpha \frac{\partial^2}{\partial x^2}\mathcal{D}_t^{1-\alpha}G(x, p, t) - pU(x)G(x, p, t). \qquad (12)$$

The initial condition is $G(x, A, t = 0) = \delta(x - x_0)\delta(A)$, or $G(x, p, t = 0) = \delta(x - x_0)$.

$\mathcal{D}_t^{1-\alpha}$ is the fractional substantial derivative operator introduced in [28]:

$$\mathcal{D}_t^{1-\alpha}G(x, p, s) = [s + pU(x)]^{1-\alpha}G(x, p, s). \qquad (13)$$

In t space,

$$\mathcal{D}_t^{1-\alpha}G(x, p, t) = \frac{1}{\Gamma(\alpha)}\left[\frac{\partial}{\partial t} + pU(x)\right]\int_0^t \frac{e^{-(t-\tau)pU(x)}}{(t-\tau)^{1-\alpha}}G(x, p, \tau)d\tau. \qquad (14)$$

Thus, due to the long waiting times, the evolution of $G(x, p, t)$ is non-Markovian and depends on the entire history.

In s space, the fractional Feynman-Kac equation reads

$$sG(x, p, s) - \delta(x - x_0) = K_\alpha \frac{\partial^2}{\partial x^2}[s + pU(x)]^{1-\alpha}G(x, p, s) - pU(x)G(x, p, s). \qquad (15)$$

A few remarks should be made.

(i) *The integer Feynman-Kac equation.*—As expected, for $\alpha = 1$ our fractional equation (12) reduces to the (integer) Feynman-Kac equation (1).

(ii) *The fractional diffusion equation.*—For $p = 0$, $G(x, p = 0, t) = \int_0^\infty G(x, A, t)dA$ reduces to $G(x, t)$, the marginal PDF of finding the particle at x at time t regardless of the value of A. Correspondingly, (10) reduces to the well-known Montroll-Weiss CTRW equation (for $x_0 = 0$) [12, 26]:

$$G(k, p = 0, s) = \frac{1 - \hat{\psi}(s)}{s}\frac{1}{1 - \cos(ka)\hat{\psi}(s)}.$$

Equation (12) reduces to the fractional diffusion equation:

$$\frac{\partial}{\partial t}G(x, t) = K_\alpha \frac{\partial^2}{\partial x^2}\mathcal{D}_{\mathrm{RL},t}^{1-\alpha}G(x, t), \qquad (16)$$

where $\mathcal{D}_{\mathrm{RL},t}^{1-\alpha}$ is the Riemann-Liouville fractional derivative operator ($\mathcal{D}_{\mathrm{RL},t}^{1-\alpha}G(x, s) \to s^{1-\alpha}G(x, s)$ in Laplace $t \to s$ space) [12, 34].

(iii) *The scaling limit.*—To derive our main result—the differential equation (12)—we used the scaling, or continuum, limit to CTRW [30–33]. In this limit, we take $a \to 0$ and

$B_\alpha \to 0$, but keep $K_\alpha = a^2/(2B_\alpha)$ finite. Recently, trajectories of this process were shown to obey a certain class of stochastic Langevin equations [35–37], hence giving these paths a mathematical meaning.

(iv) *How to solve the fractional Feynman-Kac equation.*—To obtain the PDF of a functional A, the following recipe could be followed [1]:

1. Solve (15), the fractional Feynman-Kac equation in (x, p, s) space. Equation (15) is a second order, ordinary differential equation in x.
2. Integrate the solution over all x to eliminate the dependence on the final position of the particle.
3. Invert the solution $(p, s) \to (A, t)$, to obtain $G(A, t)$, the PDF of A at time t.

We will later see (Sect. 2.2) that the second step can be circumvented by using a backward equation.

(v) *A general functional.*—When the functional is not necessarily positive, the Laplace transform $A \to p$ must be replaced by a Fourier transform. We show in the Appendix that in this case the fractional Feynman-Kac equation looks like (12), but with p replaced by $-ip$,

$$\frac{\partial}{\partial t} G(x, p, t) = K_\alpha \frac{\partial^2}{\partial x^2} \mathcal{D}_t^{1-\alpha} G(x, p, t) + ipU(x)G(x, p, t), \tag{17}$$

where $G(x, p, t)$ is the Fourier transform $A \to p$ of $G(x, A, t)$ and $\mathcal{D}_t^{1-\alpha} \to [s - ipU(x)]^{1-\alpha}$ in Laplace s space.

(vi) *Lévy flights.*—Consider CTRW with displacements Δ_x distributed according to a symmetric PDF $f(\Delta_x) \sim |\Delta_x|^{-(1+\mu)}$, with $0 < \mu < 2$. For this distribution, the characteristic function is $f(k) \sim 1 - C_\mu |k|^\mu$ [12]. This process is known as a Lévy flight, and as we show in the Appendix, the fractional Feynman-Kac equation for this case is (for $A \geq 0$)

$$\frac{\partial}{\partial t} G(x, p, t) = K_{\alpha,\mu} \nabla_x^\mu \mathcal{D}_t^{1-\alpha} G(x, p, t) - pU(x)G(x, p, t), \tag{18}$$

where $K_{\alpha,\mu} = C_\mu/B_\alpha$ (units m$^\mu$/sec$^\alpha$), and $\mathcal{D}_t^{1-\alpha}$ is the substantial fractional derivative operator defined above (13), (14). ∇_x^μ is the Riesz spatial fractional derivative operator defined in Fourier $x \to k$ space as $\nabla_x^\mu \to -|k|^\mu$ [12].

2.2 A Backward Equation

In many cases we are only interested in the distribution of the functional, A, regardless of the final position of the particle, x. Therefore, it turns out quite convenient (see Sect. 3) to obtain an equation for $G_{x_0}(A, t)$—the PDF of A at time t, given that the process has started at x_0.

According to the CTRW model, the particle, after its first jump at time τ, is at either $x_0 - a$ or $x_0 + a$. Alternatively, the particle does not move at all during the measurement time $[0, t]$. Hence,

$$G_{x_0}(A, t) = \int_0^t \psi(\tau) \left\{ \frac{1}{2} G_{x_0+a}[A - \tau U(x_0), t - \tau] + \frac{1}{2} G_{x_0-a}[A - \tau U(x_0), t - \tau] \right\} d\tau$$

$$+ W(t)\delta[A - tU(x_0)]. \tag{19}$$

Here, $\tau U(x_0)$ is the contribution to A from the pausing time at x_0 in the time interval $[0, \tau]$. The last term on the right hand side of (19) describes a motionless particle, for which $A(t) =$

$tU(x_0)$. We now Laplace transform (19) with respect to A and t, using techniques similar to those used in the previous subsection. This leads to (for $A \geq 0$)

$$G_{x_0}(p, s) = \frac{1}{2} \hat{\psi}[s + pU(x_0)] \left[G_{x_0+a}(p, s) + G_{x_0-a}(p, s) \right] + \frac{1 - \hat{\psi}[s + pU(x_0)]}{s + pU(x_0)}.$$

Fourier transform $x_0 \to k_0$ of the last equation results in

$$G_{k_0}(p, s) = \hat{\psi}\left[s + pU\left(-i\frac{\partial}{\partial k_0}\right)\right] \cos(k_0 a) G_{k_0}(p, s) + \frac{1 - \hat{\psi}\left[s + pU\left(-i\frac{\partial}{\partial k_0}\right)\right]}{s + pU\left(-i\frac{\partial}{\partial k_0}\right)} \delta(k_0).$$

As before, writing $\hat{\psi}(s) \sim 1 - B_\alpha s^\alpha$ and $\cos(k_0 a) \sim 1 - a^2 k_0^2/2$, we have

$$\left[s + pU\left(-i\frac{\partial}{\partial k_0}\right)\right]^\alpha G_{k_0}(p, s) + K_\alpha k_0^2 G_{k_0}(p, s) = \left[s + pU\left(-i\frac{\partial}{\partial k_0}\right)\right]^{\alpha-1} \delta(k_0),$$

where we used the generalized diffusion coefficient $K_\alpha = a^2/(2B_\alpha)$. Operating on both sides with $[s + pU(-i\frac{\partial}{\partial k_0})]^{1-\alpha}$,

$$sG_{k_0}(p, s) - \delta(k_0) = -K_\alpha \left[s + pU\left(-i\frac{\partial}{\partial k_0}\right)\right]^{1-\alpha} k_0^2 G_{k_0}(p, s)$$

$$- pU\left(-i\frac{\partial}{\partial k_0}\right) G_{k_0}(p, s).$$

Inverting $k_0 \to x_0$ and $s \to t$, we obtain the backward fractional Feynman-Kac equation:

$$\frac{\partial}{\partial t} G_{x_0}(p, t) = K_\alpha \mathcal{D}_t^{1-\alpha} \frac{\partial^2}{\partial x_0^2} G_{x_0}(p, t) - pU(x_0) G_{x_0}(p, t). \tag{20}$$

Here, $\mathcal{D}_t^{1-\alpha}$ equals in Laplace $t \to s$ space $[s + pU(x_0)]^{1-\alpha}$. The initial condition is $G_{x_0}(A, t = 0) = \delta(A)$, or $G_{x_0}(p, t = 0) = 1$. In (12) the operators depend on x while in (20) they depend on x_0. Therefore, (12) is called the forward equation while (20) is called the backward equation. Notice that here, the fractional derivative operator appears to the left of the Laplacian $\partial^2/\partial x_0^2$, in contrast to the forward equation (12).

In the general case when the functional is not necessarily positive and jumps are distributed according to a symmetric PDF $f(\Delta_x) \sim |\Delta_x|^{-(1+\mu)}$, $0 < \mu < 2$, the backward equation becomes (see the Appendix)

$$\frac{\partial}{\partial t} G_{x_0}(p, t) = K_{\alpha,\mu} \mathcal{D}_t^{1-\alpha} \nabla_{x_0}^\mu G_{x_0}(p, t) + ipU(x_0) G_{x_0}(p, t). \tag{21}$$

Here, p is the Fourier pair of A, $\mathcal{D}_t^{1-\alpha} \to [s - ipU(x_0)]^{1-\alpha}$ in Laplace $t \to s$ space, and $\nabla_{x_0}^\mu \to -|k_0|^\mu$ in Fourier $x_0 \to k_0$ space (see also comments (v) and (vi) at the end of Sect. 2.1 above).

3 Applications

In this section, we describe a number of ways by which our equations can be solved to obtain the distribution, the moments, and other properties of functionals of interest.

3.1 Occupation time in Half-Space

Define the occupation time of a particle in the positive half-space as $T_+ = \int_0^t \Theta[x(\tau)]d\tau$ ($\Theta(x) = 1$ for $x \geq 0$ and is zero otherwise) [15, 16, 23]. To find the distribution of occupation times, we consider the backward equation ((20), transformed $t \to s$):

$$sG_{x_0}(p,s) - 1 = \begin{cases} K_\alpha s^{1-\alpha} \frac{\partial^2}{\partial x_0^2} G_{x_0}(p,s) & x_0 < 0, \\ K_\alpha(s+p)^{1-\alpha} \frac{\partial^2}{\partial x_0^2} G_{x_0}(p,s) - pG_{x_0}(p,s) & x_0 > 0. \end{cases} \tag{22}$$

These are second order, ordinary differential equations in x_0. Solving the equations in each half-space separately, demanding that $G_{x_0}(p,s)$ is finite for $|x_0| \to \infty$,

$$G_{x_0}(p,s) = \begin{cases} C_0 \exp(x_0 s^{\alpha/2}/\sqrt{K_\alpha}) + \frac{1}{s} & x_0 < 0, \\ C_1 \exp[-x_0(s+p)^{\alpha/2}/\sqrt{K_\alpha}] + \frac{1}{s+p} & x_0 > 0. \end{cases} \tag{23}$$

For $x_0 \to -\infty$, the particle is never at $x > 0$ and thus $G_{x_0}(T_+,t) = \delta(T_+)$ and $G_{x_0}(p,s) = s^{-1}$, in accordance with (23). Similarly, for $x_0 \to +\infty$, $G_{x_0}(T_+,t) = \delta(T_+ - t)$ and $G_{x_0}(p,s) = (s+p)^{-1}$. Demanding that $G_{x_0}(p,s)$ and its first derivative are continuous at $x_0 = 0$, we obtain a pair of equations for C_0, C_1:

$$C_0 + s^{-1} = C_1 + (s+p)^{-1}; \qquad C_0 s^{\alpha/2} = -C_1(s+p)^{\alpha/2},$$

whose solution is

$$C_0 = -\frac{p(s+p)^{\alpha/2-1}}{s[s^{\alpha/2} + (s+p)^{\alpha/2}]}; \qquad C_1 = \frac{ps^{\alpha/2-1}}{(s+p)[s^{\alpha/2} + (s+p)^{\alpha/2}]}.$$

Assuming the process starts at $x_0 = 0$, $G_0(p,s) = C_1 + (s+p)^{-1}$, or, after some simplifications:

$$G_0(p,s) = \frac{s^{\alpha/2-1} + (s+p)^{\alpha/2-1}}{s^{\alpha/2} + (s+p)^{\alpha/2}}. \tag{24}$$

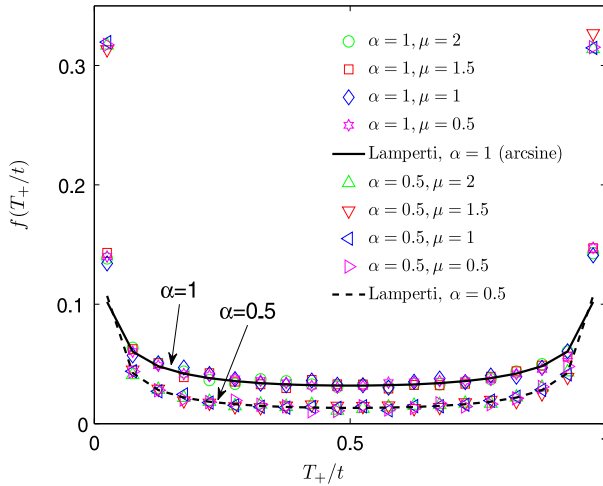Using [38], the PDF of $p_+ \equiv T_+/t$, for long times, is the (symmetric) *Lamperti* PDF:

$$f(p_+) = \frac{\sin(\pi\alpha/2)}{\pi} \frac{(p_+)^{\alpha/2-1}(1-p_+)^{\alpha/2-1}}{(p_+)^\alpha + (1-p_+)^\alpha + 2(p_+)^{\alpha/2}(1-p_+)^{\alpha/2}\cos(\pi\alpha/2)}. \tag{25}$$

This equation has been previously derived using different methods [16, 22, 38, 39] and was also shown to describe occupation times of on and off states in blinking quantum dots [40–42]. Naively, one expects the particle to spend about half the time at $x > 0$. In contrast, we learn from (25) that the particle tends to spend most of the time at either $x > 0$ or $x < 0$: $f(p_+)$ has two peaks at $p_+ = 1$ and $p_+ = 0$ (Fig. 1). This is exacerbated in the limit $\alpha \to 0$, where the distribution converges to two delta functions at $p_+ = 1$ and at $p_+ = 0$. For $\alpha = 1$ (Brownian motion) we recover the well-known arcsine law of Lévy [1, 15, 16, 43].

We note that the PDF (25) is a special case of the more general, two-parameter Lamperti PDF [16]:

$$f(\mathcal{R}, p_+) = \frac{\sin(\pi\alpha/2)}{\pi}$$
$$\times \frac{\mathcal{R}(p_+)^{\alpha/2-1}(1-p_+)^{\alpha/2-1}}{(p_+)^\alpha + \mathcal{R}^2(1-p_+)^\alpha + 2\mathcal{R}(p_+)^{\alpha/2}(1-p_+)^{\alpha/2}\cos(\pi\alpha/2)}, \tag{26}$$

Fig. 1 (Color online) The PDF of the occupation fractions in half-space T_+/t. Trajectories of diffusing particles were generated using the methods of [36, 37, 45] with parameter values $\Delta\tau = \overline{\Delta\tau} = 10^{-3}$, $\Delta t = 10^{-2}$ (as defined in [36]), $K_\alpha = 1$, and $x_0 = 0$. Simulations ended at $t = 10^4$ and included 10^4 trajectories. Simulation results for $\alpha = 0.5, 1$ and $\mu = 0.5, 1, 1.5, 2$ (see (21)) are shown as symbols (see legend). Theoretical curves correspond to Lamperti's PDF, (25) (the arcsine distribution for $\alpha = 1$), and are plotted as a *solid line* for $\alpha = 1$ and as a *dashed line* for $\alpha = 0.5$. It can be seen that the distribution of occupation fractions is determined by α but not by μ

where $\mathcal{R}$ is the asymmetry parameter. In (25), $\mathcal{R} = 1$ as a result of the symmetry of the walk. Consider, for example, the case when in (22) the diffusion coefficient is $K_\alpha^<$ for $x < 0$ and $K_\alpha^>$ for $x > 0$. Solving the equations as above, we obtain for $f(p_+)$ the two-parameter Lamperti distribution, (26), with $\mathcal{R} = \sqrt{K_\alpha^< / K_\alpha^>}$.

Kac proved in 1951 that for $\alpha = 1$ (Markovian random-walk), the occupation time distributions of both Brownian motion and Lévy flights obey the same arcsine law [44]. It was therefore interesting to find out whether a similar statement holds for $\alpha < 1$. We could not solve the Lévy flights analog of (22); therefore, we simulated trajectories whose PDF satisfies the fractional diffusion equation (16) and its generalization to Lévy flights ((18) with $p = 0$). Simulations were performed using the subordination method described in [36, 37, 45]. The results are presented in Fig. 1 and demonstrate that indeed, for $\alpha < 1$, the occupation time distribution is Lamperti's (25) for both $\mu = 2$ and $\mu < 2$ (Lévy flights). This result may be related to the recent finding that the first passage time distribution is also invariant to the value of μ [46].

3.2 First Passage Time

The time t_f when a particle starting at $x_0 = 0$ first hits $x = b$ is called the first passage time and is a quantity subject to many studies in physics and other fields [47]. The distribution of first passage times for anomalous paths can be obtained from our fractional Feynman-Kac equation using an identity due to Kac [44]:

$$\Pr\{t_f > t\} = \Pr\left\{\max_{0 \le \tau \le t} x(\tau) < b\right\} = \lim_{p \to \infty} G_{x_0}(p, t), \qquad (27)$$

where the functional is $A_f = \int_0^t U[x(\tau)]d\tau$, and

$$U(x) = \begin{cases} 0 & x < b, \\ 1 & x > b. \end{cases} \qquad (28)$$

This is true since $G_{x_0}(p,t) = \int_0^\infty e^{-pA_f} G_{x_0}(A_f,t)dA_f$, and thus, if the particle has never crossed $x = b$, we have $A_f = 0$ and $e^{-pA_f} = 1$, while otherwise, $A_f > 0$ and for $p \to \infty$, $e^{-pA_f} = 0$. To find $G_{x_0}(p,t)$ we solve the following backward equation

$$sG_{x_0}(p,s) - 1 = \begin{cases} K_\alpha s^{1-\alpha} \frac{\partial^2}{\partial x_0^2} G_{x_0}(p,s) & x_0 < b, \\ K_\alpha(s+p)^{1-\alpha} \frac{\partial^2}{\partial x_0^2} G_{x_0}(p,s) - pG_{x_0}(p,s) & x_0 > b. \end{cases}$$

Solving these equations as in the previous subsection, demanding that $G_{x_0}(p,s)$ is finite for $|x_0| \to \infty$ and demanding continuity of $G_{x_0}(p,s)$ and its first derivative at $x_0 = b$, we obtain for $x_0 = 0$

$$G_0(p,s) = \frac{1}{s}\left[1 - e^{-\frac{b}{\sqrt{K_\alpha}} s^{\alpha/2}} \frac{p(s+p)^{\alpha/2-1}}{s^{\alpha/2} + (s+p)^{\alpha/2}}\right].$$

To find the first passage time distribution we take the limit of infinite p,

$$\lim_{p\to\infty} G_0(p,s) = \frac{1}{s}\left(1 - e^{-\frac{b}{\sqrt{K_\alpha}} s^{\alpha/2}}\right). \qquad (29)$$

Defining $\tau_f = (b^2/K_\alpha)^{1/\alpha}$, we invert $s \to t$:

$$\lim_{p\to\infty} G_0(p,t) = \Pr\{t_f > t\} = 1 - \int_0^t \frac{1}{\tau_f} l_{\alpha/2}\left(\frac{\tau}{\tau_f}\right)d\tau,$$

where $l_{\alpha/2}(t)$ is the one-sided Lévy distribution of order $\alpha/2$, whose Laplace transform is $l_{\alpha/2}(s) = e^{-s^{\alpha/2}}$. The PDF of the first passage times, $f(t)$, satisfies $f(t) = \frac{\partial}{\partial t}(\Pr\{t_f < t\}) = \frac{\partial}{\partial t}(1 - \Pr\{t_f > t\})$. Thus,

$$f(t) = \frac{1}{\tau_f} l_{\alpha/2}\left(\frac{t}{\tau_f}\right). \qquad (30)$$

This result has been previously derived using different methods (e.g., equation (53) of [48]). The long times behavior of $f(t)$ is obtained from the $s \to 0$ limit:

$$f(s) \sim 1 - \frac{b}{\sqrt{K_\alpha}} s^{\alpha/2}.$$

Therefore, for long times

$$f(t) \sim \frac{b}{|\Gamma\left(-\frac{\alpha}{2}\right)|\sqrt{K_\alpha}} t^{-(1+\alpha/2)}. \qquad (31)$$

For $\alpha = 1$, we reproduce the famous $t^{-3/2}$ decay law of a one-dimensional random walk [47].

3.3 The Maximal Displacement

The maximal displacement of a diffusing particle is a random variable whose study has been of recent interest (see, e.g., [49–52] and references therein). To obtain the distribution of this variable, we use the functional defined in the previous subsection (28). Let $x_m \equiv \max_{0 \le \tau \le t} x(\tau)$, and recall from (27) that $\Pr\{x_m < b\} = \lim_{p \to \infty} G_{x_0}(p, t)$. From the previous subsection we have, for $x_0 = 0$ (29)

$$\Pr\{x_m < b\} = \frac{1}{s}\left(1 - e^{-\frac{b}{\sqrt{K_\alpha}}s^{\alpha/2}}\right).$$

Hence, the PDF of x_m is

$$P(x_m, s) = \frac{s^{\alpha/2-1}}{\sqrt{K_\alpha}} e^{-\frac{x_m}{\sqrt{K_\alpha}}s^{\alpha/2}}.$$

Inverting $s \to t$, we obtain

$$P(x_m, t) = \frac{2}{\alpha\sqrt{K_\alpha}} \frac{t}{(x_m/\sqrt{K_\alpha})^{1+2/\alpha}} l_{\alpha/2}\left[\frac{t}{(x_m/\sqrt{K_\alpha})^{2/\alpha}}\right]; \quad x_m > 0. \tag{32}$$

This PDF has the same shape as the PDF of x up to a scale factor of 2 [30], and it is in agreement with the very recent result of [51], derived using a renormalization group method.

3.4 The Hitting Probability

The probability $Q_L(x_0)$ of a particle starting at $0 < x_0 < L$ to hit L before hitting 0 is called the hitting (or exit) probability. The hitting probability has been investigated long time ago for Brownian particles [47] and more recently for some anomalous processes [53]. For CTRW, it can be calculated using the following functional:

$$U(x) = \begin{cases} 0 & 0 < x < L, \\ \infty & \text{otherwise.} \end{cases} \tag{33}$$

With (33), $A = \int_0^t U[x(\tau)]d\tau = 0$ as long as the particle did not leave the interval $[0, L]$ and is otherwise infinite. Therefore, $G(x, p, t) = \int_0^\infty e^{-pA} G(x, A, t)dA$ represents the probability of the particle to be at x at time t without ever leaving $[0, L]$. This is true for all p, since e^{-pA} is either 0 or 1 regardless of p. At the boundaries, $G(x = 0, p, t) = G(x = L, p, t) = 0$. At $(0, L)$, the forward fractional Feynman-Kac equation (15) reads, in s space,

$$sG(x, s) - \delta(x - x_0) = K_\alpha s^{1-\alpha} \frac{\partial^2}{\partial x^2} G(x, s). \tag{34}$$

Note that (34) does not depend on p and is equivalent to the fractional diffusion equation, (16), with absorbing boundary conditions. The solution of (34) for $x \ne x_0$ is

$$G(x, s) = \begin{cases} C_0 \sinh\left[\frac{s^{\alpha/2}}{\sqrt{K_\alpha}}x\right] & x < x_0, \\ C_1 \sinh\left[\frac{s^{\alpha/2}}{\sqrt{K_\alpha}}(L - x)\right] & x > x_0. \end{cases}$$

Matching the solution at $x = x_0$ and demanding $\frac{\partial}{\partial x} G(x = x_0^+, s) - \frac{\partial}{\partial x} G(x = x_0^-, s) = -\frac{1}{K_\alpha s^{1-\alpha}}$ (from (34)), we have, for $x > x_0$,

$$G(x, s) = \frac{1}{\sqrt{K_\alpha} s^{1-\alpha/2}} \frac{\sinh\left(\frac{s^{\alpha/2}}{\sqrt{K_\alpha}} x_0\right)}{\sinh\left(\frac{s^{\alpha/2}}{\sqrt{K_\alpha}} L\right)} \sinh\left[\frac{s^{\alpha/2}}{\sqrt{K_\alpha}} (L - x)\right]; \quad x > x_0. \tag{35}$$

The flux of particles that have never before left $[0, L]$ and that are leaving $[0, L]$ at time t through the right boundary is [54]

$$J(L, t) = -K_\alpha \mathcal{D}_{\text{RL},t}^{1-\alpha} \frac{\partial}{\partial x} G(x = L, t),$$

where $\mathcal{D}_{\text{RL},t}^{1-\alpha}$ is the Riemann-Liouville fractional derivative, equal to $s^{1-\alpha}$ in Laplace $t \to s$ space (see (16)). The hitting probability is the sum over all times of the flux through L [47]:

$$Q_L(x_0) = \int_0^\infty J(L, t) dt = -K_\alpha s^{1-\alpha} \frac{\partial}{\partial x} G(x = L, s)\bigg|_{s=0}.$$

Using (35), we have

$$Q_L(x_0) = \frac{x_0}{L}. \tag{36}$$

The hitting probability for anomalous diffusion, $\alpha < 1$, is the same as in the Brownian case [47]. This is expected, since the hitting probability should not depend on the waiting time PDF $\psi(\tau)$.

Note that a backward equation for $Q_L(x_0)$ can be obtained by the much simpler argument that for unbiased CTRW on a lattice, $Q_L(x_0) = [Q_L(x_0 + a) + Q_L(x_0 - a)]/2$. In the continuum limit, $a \to 0$, this gives $\frac{\partial^2 Q_L(x_0)}{\partial x_0^2} = 0$. With the boundary conditions $Q_L(x_0 = 0) = 0$ and $Q_L(x_0 = L) = 1$, (36) immediately follows (see [47] for a binomial random walk).

3.5 The Time in an Interval

Consider the time-in-interval functional $T_i = \int_0^t U[x(\tau)] d\tau$, where

$$U(x) = \begin{cases} 1 & |x| < b, \\ 0 & |x| > b. \end{cases} \tag{37}$$

Namely, T_i is the total residence time of the particle in the interval $[-b, b]$. Denote by $G_{x_0}(T_i, t)$ the PDF of T_i at time t when the process starts at x_0, and denote by $G_{x_0}(p, s)$ the Laplace transform $T_i \to p$, $t \to s$ of $G_{x_0}(T_i, t)$. $G_{x_0}(p, s)$ satisfies the backward fractional Feynman-Kac equation:

$$s G_{x_0}(p, s) - 1 = \begin{cases} K_\alpha (s + p)^{1-\alpha} \frac{\partial^2}{\partial x_0^2} G_{x_0}(p, s) - p G_{x_0}(p, s) & |x_0| < b, \\ K_\alpha s^{1-\alpha} \frac{\partial^2}{\partial x_0^2} G_{x_0}(p, s) & |x_0| > b. \end{cases} \tag{38}$$

We solve this equation demanding that the solution is finite for $|x_0| \to \infty$,

$$G_{x_0}(p, s) = \begin{cases} C_1 \cosh[x_0(s + p)^{\alpha/2}/\sqrt{K_\alpha}] + \frac{1}{s+p} & |x_0| < b, \\ C_0 \exp[-|x_0| s^{\alpha/2}/\sqrt{K_\alpha}] + \frac{1}{s} & |x_0| > b. \end{cases} \tag{39}$$

Demanding continuity of $G_{x_0}(p, s)$ and its first derivative at $x_0 = b$ we solve for C_1 and then obtain for $x_0 = 0$

$$G_0(p, s) = \frac{p + s\left\{\cosh\left[\frac{(s+p)^{\alpha/2}}{\sqrt{K_\alpha}}b\right] + \frac{(s+p)^{\alpha/2}}{s^{\alpha/2}}\sinh\left[\frac{(s+p)^{\alpha/2}}{\sqrt{K_\alpha}}b\right]\right\}}{s(s + p)\left\{\cosh\left[\frac{(s+p)^{\alpha/2}}{\sqrt{K_\alpha}}b\right] + \frac{(s+p)^{\alpha/2}}{s^{\alpha/2}}\sinh\left[\frac{(s+p)^{\alpha/2}}{\sqrt{K_\alpha}}b\right]\right\}}. \tag{40}$$

In principle, the PDF $G_0(T_i, t)$ can be obtained from (40) by inverse Laplace transforming $p \to T_i$ and $s \to t$. However, we could invert (40) only for $\alpha \to 0$:

$$G_0(T_i, t)_{\alpha \to 0} = (1 - e^{-b/\sqrt{K_0}})\delta(T_i - t) + e^{-b/\sqrt{K_0}}\delta(T_i). \tag{41}$$

This can be intuitively explained as follows. For $\alpha \to 0$, the PDF of x becomes time-independent and approaches $G(x, t) \approx \exp(-|x|/\sqrt{K_0})/(2\sqrt{K_0})$ (equation (A1) in [30]). With probability $\int_{-b}^{b} G(x, t)dx = 1 - e^{-b/\sqrt{K_0}}$, the particle never leaves the region $[-b, b]$ and thus $T_i = t$; with probability $e^{-b/\sqrt{K_0}}$, the particle is almost never at $[-b, b]$ and thus $T_i = 0$.

The first two moments of T_i can be obtained from (40) by

$$\langle T_i \rangle(s) = -\left.\frac{\partial}{\partial p}G_0(p, s)\right|_{p=0} \quad; \quad \langle T_i^2 \rangle(s) = \left.\frac{\partial^2}{\partial p^2}G_0(p, s)\right|_{p=0}.$$

Calculating the derivatives, substituting $p = 0$, and inverting, we obtain, in the long times limit,

$$\begin{aligned}
\langle T_i \rangle &\sim t^{1-\alpha/2}\frac{b}{\sqrt{K_\alpha}\Gamma(2 - \alpha/2)}, \\
\langle T_i^2 \rangle &\sim t^{2-\alpha/2}\frac{2b(1 - \alpha)}{\sqrt{K_\alpha}\Gamma(3 - \alpha/2)} + t^{2-\alpha}\frac{b^2(3\alpha - 1)}{K_\alpha\Gamma(3 - \alpha)}.
\end{aligned} \tag{42}$$

We verified that (42) agrees with simulations (Fig. 2). The average time at $[-b, b]$ scales as $t^{1-\alpha/2}$ since this is the product of the average number of returns to the interval $[-b, b]$ ($\sim t^{\alpha/2}$) and the average time spent at $[-b, b]$ on each visit ($\sim t^{1-\alpha}$; see equation (61) in [16]). We also see that for $\alpha < 1$, the PDF of T_i cannot have a scaling form since $\langle T_i^2 \rangle \sim t^{2-\alpha/2} \not\propto \langle T_i \rangle^2 \sim t^{2-\alpha}$. For $\alpha = 1$, $\langle T_i \rangle \sim t^{1/2}$ and $\langle T_i^2 \rangle \sim t$.

3.6 Survival in a Medium with an Absorbing Interval

A problem related to that of the previous subsection is a medium in which a diffusing particle is absorbed at rate R whenever it is in the interval $[-b, b]$. The survival probability of the particle, S, is related to T_i, the total time at $[-b, b]$, through $S = \exp(-RT_i)$. Thus, if $G_{x_0}(T_i, t)$ is the PDF of T_i at time t, then the $T_i \to R$ Laplace transform $G_{x_0}(R, t) = \int_0^\infty e^{-RT_i}G_{x_0}(T_i, t)dT_i$ equals $\langle S \rangle$, the survival probability averaged over all trajectories [21]. From (40) of the previous subsection we immediately obtain (in Laplace $t \to s$ space and for $x_0 = 0$)

$$\langle S \rangle = G_0(R, s) = \frac{R + s\left\{\cosh\left[\frac{(s+R)^{\alpha/2}}{\sqrt{K_\alpha}}b\right] + \frac{(s+R)^{\alpha/2}}{s^{\alpha/2}}\sinh\left[\frac{(s+R)^{\alpha/2}}{\sqrt{K_\alpha}}b\right]\right\}}{s(s + R)\left\{\cosh\left[\frac{(s+R)^{\alpha/2}}{\sqrt{K_\alpha}}b\right] + \frac{(s+R)^{\alpha/2}}{s^{\alpha/2}}\sinh\left[\frac{(s+R)^{\alpha/2}}{\sqrt{K_\alpha}}b\right]\right\}}, \tag{43}$$

Fig. 2 (Color online) The first two moments of the time-in-interval functional T_i. *Top panel*—first moment; *bottom panel*—second moment. Simulations (*circles*) were performed using the method of [36, 37] with parameters as in Fig. 1. The theoretical curves (*lines*) correspond to the leading terms of (42). The width of the interval (see (37)) is $b = 0.1$
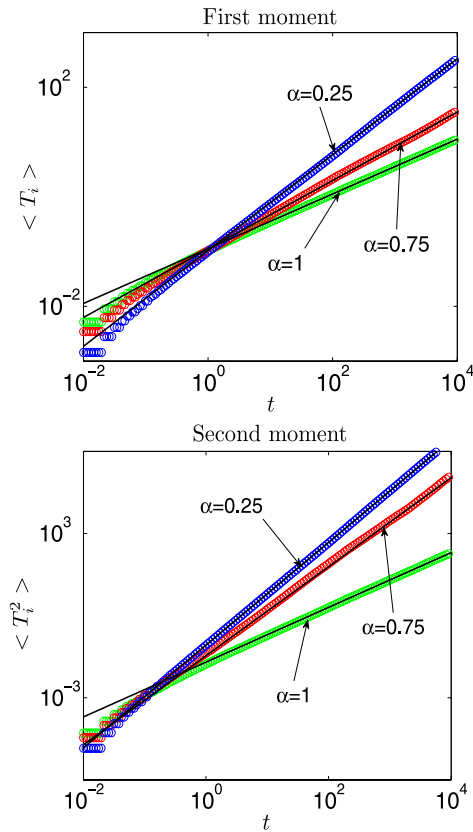
where here R is a parameter (the absorption rate) and thus the equation needs to be inverted only with respect to s. We could invert (43) for a few limiting cases.

(i) $t \to \infty$. The long time behavior is obtained by taking the $s \to 0$ limit and inverting:

$$\langle S \rangle \sim \left[\Gamma(1 - \alpha/2) \sinh\left(\frac{bR^{\alpha/2}}{\sqrt{K_\alpha}} \right) \right]^{-1} (Rt)^{-\alpha/2} + \mathcal{O}\left[(Rt)^{-\alpha} \right]. \tag{44}$$

Thus, the survival probability of the particle in the absorbing domain decays as $t^{-\alpha/2}$. We verified (44) using simulations (Fig. 3).

(ii) $\alpha \to 0$. Inverting (43) yields

$$\langle S \rangle_{\alpha \to 0} = (1 - e^{-b/\sqrt{K_0}})e^{-Rt} + e^{-b/\sqrt{K_0}}. \tag{45}$$

This can be explained as in the previous subsection. For $\alpha \to 0$, the PDF of x approaches $G(x, t) \approx \exp(-|x|/\sqrt{K_0})/(2\sqrt{K_0})$. With probability $(1 - e^{-b/\sqrt{K_0}})$, the particle never leaves the region $[-b, b]$. Thus, its probability of survival is just e^{-Rt}. With probability $e^{-b/\sqrt{K_0}}$, the particle is almost never in the absorbing zone, and it survives with probability 1.

(iii) *Other limiting cases*. It can be shown that for $b \to 0$ or $R \to 0$, $\langle S \rangle = 1$; for $R \to \infty$, $\langle S \rangle = 0$; and for $b \to \infty$, $\langle S \rangle = e^{-Rt}$.

Fig. 3 (Color online) Survival probability in an absorbing medium. We simulated anomalous diffusion trajectories as in Fig. 1 [36, 37], with total time $t = 10^3$. We plot $\langle e^{-RT_i} \rangle$, where T_i is the total time at $[-b, b]$, $R = 10$, and $b = 1$. Simulation results (*symbols*) agree with theory (*lines*, see (44)), for $Rt \gg 1$
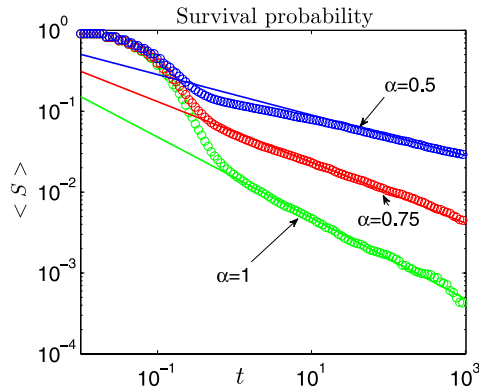
3.7 The Area Under the Random Walk Curve

The functional $A_x = \int_0^t x(\tau)d\tau$ $(U(x) = x)$ represents the total area under the random walk curve $x(t)$ [5, 25], and it is also related to the phase accumulated by spins in an NMR experiment [25]. In this subsection we obtain the first two moments of this functional, and for a couple of special cases, also its PDF. Since A_x is not necessarily positive, we use the generalized forward equation ((17) Laplace transformed $t \to s$),

$$sG(x, p, s) - \delta(x) = K_\alpha \frac{\partial^2}{\partial x^2}(s - ipx)^{1-\alpha}G(x, p, s) + ipxG(x, p, s). \tag{46}$$

Here, $G(x, p, s)$ is the Fourier-Laplace transform of $G(x, A_x, t)$ and we assumed $x_0 = 0$. Since the walk is unbiased, $\langle A_x \rangle = 0$. To find the second moment of A_x, we use

$$\langle A_x^2 \rangle(t) = \int_{-\infty}^{\infty} -\frac{\partial^2}{\partial p^2}G(x, p, t)\bigg|_{p=0} dx.$$

Integrating (46) over all x, taking the derivatives with respect to p and substituting $p = 0$, we obtain

$$s\langle A_x^2 \rangle(s) = 2\langle xA_x \rangle(s), \tag{47}$$

which is in fact obvious since $\frac{d}{dt}(A_x) = \frac{d}{dt}(\int_0^t x(\tau)d\tau) = x$, and thus $\frac{d}{dt}\langle A_x^2 \rangle = 2\langle xA_x \rangle$. Hence, the problem of finding $\langle A_x^2 \rangle$ reduces to that of finding $\langle xA_x \rangle$, for which we have $\langle xA_x \rangle = \int_{-\infty}^{\infty} -ix\frac{\partial}{\partial p}G(x, p, t)|_{p=0}dx$. This leads to
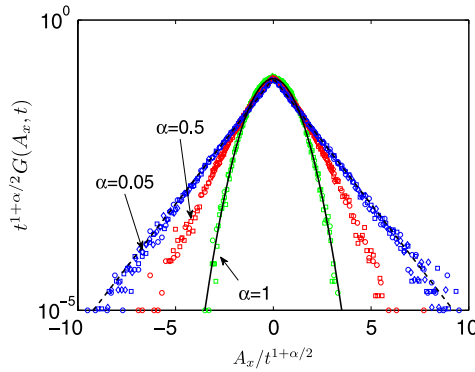
$$s\langle xA_x \rangle(s) = \langle x^2 \rangle(s). \tag{48}$$

Similarly,

$$s\langle x^2 \rangle(s) = 2K_\alpha s^{-\alpha}. \tag{49}$$

Combining (47), (48), and (49), we find $\langle A_x^2 \rangle(s) = 4K_\alpha s^{-(3+\alpha)}$, or, in t space,

$$\langle A_x^2 \rangle(t) = \frac{4K_\alpha}{\Gamma(3 + \alpha)}t^{2+\alpha}. \tag{50}$$

Fig. 4 (Color online) The area under the random walk curve A_x. We simulated diffusion trajectories as in Fig. 1 [36, 37] (10^5 trajectories) and calculated the PDF $G(A_x, t)$. To illustrate the scaling, we plot $t^{1+\alpha/2}G(A_x, t)$ vs. $A_x/t^{1+\alpha/2}$ ($K_\alpha = 1$), collapsing all curves with the same α but different times: $t = 1$ (*circles*), $t = 10$ (*squares*), and $t = 100$ (*diamonds*). Theory for $\alpha = 1$ is from (51) (Gaussian, *solid line*); theory for $\alpha \to 0$ is from (52) (exponential, *dashed line*)

Higher moments of A_x can be similarly calculated (see next subsection). The distribution of A_x can be obtained for a few limiting cases. For $\alpha = 1$, A_x is normally distributed (equation (61) in [5]):

$$G(A_x, t)_{\alpha=1} = \sqrt{\frac{3}{4\pi K_1 t^3}} \exp\left(-\frac{3A_x^2}{4K_1 t^3}\right). \tag{51}$$

For $\alpha \to 0$, the PDF of x is $G(x, t) \approx \exp(-|x|/\sqrt{K_0})/(2\sqrt{K_0})$ ([30] and Sect. 3.5) and is independent of t. In other words, the particle is found at $x(t)$ for most of the time interval $[0, t]$. Hence, $A_x(t) \approx tx(t)$ and

$$G(A_x, t)_{\alpha \to 0} \approx \frac{1}{2\sqrt{K_0}t} \exp\left(-\frac{|A_x|}{\sqrt{K_0}t}\right). \tag{52}$$

To confirm (51) and (52), we plot in Fig. 4 the PDF of A_x for various values of α as obtained from simulation of diffusion trajectories. It can also be seen from Fig. 4 that the PDF of A_x obeys a scaling relation, as we show in the next subsection.

3.8 The Moments of the Functionals $U(x) = x^k$

In the previous subsection we derived the first two moments of the $U(x) = x$ functional; but in fact, all moments of all functionals $A_{x^k} = \int_0^t x^k(\tau)d\tau$, $k = 1, 2, 3, \ldots$ can be obtained, leading to a scaling form of their PDF. As explained above, the functionals with $k = 1, 2$ arise in the context of NMR and are therefore particularly interesting.

We assume $x_0 = 0$ and consider the forward equation (15) for even k's:

$$sG(x, p, s) - \delta(x) = K_\alpha \frac{\partial^2}{\partial x^2} \left(s + px^k\right)^{1-\alpha} G(x, p, s) - px^k G(x, p, s). \tag{53}$$

Here, $G(x, p, s)$ is the double Laplace transform of $G(x, A_{x^k}, t)$ since for even k's A_{x^k} is always positive. We are interested in the moments $\langle A_{x^k}^n \rangle$, $n = 0, 1, 2, \ldots$; however, to find these, we must first obtain the more general moments $\langle A^n x^m \rangle$, $n, m = 0, 1, 2, \ldots$. Operating

on each term of (53) with $(-1)^n \frac{\partial^n}{\partial p^n}$, substituting $p = 0$, multiplying each term by x^m, and integrating over all x, (53) becomes

$$s\langle A^n x^m \rangle(s) = \delta_{n,0}\delta_{m,0} + H_{n-1}n\langle A^{n-1} x^{m+k} \rangle(s)$$

$$+ H_{m-2}K_\alpha m(m-1)\sum_{j=0}^{n} \binom{n}{j} \left[\prod_{l=0}^{j-1}(1-\alpha-l)\right](-1)^j s^{1-\alpha-j}$$

$$\times \langle A^{n-j} x^{m+jk-2} \rangle(s), \tag{54}$$

where $\delta_{i,j}$ is Kronecker's delta function—$\delta_{i,j}$ equals 1 for $i = j$ and equals zero otherwise; and H_i is the discrete Heaviside function—H_i equals 1 for $i \geq 0$ and equals zero otherwise. It can be proved that (54) remains true also for odd k's, when A_{x^k} can be either positive or negative. Equation (54) is satisfied by the following choice of $\langle A^n x^m \rangle$:

$$\langle A^n x^m \rangle(s) = c_{n,m}(k)K_\alpha^{\frac{m+nk}{2}} s^{-(1+n+\frac{m+nk}{2}\alpha)}, \tag{55}$$

for all n and even m when k is even and for even $(n + m)$ when k is odd. In all other cases $\langle A^n x^m \rangle = 0$ due to symmetry. The $c_{n,m}$'s are k-dependent dimensionless constants that satisfy the following recursion equation:

$$c_{n,m}(k) = \delta_{n,0}\delta_{m,0} + H_{n-1}nc_{n-1,m+k}(k)$$

$$+ H_{m-2}m(m-1)\sum_{j=0}^{n} \binom{n}{j} \left[\prod_{l=0}^{j-1}(1-\alpha-l)\right](-1)^j c_{n-j,m+jk-2}(k), \tag{56}$$

with initial conditions $c_{0,0}(k) = 1$ and $c_{0,1}(k) = 0$. The moments of A_{x^k} are therefore given in t space by

$$\langle A_{x^k}^n \rangle(t) = c_{n,0}(k)\frac{K_\alpha^{\frac{nk}{2}}}{\Gamma\left(1+n+\frac{n\alpha k}{2}\right)} t^{n(1+\frac{\alpha k}{2})}. \tag{57}$$

For example, for $k = 1$, $\langle A_x \rangle = \langle A_x^3 \rangle = 0$, $\langle A_x^2 \rangle = 4K_\alpha t^{2+\alpha}/\Gamma(3+\alpha)$ (50), and $\langle A_x^4 \rangle = 48(\alpha^2 + 7\alpha + 12)K_\alpha^2 t^{4+2\alpha}/\Gamma(5+2\alpha)$; while for $k = 2$, $\langle A_{x^2} \rangle = 2K_\alpha t^{1+\alpha}/\Gamma(2+\alpha)$ and $\langle A_{x^2}^2 \rangle = (48 + 8\alpha)K_\alpha^2 t^{2+2\alpha}/\Gamma(3+2\alpha)$.

Equation (57) suggests that the PDF of A_{x^k} obeys the scaling relation

$$G(A_{x^k}, t) = \frac{1}{K_\alpha^{k/2} t^{1+\alpha k/2}} g_{\alpha,k}\left(\frac{A_{x^k}}{K_\alpha^{k/2} t^{1+\alpha k/2}}\right), \tag{58}$$

where $g_{\alpha,k}(x)$ is a dimensionless scaling function. To verify the scaling form of (58), we plot in Fig. 4 simulation results for the PDF of A_x ($k = 1$) for $\alpha \approx 0$ and $\alpha = 1$ (for which $G(A_x, t)$ is known—(51) and (52) in the previous subsection), and for an intermediate value, $\alpha = 0.5$. In all cases the simulated PDF satisfies the scaling form (58).

4 Summary and Discussion

Functionals of the path of a Brownian particle have been investigated in numerous studies since the development of the Feynman-Kac equation in 1949. However, an analog equation

for functionals of non-Brownian particles has been missing. Here, we developed such an equation based on the CTRW model with broadly distributed waiting times. We derived forward and backward equations ((12) and (20)) and generalizations to Lévy flights ((18) and (21)). Using the backward equation, we derived the PDFs of the occupation time in half-space, the first passage time, and the maximal displacement, and calculated the average survival probability in an absorbing medium. Using the forward equation, we calculated the hitting probability and all the moments of $U(x) = x^k$ functionals.

The fractional Feynman-Kac equation (12) can be obtained from the integer equation (1) by insertion of a substantial fractional derivative operator [28]. In that sense, our work is a natural generalization of that of Kac's. The distributions we obtained for specific functionals are also the expected extensions of their Brownian counterparts: the arcsine law for the occupation time in half-space [1, 43] was replaced by Lamperti's PDF (25) [22], and the famous $t^{-3/2}$ decay of the one-dimensional first passage time PDF [47] became $t^{-(1+\alpha/2)}$ (31). Thus, our analysis supports the notion that CTRW and the emerging fractional paths [36, 37] are elegant generalizations of ordinary Brownian motion. Nevertheless, other non-Brownian processes are also important. For example, it would be interesting to find an equation for the PDF of anomalous functionals when the underlying process is fractional Brownian motion [14].

Our fractional Feynman-Kac equation (12) has the form of a fractional Schrödinger equation in imaginary time. Real time, fractional Schrödinger equations for the wave function have also been recently proposed [55–59]. However, these are very different from our fractional Feynman-Kac equation. In [55–57], the Laplacian was replaced with a fractional spatial derivative which would correspond to a *Markovian* CTRW with heavy tailed distribution of jump lengths (Lévy flights; see also the Appendix below). The approach in [58, 59] is based on a temporal fractional Riemann-Liouville derivative—however not substantial—which leads to non-Hermitian evolution and hence non-normalizable quantum mechanics. It is unclear yet whether all these fractional Schrödinger equations actually describe any physical phenomenon (see [60] for discussion). In principle, a fractional Schrödinger equation can also be written using the substantial fractional derivative we used here. If there is a physical process behind such a quantum mechanical analog of our equation remains at this stage unclear.

In this paper we considered only the case of a free particle. In [29], we reported a fractional Feynman-Kac equation for a particle under the influence of a binding force, where anomalous diffusion can lead to weak ergodicity breaking [61–63]. The derivation of an equation for the distribution of general functionals and the treatment of specific functionals for bounded particles will be published elsewhere.

Appendix: Generalization to Arbitrary Functionals and Lévy Flights

Here we generalize our forward and backward fractional Feynman-Kac equations ((12) and (20), respectively) to the case when the functional is not necessarily positive and to the case when the CTRW jump length distribution is arbitrary, and in particular, heavy tailed.

In our generalized CTRW model, the particle moves, after waiting at x, to $x + \Delta_x$, where Δ_x is distributed according to $f(\Delta_x)$. The PDF $f(\Delta_x)$ must be symmetric: $f(\Delta_x) =$

$f(-\Delta_x)$ but can be otherwise arbitrary. Let us rederive the forward equation for this model. We replace (4) with

$$Q_{n+1}(x, A, t) = \int_0^t \psi(\tau) \int_{-\infty}^\infty f(\Delta_x) Q_n[x - \Delta_x, A - \tau U(x - \Delta_x), t - \tau] d\Delta_x d\tau.$$

Since A can be negative, we *Fourier* transform the last equation $A \to p$

$$Q_{n+1}(x, p, t) = \int_0^t \psi(\tau) \int_{-\infty}^\infty f(\Delta_x) e^{ip\tau U(x - \Delta_x)} Q_n(x - \Delta_x, p, t - \tau) d\Delta_x d\tau.$$

Laplace transforming $t \to s$ and Fourier transforming $x \to k$ we have

$$Q_{n+1}(k, p, s) = \int_{-\infty}^\infty e^{ikx} \int_{-\infty}^\infty f(\Delta_x) \hat\psi[s - ipU(x - \Delta_x)] Q_n(x - \Delta_x, p, s) d\Delta_x dx.$$

Changing variables: $x' = x - \Delta_x$,

$$Q_{n+1}(k, p, s) = \int_{-\infty}^\infty e^{ik\Delta_x} f(\Delta_x) d\Delta_x \int_{-\infty}^\infty e^{ikx'} \hat\psi[s - ipU(x')] Q_n(x', p, s) dx'$$

$$= f(k) \hat\psi\left[s - ipU\left(-i\frac{\partial}{\partial k}\right)\right] Q_n(k, p, s).$$

Summing over all n and using the initial condition $Q_0(k, p, s) = e^{ikx_0}$,

$$\sum_{n=0}^\infty Q_n(k, p, s) = \left\{1 - f(k)\hat\psi\left[s - ipU\left(-i\frac{\partial}{\partial k}\right)\right]\right\}^{-1} e^{ikx_0}.$$

Note that this agrees with (8) since for nearest neighbor hopping $f(k) = \int_{-\infty}^\infty e^{ik\Delta_x} [\frac{1}{2}\delta(\Delta_x - a) + \frac{1}{2}\delta(\Delta_x + a)] d\Delta_x = \cos(ka)$. Next, we observe that (3) of Sect. 2.1 remains the same even under the general conditions. Calculating the transformed $G(k, p, s)$ as above, and using the result of the last equation, we obtain the formal solution

$$G(k, p, s) = \frac{1 - \hat\psi\left[s - ipU\left(-i\frac{\partial}{\partial k}\right)\right]}{s - ipU\left(-i\frac{\partial}{\partial k}\right)}$$

$$\times \left\{1 - f(k)\hat\psi\left[s - ipU\left(-i\frac{\partial}{\partial k}\right)\right]\right\}^{-1} e^{ikx_0}.$$

We now assume that $f(\Delta_x)$ has a finite second moment and thus its characteristic function can be written, for small k, as $f(k) \sim 1 - \sigma^2 k^2/2$. This characteristic function is identical to that of nearest neighbor hopping (with $\sigma = a$); we can thus proceed as in Sect. 2.1 to obtain

$$\frac{\partial}{\partial t} G(x, p, t) = K_\alpha \frac{\partial^2}{\partial x^2} \mathcal{D}_t^{1-\alpha} G(x, p, t) + ipU(x)G(x, p, t), \tag{59}$$

where here $\mathcal{D}_t^{1-\alpha} \to [s - ipU(x)]^{1-\alpha}$ in Laplace s space and $K_\alpha = \sigma^2/(2B_\alpha)$.

Consider now the case of *Lévy flights*—$f(\Delta_x) \sim |\Delta_x|^{-(1+\mu)}$ (for large Δ_x) with $0 < \mu < 2$, and thus jump lengths have a diverging second moment. The characteristic function is $f(k) \sim 1 - C_\mu |k|^\mu$, and the fractional Feynman-Kac equation becomes

$$\frac{\partial}{\partial t} G(x, p, t) = K_{\alpha,\mu} \nabla_x^\mu \mathcal{D}_t^{1-\alpha} G(x, p, t) + ipU(x)G(x, p, t), \tag{60}$$

where $K_{\alpha,\mu} = C_\mu / B_\alpha$ and ∇_x^μ is the Riesz spatial fractional derivative operator: $\nabla_x^\mu \to -|k|^\mu$ in Fourier k space.

Repeating the calculations of Sect. 2.2 for a non-necessarily-positive functional and for Lévy flights, it can be shown that the generalized backward equation is:

$$\frac{\partial}{\partial t} G_{x_0}(p,t) = K_{\alpha,\mu} \mathcal{D}_t^{1-\alpha} \nabla_{x_0}^\mu G_{x_0}(p,t) + ip U(x_0) G_{x_0}(p,t). \tag{61}$$

Here, $\mathcal{D}_t^{1-\alpha} \to [s - ip U(x_0)]^{1-\alpha}$ in Laplace s space and $\nabla_{x_0}^\mu \to -|k_0|^\mu$ in Fourier k_0 space.

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