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Chapter 8

Fractional Feynman–Kac Equation for Anomalous Diffusion Functionals

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Functionals of the path of a Brownian particle are known to obey the celebrated Feynman–Kac equation. We develop here a fractional Feynman–Kac equation for functionals of the sub-diffusive continuous-time random walk process. Several simple examples of functionals are explicitly treated such as the occupation time, the first passage time, and the maximum of the walk. In the presence of a binding field, the fractional Feynman–Kac equation describes the route to weak ergodicity breaking.

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1. Introduction

In nature, a noisy signal $x(t)$ represents a physical observable that is difficult to predict. However, the time-average of the signal, $\int_0^t x(\tau)d\tau/t$, is in many cases non-random. Consider for example a Brownian particle attached to a

spring and embedded in a thermal heat bath. The trajectory of the particle $x(t)$ is rather noisy and erratic, but yet, we expect the time-averages

$$\overline{x^n(t)} = \int_0^t x^n(\tau) d\tau / t$$

to converge, in the long time limit, to their corresponding ensemble averages

$$\lim_{t \rightarrow \infty} \overline{x^n(t)} = \langle x^n \rangle,$$

where in thermal equilibrium, ensemble averages are described by Boltzmann statistics

$$\langle x^n \rangle = \frac{1}{Z} \int_{-\infty}^{\infty} x^n e^{-V(x)/(k_B T)} dx. \quad (1)$$

Here, Z is the normalizing partition function and $V(x)$ is a binding potential, for example, $V(x) = \frac{1}{2} m \omega^2 x^2$ for a particle attached to a spring. Boltzmann statistics is beautiful since it is not sensitive to the dynamics of the particle. For example, the underlying dynamics can be either Markovian or non-Markovian [1] (e.g., a Langevin equation with either white or colored noise); in both cases, the ensemble average will be distributed according to Boltzmann statistics.

In recent years there is growing interest in anomalous diffusion processes modeled with fractional kinetic equations, such as the fractional Fokker–Planck equation for subdiffusion in a binding potential [2–9]. Fractional kinetics exhibits ergodicity breaking: time averages remain random variables, even in the long time limit [10–16]. This ergodicity breaking is weak; there are no inaccessible regions in the phase space, as in strong ergodicity breaking.

To investigate weak ergodicity breaking, we study in this chapter the more general problem of functionals of the process $x(t)$, defined as

$$A = \int_0^t U[x(\tau)] d\tau, \quad (2)$$

where $U(x)$ is a prescribed function. For example, with $U(x) = x^n$, the time-averages are $\overline{x^n(t)} = A/t$. We consider paths of sub-diffusive continuous-time random walk (CTRW), an important and widely investigated process that is frequently used to describe the motion of particles in disordered systems [17–20]. We then obtain an equation for the probability density function (PDF) of functionals of these paths. Our new equation turns to be a powerful tool when studying functionals of subdiffusive CTRW processes. In

particular, using our equation we obtain the fluctuations of the time-average of $x(t)$ and thereby learn about the kinetics of the weak ergodicity breaking.

When $x(t)$ describes a trajectory of a Brownian particle, A is called a Brownian functional [21]. Functionals of Brownian motion arise in numerous problems across a variety of scientific fields from condensed matter physics [22–25], to hydrodynamics [26], meteorology [27], and finance [28, 29]. The PDF of A satisfies a Schrödinger-like equation, derived in 1949 by Kac inspired by Feynman’s path integrals [30].

Denote by $G(x, A, t)$ the joint PDF of finding, at time t , the particle at x and the functional at A . The Feynman–Kac theory shows that (for a free Brownian particle and for $U(x) \geq 0$) [21, 30],

$$\frac{\partial}{\partial t} G(x, p, t) = K \frac{\partial^2}{\partial x^2} G(x, p, t) - pU(x)G(x, p, t), \quad (3)$$

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

We generalize the Feynman–Kac equation to non-Brownian functionals. We consider CTRW as the underlying process leading to anomalous diffusion. In the continuum limit of this process, we derive the following *fractional* Feynman–Kac equation [31],

$$\frac{\partial}{\partial t} G(x, p, t) = K_\alpha \mathcal{L}_{\text{FP}} \mathcal{D}_t^{1-\alpha} G(x, p, t) - pU(x)G(x, p, t), \quad (4)$$

where K_α is a generalized diffusion coefficient and the symbol $\mathcal{D}_t^{1-\alpha}$ is Friedrich’s *substantial fractional derivative* and is equal in Laplace space $t \rightarrow s$ to $[s + pU(x)]^{1-\alpha}$ [32]. $\mathcal{L}_{\text{FP}} = \frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x} \frac{F(x)}{k_B T}$ is the Fokker–Planck operator, where $F(x) = -V'(x)$ is the force at x and T is the temperature. When $\alpha = 1$ and $F(x) = 0$, Eq. (4) reduces to the celebrated Feynman–Kac equation (3).

With our fractional Feynman–Kac equation (4), we investigate functionals of subdiffusive CTRW processes both in the absence and in the presence of a binding force field. In the force-free case, questions of ergodicity are irrelevant since $Z \rightarrow \infty$. There are however several functionals 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 [33, 34]. This functional is useful in kinetic studies of chemical reactions that take place exclusively in a domain [35, 36]. In the presence of a binding force, we use our equation

to study the time average of $x(t)$, a random variable that exhibits weak ergodicity breaking.

The rest of the chapter is organized as follows. In Sec. 2, we derive Eq. (4) and a *backward* equation that depends on the initial position rather than the final one. In Sec. 3, we demonstrate solutions of our equations for a few functionals of interest of free particles. In Sec. 4, we investigate functionals of bounded particles and illustrate how our equation leads to weak ergodicity breaking. We summarize in Sec. 5. A short description of our work appeared in [31] more details can be found in [37].

2. Derivation of the Equations

2.1. Fractional Feynman–Kac equation

The continuous-time random walk model [2, 17–20] considers an infinite one-dimensional lattice with spacing a on which a particle is allowed to jump to its nearest neighbors only. The probabilities of jumping left $L(x)$ and right $R(x)$ depend on the force at the point. Denote by $V(x)$ the potential at point x . We assume thermal equilibrium at temperature T and detailed balance. Namely, that

$$L(x)e^{-V(x)/(k_B T)} = R(x-a)e^{-V(x-a)/(k_B T)} \quad (5)$$

holds true for every lattice point x [14].

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 to either $x_0 + a$ (with probability $R(x)$) or $x_0 - a$ (with probability $L(x)$), after which the process is renewed. If $F(x) = 0$, then $R(x) = L(x) = 1/2$. We assume that for long waiting times,

$$\psi(\tau) \sim \frac{B_\alpha}{|\Gamma(-\alpha)|} \tau^{-(1+\alpha)}. \quad (6)$$

For $0 < \alpha < 1$, the average waiting time is infinite and the process is subdiffusive with (for $F(x) = 0$) $\langle x^2 \rangle = 2K_\alpha t^\alpha / \Gamma(1 + \alpha)$ ($K_\alpha = a^2 / (2B_\alpha)$, units $\text{m}^2/\text{sec}^\alpha$) [8]. We look for the differential equation that describes the distribution of functionals in the continuum limit of this model, focusing on $0 < \alpha < 1$.

Recall that the functional is defined as $A = \int_0^t U[x(\tau)] d\tau$ with the arbitrary function $U(x)$ 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 $t - \tau$ when the last jump was made. Let $\chi(x, A, t)dt$ be the probability of the particle to jump into (x, A) in the time interval $[t, t + dt]$. We have,

$$G(x, A, t) = \int_0^t W(\tau) \chi[x, A - \tau U(x), t - \tau] d\tau, \quad (7)$$

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 calculate χ , we note that to *arrive to* (x, A) at time t , the particle must have arrived to either $[x - a, A - \tau U(x - a)]$ or $[x + a, A - \tau U(x + a)]$ at the time $t - \tau$ when the previous jump was made. Given the probabilities of jumping left and right,

$$\begin{aligned} \chi(x, A, t) = & \int_0^t \psi(\tau) \{ L(x + a) \chi[x + a, A - \tau U(x + a), t - \tau] \\ & + R(x - a) \chi[x - a, A - \tau U(x - a), t - \tau] \} d\tau \\ & + \delta(x - x_0) \delta(A) \delta(t), \end{aligned} \quad (8)$$

where $\psi(\tau)$ is the PDF of τ , the time between jumps. The term $\delta(x - x_0) \delta(A) \delta(t)$ corresponds to no jumps.

Assume that $U(x) \geq 0$ for all x and thus $A \geq 0$ (an assumption we will relax later). Let $\chi(x, p, t) = \int_0^\infty e^{-pA} \chi(x, A, t) dA$ be the Laplace transform $A \rightarrow p$ of $\chi(x, A, t)$, we use along this work the convention that the variables in parentheses define the space we are working in. We note that

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

where we used the fact that $\chi(x, A, t) = 0$ for $A < 0$. Thus, Laplace transforming ($A \rightarrow p$) Eq. (8), we find

$$\begin{aligned} \chi(x, p, t) = & L(x + a) \int_0^t \psi(\tau) e^{-p\tau U(x+a)} \chi(x + a, p, t - \tau) d\tau \\ & + R(x - a) \int_0^t \psi(\tau) e^{-p\tau U(x-a)} \chi(x - a, p, t - \tau) d\tau \\ & + \delta(x - x_0) \delta(t). \end{aligned} \quad (9)$$

Laplace transforming $t \rightarrow s$ Eq. (9) using the convolution theorem,

$$\begin{aligned}\chi(x, p, s) = & L(x+a)\hat{\psi}[s+pU(x+a)]\chi(x+a, p, s) \\ & + R(x-a)\hat{\psi}[s+pU(x-a)]\chi(x-a, p, s) + \delta(x-x_0),\end{aligned}\quad (10)$$

where $\hat{\psi}(s)$ is the Laplace transform of the waiting time PDF. Let $\chi(k, p, s) = \int_{-\infty}^{\infty} e^{ikx}\chi(x, p, s)dx$ be the Fourier transform $x \rightarrow k$ of $\chi(x, p, s)$. Fourier transforming Eq. (10) and changing variables $x \rightarrow x \pm a$,

$$\begin{aligned}\chi(k, p, s) = & e^{-ika} \int_{-\infty}^{\infty} e^{ikx} L(x)\hat{\psi}[s+pU(x)]\chi(x, p, s)dx \\ & + e^{ika} \int_{-\infty}^{\infty} e^{ikx} R(x)\hat{\psi}[s+pU(x)]\chi(x, p, s)dx + e^{ikx_0}.\end{aligned}$$

If the lattice spacing is small enough such that $aF(x) \ll k_B T$ and $R(x-a) \approx R(x)$, we can use $L(x) = 1 - R(x)$ and the detailed balance equation (5) to show that [8]

$$R(x) \approx \frac{1}{2} \left[1 + \frac{aF(x)}{2k_B T} \right] \quad L(x) \approx \frac{1}{2} \left[1 - \frac{aF(x)}{2k_B T} \right]. \quad (11)$$

Using (11) and applying the Fourier transform identity $\mathcal{F}\{xf(x)\} = -i\frac{\partial}{\partial k}f(k)$,

$$\begin{aligned}\chi(k, p, s) = & \left[\cos(ka) + i \sin(ka) \frac{aF(-i\frac{\partial}{\partial k})}{2k_B T} \right] \\ & \times \hat{\psi} \left[s + pU \left(-i\frac{\partial}{\partial k} \right) \right] \chi(k, p, s) + e^{ikx_0}.\end{aligned}\quad (12)$$

Note that the order of the terms is important: for example, $\cos(ka)$ does not commute with $\hat{\psi}[s+pU(-i\frac{\partial}{\partial k})]$. The formal solution of Eq. (12) is

$$\begin{aligned}\chi(k, p, s) = & \left\{ 1 - \left[\cos(ka) + i \sin(ka) \frac{aF(-i\frac{\partial}{\partial k})}{2k_B T} \right] \right. \\ & \left. \times \hat{\psi} \left[s + pU \left(-i\frac{\partial}{\partial k} \right) \right] \right\}^{-1} e^{ikx_0}.\end{aligned}\quad (13)$$

We next use our expression for χ to calculate $G(x, A, t)$. Transforming Eq. (7) $(x, A, t) \rightarrow (k, p, s)$,

$$G(k, p, s) = \frac{1 - \hat{\psi} \left[s + pU \left(-i\frac{\partial}{\partial k} \right) \right]}{s + pU \left(-i\frac{\partial}{\partial k} \right)} \chi(k, p, s), \quad (14)$$

where we used $\hat{W}(s) = \int_0^\infty e^{-st} W(t) dt = [1 - \hat{\psi}(s)]/s$. Substituting Eq. (13) into (14), we find

$$\begin{aligned}
 G(k, p, s) &= \frac{1 - \hat{\psi} \left[s + pU \left(-i \frac{\partial}{\partial k} \right) \right]}{s + pU \left(-i \frac{\partial}{\partial k} \right)} \\
 &\times \left\{ 1 - \left[\cos(ka) + i \sin(ka) \frac{aF \left(-i \frac{\partial}{\partial k} \right)}{2k_B T} \right] \right. \\
 &\times \left. \hat{\psi} \left[s + pU \left(-i \frac{\partial}{\partial k} \right) \right] \right\}^{-1} e^{ikx_0}. \quad (15)
 \end{aligned}$$

To derive a differential equation for $G(x, p, t)$, we recall the waiting time distribution is $\psi(t) \sim B_\alpha t^{-(1+\alpha)}/|\Gamma(-\alpha)|$ (Eq. (6)), and write its Laplace transform $\hat{\psi}(s)$ for $s \rightarrow 0$ as [2]

$$\hat{\psi}(s) \sim 1 - B_\alpha s^\alpha, \quad 0 < \alpha < 1, \quad s \rightarrow 0. \quad (16)$$

Substituting Eq. (16) into Eq. (15), applying the small k expansions $\cos(ka) \sim 1 - k^2 a^2/2$ and $\sin(ka) \sim ka$, and neglecting the high order terms,

$$\begin{aligned}
 G(k, p, s) &= \left[s + pU \left(-i \frac{\partial}{\partial k} \right) \right]^{\alpha-1} \\
 &\times \left\{ K_\alpha \left[k^2 - ik \frac{F \left(-i \frac{\partial}{\partial k} \right)}{k_B T} \right] + \left[s + pU \left(-i \frac{\partial}{\partial k} \right) \right]^\alpha \right\}^{-1} e^{ikx_0},
 \end{aligned}$$

where we used the generalized diffusion coefficient [8]

$$K_\alpha \equiv \lim_{a^2, B_\alpha \rightarrow 0} \frac{a^2}{2B_\alpha}. \quad (17)$$

By neglecting the high order terms in s and k , we effectively reached the continuum limit of the lattice walk [38]. Rearranging the expression in the last equation we find

$$\begin{aligned}
 sG(k, p, s) - e^{ikx_0} &= -K_\alpha \left[k^2 - ik \frac{F \left(-i \frac{\partial}{\partial k} \right)}{k_B T} \right] \left[s + pU \left(-i \frac{\partial}{\partial k} \right) \right]^{1-\alpha} \\
 &\times G(k, p, s) - pU \left(-i \frac{\partial}{\partial k} \right) G(k, p, s).
 \end{aligned}$$

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

$$\frac{\partial}{\partial t} G(x, p, t) = K_\alpha \mathcal{L}_{\text{FP}} \mathcal{D}_t^{1-\alpha} G(x, p, t) - pU(x)G(x, p, t), \quad (18)$$

where

$$\mathcal{L}_{\text{FP}} = \frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x} \frac{F(x)}{k_B T} \quad (19)$$

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

The symbol $\mathcal{D}_t^{1-\alpha}$ represents the fractional substantial derivative operator introduced in [32]:

$$\mathcal{L}\{\mathcal{D}_t^{1-\alpha} G(x, p, t)\} = [s + pU(x)]^{1-\alpha} G(x, p, s), \quad (20)$$

where $\mathcal{L}\{f(t)\} = \int_0^t e^{-st} f(t) dt$ is the Laplace transform $t \rightarrow s$ (see also [39]). In t space,

$$\mathcal{D}_t^{1-\alpha} G(x, p, t) = \frac{1}{\Gamma(\alpha)} \left[\frac{\partial}{\partial t} + pU(x) \right] \int_0^t \frac{e^{-(t-\tau)pU(x)}}{(t-\tau)^{1-\alpha}} G(x, p, \tau) d\tau. \quad (21)$$

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

$$sG(x, p, s) - \delta(x - x_0) = K_\alpha \mathcal{L}_{\text{FP}} [s + pU(x)]^{1-\alpha} G(x, p, s) - pU(x)G(x, p, s). \quad (22)$$

A few remarks should be made.

(i) *The integer Feynman–Kac equation.* Consider the force-free case $F(x) = 0$. As expected, for $\alpha = 1$ our fractional equation (18) reduces to the (integer) Feynman–Kac equation (3).

(ii) *The fractional Fokker–Planck 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, Eq. (18) reduces

to the fractional Fokker–Planck equation:

$$\frac{\partial}{\partial t}G(x, t) = K_\alpha \mathcal{L}_{\text{FP}} \mathcal{D}_{\text{RL}, t}^{1-\alpha} G(x, t), \quad (23)$$

where $\mathcal{D}_{\text{RL}, t}^{1-\alpha}$ is the Riemann–Liouville fractional derivative operator ($\mathcal{D}_{\text{RL}, t}^{1-\alpha} G(x, s) \rightarrow s^{1-\alpha} G(x, s)$ in Laplace $t \rightarrow s$ space) [2, 7, 8].

(iii) *A general functional.* When the functional is not necessarily positive, the Laplace transform $A \rightarrow p$ must be replaced by a Fourier transform $G(x, p, t) = \int_{-\infty}^{\infty} e^{ipA} G(x, A, t) dA$. It can be shown [37] that the fractional Feynman–Kac equation looks like (18), but with p replaced by $-ip$,

$$\frac{\partial}{\partial t}G(x, p, t) = K_\alpha \mathcal{L}_{\text{FP}} \mathcal{D}_t^{1-\alpha} G(x, p, t) + ipU(x)G(x, p, t), \quad (24)$$

where $\mathcal{D}_t^{1-\alpha} \rightarrow [s - ipU(x)]^{1-\alpha}$ in Laplace s space.

(iv) *Lévy flights.* Consider CTRW with $F(x) = 0$ and displacements Δ_x distributed according to a symmetric PDF $f(\Delta_x) \sim |\Delta_x|^{-(1+\mu)}$, with $0 < \mu < 2$. The Fourier transform of this distribution is $f(k) \sim 1 - C_\mu |k|^\mu$ [2]. This process is known as a Lévy flight, and it can be shown to obey the following fractional Feynman–Kac equation (for $U(x) \geq 0$) [37]

$$\frac{\partial}{\partial t}G(x, p, t) = K_{\alpha, \mu} \nabla_x^\mu \mathcal{D}_t^{1-\alpha} G(x, p, t) - pU(x)G(x, p, t), \quad (25)$$

where $K_{\alpha, \mu} = C_\mu/B_\alpha$ (units $\text{m}^\mu/\text{sec}^\alpha$), and $\mathcal{D}_t^{1-\alpha}$ is the substantial fractional derivative operator defined above (Eqs. (20) and (21)). ∇_x^μ is the Riesz spatial fractional derivative operator defined in Fourier $x \rightarrow k$ space as $\nabla_x^\mu \rightarrow -|k|^\mu$ [2].

(v) *Fractional Schrödinger equations.* Our fractional Feynman–Kac equation (18) 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 [40–44]. However, these are different from our fractional Feynman–Kac equation because they are either based on a fractional *spatial* derivative, or on a *non-substantial* temporal fractional derivative that leads to non-Hermitian evolution and hence non-normalizable quantum mechanics. Whether these fractional Schrödinger equations actually describe any physical reality is still unclear [45].

(vi) *How to solve the fractional Feynman–Kac equation.* To obtain the PDF of a functional A , the following recipe could be followed [21]:

- (1) Solve Eq. (22), the fractional Feynman–Kac equation in (x, p, s) space. Equation (22) 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 $(p, s) \rightarrow (A, t)$, to obtain $G(A, t)$, the PDF of A at time t .

In the next section we will see that the second step can be circumvented by using a backward equation.

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 Sec. 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,

$$\begin{aligned} G_{x_0}(A, t) = & \int_0^t \psi(\tau) \{ R(x_0) G_{x_0+a}[A - \tau U(x_0), t - \tau] \\ & + L(x_0) G_{x_0-a}[A - \tau U(x_0), t - \tau] \} d\tau \\ & + W(t) \delta[A - tU(x_0)]. \end{aligned} \quad (26)$$

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 Eq. (26) describes a motionless particle, for which $A(t) = tU(x_0)$. We now transform Eq. (26) $(x_0, A, t) \rightarrow (k_0, p, s)$, using techniques similar to those used in the previous subsection. This leads to, for $U(x) \geq 0$,

$$\begin{aligned} G_{k_0}(p, s) = & \hat{\psi} \left[s + pU \left(-i \frac{\partial}{\partial k_0} \right) \right] \left[\cos(k_0 a) - \frac{aF \left(-i \frac{\partial}{\partial k_0} \right)}{2k_B T} i \sin(k_0 a) \right] \\ & \times G_{k_0}(p, s) + \frac{1 - \hat{\psi} \left[s + pU \left(-i \frac{\partial}{\partial k_0} \right) \right]}{s + pU \left(-i \frac{\partial}{\partial k_0} \right)} \delta(k_0). \end{aligned}$$

To derive the last equation, we used the approximations (11). To reach the continuum limit we expand $\hat{\psi}(s) \sim 1 - B_\alpha s^\alpha$, $\cos(k_0 a) \sim 1 - k_0^2 a^2/2$, and

$\sin(k_0 a) \sim k_0 a$. After some rearrangements,

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

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

$$\frac{\partial}{\partial t} G_{x_0}(p, t) = K_\alpha \mathcal{D}_t^{1-\alpha} \mathcal{L}_{\text{FP}}^{(\text{B})} G_{x_0}(p, t) - pU(x_0) G_{x_0}(p, t), \quad (27)$$

where

$$\mathcal{L}_{\text{FP}}^{(\text{B})} = \frac{\partial^2}{\partial x_0^2} + \frac{F(x_0)}{k_B T} \frac{\partial}{\partial x_0} \quad (28)$$

is the *backward* Fokker–Planck operator. Here, $\mathcal{D}_t^{1-\alpha}$ equals in Laplace $t \rightarrow s$ 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 Eq. (18) the operators depend on x while in Eq. (27) they depend on x_0 . Therefore, Eq. (18) is called the forward equation while Eq. (27) is called the backward equation. Notice that here, the fractional derivative operator appears to the left of the Fokker–Planck operator $\mathcal{L}_{\text{FP}}^{(\text{B})}$, in contrast to the forward equation (18). Also, note the different sign and order of terms in $\mathcal{L}_{\text{FP}}^{(\text{B})}$ (Eq. (28)) compared to $\mathcal{L}_{\text{FP}}$ (Eq. (19)).

3. Functionals of Free Particles

In this Section, we illustrate a number of applications of our equation in the force-free case, $F(x) = 0$. For more applications, see [37].

3.1. Occupation time in half-space

The occupation time of a particle in the positive half-space has wide applications in both physics [16, 46, 47] and mathematics [48]. Formally, the occupation time is defined as $T_+ = \int_0^t \Theta[x(\tau)] d\tau$, where $\Theta(x) = 1$ for $x \geq 0$ and is zero otherwise. To find the PDF of the occupation time, consider the

backward equation ((27), transformed $t \rightarrow s$):

$$sG_{x_0}(p, s) - 1 = \begin{cases} K_\alpha s^{1-\alpha} \frac{\partial^2}{\partial x_0^2} G_{x_0}(p, s) & x_0 < 0, \\ K_\alpha (s+p)^{1-\alpha} \frac{\partial^2}{\partial x_0^2} G_{x_0}(p, s) - pG_{x_0}(p, s) & x_0 > 0. \end{cases} \quad (29)$$

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 $|x_0| \rightarrow \infty$,

$$G_{x_0}(p, s) = \begin{cases} C_0 \exp(x_0 s^{\alpha/2} / \sqrt{K_\alpha}) + \frac{1}{s} & x_0 < 0, \\ C_1 \exp[-x_0 (s+p)^{\alpha/2} / \sqrt{K_\alpha}] + \frac{1}{s+p} & x_0 > 0. \end{cases} \quad (30)$$

For $x_0 \rightarrow -\infty$, 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 Eq. (30). Similarly, for $x_0 \rightarrow +\infty$, $G_{x_0}(T_+, t) = \delta(T_+ - t)$ 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 :

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

whose solution is

$$C_0 = -\frac{p(s+p)^{\alpha/2-1}}{s[s^{\alpha/2} + (s+p)^{\alpha/2}]}, \quad C_1 = \frac{ps^{\alpha/2-1}}{(s+p)[s^{\alpha/2} + (s+p)^{\alpha/2}]} \quad (31)$$

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

$$G_0(p, s) = \frac{s^{\alpha/2-1} + (s+p)^{\alpha/2-1}}{s^{\alpha/2} + (s+p)^{\alpha/2}}. \quad (32)$$

Using [49], the PDF of $\lambda \equiv T_+/t$, for long times, is the symmetric *Lamperti* PDF [50, 51]:

$$f(\lambda) = \frac{\sin(\pi\alpha/2)}{\pi} \frac{\lambda^{\alpha/2-1}(1-\lambda)^{\alpha/2-1}}{\lambda^\alpha + (1-\lambda)^\alpha + 2\lambda^{\alpha/2}(1-\lambda)^{\alpha/2} \cos(\pi\alpha/2)}. \quad (33)$$

This equation has also been derived using other methods [47]. Naively, one expects the particle to spend about half the time at $x > 0$. In contrast, we learn from Eq. (33) that the particle tends to spend most of the time at either $x > 0$ or $x < 0$: $f(\lambda)$ has two peaks at $\lambda = 1$ and $\lambda = 0$. This is exacerbated in the limit $\alpha \rightarrow 0$, where the distribution converges to two delta functions at $T^+/t = 1$ and at $T^+/t = 0$. For $\alpha = 1$ (Brownian motion) we recover the well-known arcsine law of Lévy [21, 46, 47].

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 [52]. The distribution of first passage times for anomalous paths can be obtained from the fractional Feynman–Kac equation using an identity due to Kac [53]:

$$\Pr\{t_f > t\} = \Pr\left\{\max_{0 \leq \tau \leq t} x(\tau) < b\right\} = \lim_{p \rightarrow \infty} G_{x_0}(p, t), \quad (34)$$

where $G_{x_0}(p, t)$ describes the functional $A_f = \int_0^t U[x(\tau)]d\tau$ with

$$U(x) = \begin{cases} 0 & x < b, \\ 1 & x > b. \end{cases} \quad (35)$$

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 $p \rightarrow \infty$, $e^{-pA_f} = 0$. The functional (35) is similar to the functional studied in the previous section. 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 ,

$$\lim_{p \rightarrow \infty} G_0(p, s) = \frac{1}{s} \left(1 - e^{-\frac{b}{\sqrt{K_\alpha}} s^{\alpha/2}} \right). \quad (36)$$

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

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

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 $f(t) = \frac{\partial}{\partial t}(\text{Pr}\{t_f < t\}) = \frac{\partial}{\partial t}(1 - \text{Pr}\{t_f > t\})$. Thus,

$$f(t) = \frac{1}{\tau_f} l_{\alpha/2}\left(\frac{t}{\tau_f}\right). \quad (37)$$

A different derivation of this equation appears in [54]. The long times behavior of $f(t)$ is obtained from the $s \rightarrow 0$ limit: $f(s) \sim 1 - \frac{b}{\sqrt{K_\alpha}} s^{\alpha/2}$. Therefore, for long times

$$f(t) \sim \frac{b}{|\Gamma(-\frac{\alpha}{2})|\sqrt{K_\alpha}} t^{-(1+\alpha/2)}. \quad (38)$$

For $\alpha = 1$, we reproduce the famous $t^{-3/2}$ decay law of a one-dimensional random walk [52].

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., [55–58] and references therein). To obtain the distribution of this variable, we use the functional defined in the previous section (Eq. (35)). Let $x_m \equiv \max_{0 \leq \tau \leq t} x(\tau)$, and recall from Eq. (34) that $\text{Pr}\{x_m < b\} = \lim_{p \rightarrow \infty} G_{x_0}(p, t)$. From the previous section we have, for $x_0 = 0$ (Eq. (36)),

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

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 $s \rightarrow t$, we obtain

$$P(x_m, t) = \frac{2}{\alpha \sqrt{K_\alpha}} \frac{t}{(x_m/\sqrt{K_\alpha})^{1+2/\alpha}} l_{\alpha/2}\left[\frac{t}{(x_m/\sqrt{K_\alpha})^{2/\alpha}}\right], \quad x_m > 0. \quad (39)$$

This PDF has the same shape as the PDF of x up to a scale factor of 2 [8], and it is in agreement with the very recent result of [57], derived using a renormalization group method.

4. Functionals of Bounded Particles: Weak Ergodicity Breaking

4.1. The fluctuations of the time-averaged position

In this section we use our equation for non-Brownian functionals in a force field to characterize weak ergodicity breaking. Consider the fractional Fokker–Planck equation (23) in the harmonic potential $V(x) = m\omega^2 x^2/2$. In thermal equilibrium, the position of an ensemble of independent particles follows the Boltzmann distribution (see Eq. (1)),

$$G(x) = \frac{1}{Z} \exp[-V(x)/(k_B T)] = \frac{1}{Z} \exp[-m\omega^2 x^2/(2k_B T)]. \quad (40)$$

We are interested in the *time-averaged* position:

$$\bar{x} = \frac{\int_0^t x(\tau) d\tau}{t}.$$

Clearly, the numerator is a functional of the anomalous path, $A_x = \int_0^t x(\tau) d\tau$, or in other words, $U(x) = x$. When the motion is Brownian, the process is ergodic since the field is binding. Due to the symmetry of the harmonic field, in the long time limit $\bar{x}$ is statistically equal to zero, namely,

$$\begin{aligned} \lim_{t \rightarrow \infty} \bar{x} &= \langle x \rangle = \int_{-\infty}^{\infty} x G(x) dx \\ &= \frac{1}{Z} \int_{-\infty}^{\infty} x \exp \left[-\frac{m\omega^2 x^2}{2k_B T} \right] dx = 0. \end{aligned} \quad (41)$$

Put differently, in an ergodic system the fluctuations of the time-averaged position vanish:

$$\lim_{t \rightarrow \infty} \langle (\Delta \bar{x})^2 \rangle = \lim_{t \rightarrow \infty} \left[\langle \bar{x}^2 \rangle - \langle \bar{x} \rangle^2 \right] = 0. \quad (42)$$

For anomalous subdiffusion ergodicity is broken [11, 13, 14] and the fluctuations of the time-averaged position do not vanish even for long times. This is illustrated in Fig. 1.

With our equation for anomalous functionals, we now treat the problem of the fluctuations of the time-average of $x(t)$,

$$\langle (\Delta \bar{x})^2 \rangle = \langle A_x^2 \rangle / t^2,$$

where we assumed $x_0 = 0$ such that $\langle \bar{x} \rangle = 0$ at all times due to symmetry. The equation that describes the distribution of the functional A_x is the

Fig. 1. Trajectories of particles in a binding harmonic field and the time-averaged position. Paths were generated for $\alpha = 1, 0.75, 0.5$ using the method described in Sec. 4.2 [59] with $a = 0.01$, $K_\alpha = 1/2$, $k_B T / (m\omega^2) = 1/2$, and $x_0 = 0$. The solid lines are the trajectories and the dashed line correspond to the time-averaged position $\bar{x} = \int_0^t x(\tau) d\tau / t$. For $\alpha = 1$, the time-average of $x(t)$ quickly converges to zero because ergodicity holds. For $\alpha < 1$, the process is non-ergodic since the average waiting time is infinite. For small enough α , the time-average approaches the position where the particle is stuck for the most time.

forward Eq. (24):

$$\frac{\partial}{\partial t} G(x, p, t) = K_\alpha \left[\frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial x} \frac{m\omega^2 x}{k_B T} \right] \mathcal{D}_t^{1-\alpha} G(x, p, t) + ipx G(x, p, t),$$

where we used $U(x) = x$, and p is the Fourier pair of A_x . Since $G(x, p, t = 0) = \delta(x)$, we have in s space,

$$sG(x, p, s) - \delta(x) = K_\alpha \left[\frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial x} \frac{m\omega^2 x}{k_B T} \right] [s - ipx]^{1-\alpha} \times G(x, p, s) + ipx G(x, p, s). \quad (43)$$

To find $\langle A_x^2 \rangle$, we use the relation

$$\langle A_x^2 \rangle_s = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A_x^2 G(x, A_x, s) dA_x dx = - \int_{-\infty}^{\infty} \frac{\partial^2}{\partial p^2} G(x, p, s) \Big|_{p=0} dx. \quad (44)$$

Operating on both sides of (43) with $-\frac{\partial^2}{\partial p^2}$, substituting $p = 0$, and integrating over all x , we obtain, in s space,

$$s \langle A_x^2 \rangle_s = 2 \langle A_x x \rangle_s, \quad (45)$$

where we used the fact that the integral over the $\mathcal{L}_{\text{FP}}$ term vanishes because $x^n G$ and $x^n \frac{\partial G}{\partial x}$ are zero for $|x| \rightarrow \infty$ for all n . Thus, the problem of finding $\langle A_x^2 \rangle_s$ reduces to that of finding $\langle A_x x \rangle_s$. We next use

$$\begin{aligned} \langle A_x x \rangle_s &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A_x x G(x, A_x, s) dA_x dx \\ &= -i \int_{-\infty}^{\infty} x \frac{\partial}{\partial p} G(x, p, s) \Big|_{p=0} dx. \end{aligned} \quad (46)$$

Operating on both sides of (43) with $-i \frac{\partial}{\partial p}$, substituting $p = 0$, and integrating over $\int_{-\infty}^{\infty} \cdots x dx$, we obtain,

$$s \langle A_x x \rangle_s = [1 + (1 - \alpha)(s\tau)^{-\alpha}] \langle x^2 \rangle_s - s(s\tau)^{-\alpha} \langle A_x x \rangle_s,$$

where we defined the relaxation time $\tau^\alpha = k_B T / (K_\alpha m \omega^2)$. Thus,

$$s \langle A_x x \rangle_s = \frac{(1 - \alpha) + (s\tau)^\alpha}{1 + (s\tau)^\alpha} \langle x^2 \rangle_s. \quad (47)$$

Finally, to find $\langle x^2 \rangle_s$, we use

$$\langle x^2 \rangle_s = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x^2 G(x, A_x, s) dA_x dx = \int_{-\infty}^{\infty} x^2 G(x, p = 0, s) dx. \quad (48)$$

Substituting $p = 0$ in (43) and integrating over $\int_{-\infty}^{\infty} \cdots x^2 dx$,

$$s \langle x^2 \rangle_s = 2K_\alpha s^{-\alpha} - 2s(s\tau)^{-\alpha} \langle x^2 \rangle_s,$$

where we used the normalization condition $\int \int G(x, A_x, s) dA_x dx = 1/s$. Thus,

$$s \langle x^2 \rangle_s = \frac{2 \langle x^2 \rangle_{\text{th}}}{2 + (s\tau)^\alpha}. \quad (49)$$

where $\langle x^2 \rangle_{\text{th}} = K_\alpha \tau^\alpha = k_B T / (m \omega^2)$ is the second moment of x in thermal equilibrium (see Eq. (40)). Combining Eqs. (45), (47), and (49), we find in

Laplace s space,

$$\langle A_x^2 \rangle_s = \frac{4}{s^3} \frac{(1-\alpha) + (s\tau)^\alpha}{1 + (s\tau)^\alpha} \frac{\langle x^2 \rangle_{\text{th}}}{2 + (s\tau)^\alpha}.$$

To invert to the time domain, we first write $\langle A_x^2 \rangle_s$ as partial fractions:

$$\langle A_x^2 \rangle_s = \frac{2 \langle x^2 \rangle_{\text{th}}}{s^3} \left[(1-\alpha) + 2\alpha \frac{(s\tau)^\alpha}{1 + (s\tau)^\alpha} - (1+\alpha) \frac{(s\tau)^\alpha}{2 + (s\tau)^\alpha} \right]. \quad (50)$$

The inverse of the last equation is

$$\langle A_x^2 \rangle = \langle x^2 \rangle_{\text{th}} t^2 \{ (1-\alpha) + 4\alpha E_{\alpha,3}[-(t/\tau)^\alpha] - 2(1+\alpha) E_{\alpha,3}[-2(t/\tau)^\alpha] \},$$

where we used the Laplace transform relation [60]

$$\int_0^\infty e^{-st} t^2 E_{\alpha,3}[-c(t/\tau)^\alpha] dt = \frac{1}{s^3} \frac{(s\tau)^\alpha}{c + (s\tau)^\alpha}$$

and $E_{\alpha,3}(z)$ is the Mittag-Leffler function, defined as [60]

$$E_{\alpha,3}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(3 + \alpha n)}. \quad (51)$$

The Mittag-Leffler function arises frequently in the context of fractional calculus as the fractional extension of the exponential function [7]. Using $\langle \bar{x}^2 \rangle = \langle A_x^2 \rangle / t^2$ we finally have

$$\langle \bar{x}^2 \rangle = \langle x^2 \rangle_{\text{th}} \{ (1-\alpha) + 4\alpha E_{\alpha,3}[-(t/\tau)^\alpha] - 2(1+\alpha) E_{\alpha,3}[-2(t/\tau)^\alpha] \}. \quad (52)$$

Equation (52) is illustrated in Fig. 2.

To find the long times behavior, we expand Eq. (50) for small s , invert, and divide by t^2 (Fig. 2),

$$\langle \bar{x}^2 \rangle \sim (1-\alpha) \langle x^2 \rangle_{\text{th}} + \frac{(3\alpha-1) \langle x^2 \rangle_{\text{th}}}{\Gamma(3-\alpha)} \left(\frac{t}{\tau} \right)^{-\alpha} + \mathcal{O} \left[\left(\frac{t}{\tau} \right)^{-2\alpha} \right]. \quad (53)$$

Thus, for $\alpha < 1$

$$\lim_{t \rightarrow \infty} \langle (\Delta \bar{x})^2 \rangle = (1-\alpha) \langle x^2 \rangle_{\text{th}} > 0 \quad (54)$$

and ergodicity is broken [13,14]. Only when $\alpha=1$, we have ergodic behavior $\lim_{t \rightarrow \infty} \langle (\Delta \bar{x})^2 \rangle = 0$. Equations (52) and (53) thus exhibit $t^{-\alpha}$ convergence of the fluctuations of the time-averaged position to its asymptotic

Fig. 2. Fluctuations of the time-average of $x(t)$, $\langle (\Delta \bar{x})^2 \rangle$, for a particle in a binding harmonic field. Except for $\alpha = 1$, the fluctuations do not vanish when $t \rightarrow \infty$ and thus ergodicity is broken. Symbols represent simulation results for (top to bottom) $\alpha = 0.25, 0.5, 0.75, 1$ (see also legend). CTRW trajectories were generated using the method described in the main text (Sec. 4.2) with parameter values $a = 0.02$, $K_\alpha = 1/2$, $\langle x^2 \rangle_{\text{th}} = 1/2$ (or $\tau^\alpha = 1$), and $x_0 = 0$. Simulations ended at $t = 10^3$ and included at least 10^4 trajectories for each α . Theory, Eq. (52), is plotted in solid lines, and agrees well with simulations without any fit. The straight dashed lines are the infinite time limit $\langle (\Delta \bar{x})^2 \rangle = (1-\alpha) \langle x^2 \rangle_{\text{th}}$ (Eq. (54)). The convergence to this limit is slowest for $\alpha = 0.25$. The dotted lines represent the short-times and long-times approximations, Eqs. (53) and (55), respectively.

value. The convergence to the long time limit is extremely slow for $\alpha \rightarrow 0$ as expected. For short times [7]

$$E_{\alpha,3}[-(t/\tau)^\alpha] \sim \frac{1}{2} - \frac{(t/\tau)^\alpha}{\Gamma(3+\alpha)}.$$

Therefore, for short times,

$$\langle \bar{x}^2 \rangle \approx \frac{4 \langle x^2 \rangle_{\text{th}}}{\Gamma(3+\alpha)} \left(\frac{t}{\tau} \right)^\alpha. \quad (55)$$

This is demonstrated in Fig. 2. For $t = 0$, $\langle \bar{x}^2 \rangle = 0$ because $x_0 = 0$.

4.2. Simulation of trajectories

The fractional Feynman–Kac equation describes the joint PDF of x and A in the continuum limit of the CTRW. In this limit, $a \rightarrow 0$ and $B_\alpha \rightarrow 0$ but the generalized diffusion coefficient $K_\alpha = a^2/(2B_\alpha)$ (Eq. (17)) is kept finite [8]. We simulate trajectories of this process as follows [59].

We place a particle on a one-dimensional lattice in initial position x_0 . We set the lattice spacing a and the generalized diffusion coefficient K_α and determine $B_\alpha = a^2/(2K_\alpha)$. Waiting times are then drawn for $\alpha = 1$ from an exponential distribution $\psi(\tau) = e^{-\tau/\tau_0}/\tau_0$ with mean $\tau_0 = B_1$. This is implemented by setting $\tau = -\tau_0 \ln(u)$, where u is a number uniformly distributed in $[0, 1]$. For $\alpha < 1$, we set $\tau_0 = [B_\alpha/\Gamma(1-\alpha)]^{1/\alpha}$ and $\tau = \tau_0 u^{-1/\alpha}$. This corresponds to $\psi(\tau) = \frac{B_\alpha}{|\Gamma(-\alpha)|} \tau^{-(1+\alpha)}$ ($\tau \geq \tau_0$) as in Sec. 2. After waiting time τ , we move the particle right or left (to $x_0 + a$ or $x_0 - a$, respectively) with probabilities $R(x)$ and $L(x)$, respectively, as given in Eq. (11). Specifically, for the harmonic potential we conveniently set $\langle x^2 \rangle_{\text{th}} = k_B T/(m\omega^2) = 1/2$ and thus $R(x) = (1 - ax)/2$ and $L(x) = (1 + ax)/2$. We then repeatedly wait and move the particle until the end of the simulation.

We implemented this algorithm to study the time-average of $x(t)$ for a particle in a harmonic potential. For each trajectory, we calculated $\bar{x}(t)$ for various time points. For each time point, we then computed the fluctuations $\langle (\Delta \bar{x})^2 \rangle$ over many trajectories. Convergence to the theoretical result was observed when we used smaller and smaller lattice spacing a , while keeping fixed the generalized diffusion coefficient K_α . The final results are presented in Fig. 2 and indeed agree with our theory, Eq. (52) without any fit. We also implemented the alternative simulation method of [61,62], to reach the same results (not shown).

5. Summary

Functionals of the path of a Brownian particle have been investigated in numerous studies since the development of the Feynman–Kac equation in 1949 [30]. We developed forward and backward equations (Eqs. (18) and (27), respectively) for functionals of anomalous diffusion based on fractional calculus [31]. In the force-free case, we studied a few functionals of interest, including the occupation time in half-space and the maximal displacement; further examples can be found in [37]. For a particle in a harmonic field, we calculated the fluctuations of the time-averaged position and demonstrated weak ergodicity breaking.

The fractional Feynman–Kac equation (18) can be obtained from the integer equation (3) by insertion of a substantial fractional derivative operator [32]. In that sense, it 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 [52] was replaced by Lamperti's PDF (Eq. (33)) [50],

and the famous $t^{-3/2}$ decay of the one-dimensional first passage time PDF [52] became $t^{-(1+\alpha/2)}$ (Eq. (38)). Instead of the usual ergodic behavior of the Brownian motion, we observed weak ergodicity breaking. Thus, our analysis supports the notion that CTRW and the emerging fractional paths 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 [63].

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