Fractional Feynman-Kac equation for weak ergodicity breaking

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The continuous-time random walk (CTRW) is a model of anomalous subdiffusion in which particles are immobilized for random times between successive jumps. A power-law distribution of the waiting times, $\psi(\tau) \sim \tau^{-(1+\alpha)}$, leads to subdiffusion ($\langle x^2 \rangle \sim t^\alpha$) for $0 < \alpha < 1$. In closed systems, the long stagnation periods cause time averages to divert from the corresponding ensemble averages, which is a manifestation of weak ergodicity breaking. The time average of a general observable $\overline{U}(t) = \frac{1}{t}\int_0^t U[x(\tau)]d\tau$ is a functional of the path and is described by the well-known Feynman-Kac equation if the motion is Brownian. Here, we derive forward and backward fractional Feynman-Kac equations for functionals of CTRW in a binding potential. We use our equations to study two specific time averages: the fraction of time spent by a particle in half-box, and the time average of the particle's position in a harmonic field. In both cases, we obtain the probability density function of the time averages for $t \to \infty$ and the first two moments. Our results show that both the occupation fraction and the time-averaged position are random variables even for long times, except for $\alpha = 1$, when they are identical to their ensemble averages. Using our fractional Feynman-Kac equation, we also study the dynamics leading to weak ergodicity breaking, namely the convergence of the fluctuations to their asymptotic values.

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I. INTRODUCTION

The time average of an observable $U(x)$ of a diffusing particle is defined as

$$\overline{U}(t) = \frac{1}{t}\int_0^t U[x(\tau)]d\tau, \tag{1}$$

where $x(t)$ is the particle's trajectory. For Brownian motion in a binding potential $V(x)$ and in contact with a heat bath, ergodicity leads to

$$\lim_{t\to\infty} \overline{U}(t) = \langle U \rangle_{\text{th}} = \int_{-\infty}^{\infty} U(x) G_{\text{eq}}(x) dx, \tag{2}$$

where $G_{\text{eq}}(x) = e^{-V(x)/(k_B T)}/Z$ is the Boltzmann distribution and $\langle U \rangle_{\text{th}}$ is the thermal average. The equality of the time and ensemble averages in ergodic systems is one of the basic presuppositions of statistical mechanics.

In the past few decades, it was found that in many systems, the diffusion of particles is anomalously slow, $\langle x^2 \rangle \sim t^\alpha$ with $0 < \alpha < 1$ [1–4]. Anomalous subdiffusion is commonly modeled as a continuous-time random walk (CTRW): nearest-neighbor hopping on a lattice, with waiting times between jumps distributed as a power-law with infinite mean [5,6].

For closed systems, the long immobilization periods of CTRW result in a deviation of time averages from ensemble averages even for long times [7–10]. Although there are no inaccessible regions in the phase space (i.e., there is no strong ergodicity breaking), the divergence of the mean waiting time results in some waiting times of the order of magnitude of the entire experiment. Therefore, particles do not sample the phase space uniformly in any single trajectory, leading to weak ergodicity breaking [11].

Two examples of particularly interesting time averages, which we study in this paper, are given below. For a particle in a bounded region, the occupation fraction is defined as $\lambda(t) = \frac{1}{t}\int_0^t \Theta[x(\tau)]d\tau$, where $\Theta(x)$ is the Heaviside function. In other words, λ is the fraction of time spent by the particle in the positive side of the region [12,13]. Generally, the occupation fraction can be defined for any given subspace. Consider, for example, a particle in a sample illuminated by a laser, where the particle emits photons only under the laser's focus. The occupation fraction is proportional to the total emitted light [14,15]. Next, the time-averaged position of a particle is defined as $\overline{x}(t) = \frac{1}{t}\int_0^t x(\tau)d\tau$. Recent advances in single-particle tracking technologies enable the experimental determination of this quantity for beads in polymer networks [16,17] and for biological macromolecules and small organelles in living cells [18–21]. Since in many physical and biological systems the diffusion is anomalous, the study of occupation fractions or time-averaged positions in subdiffusive processes such as CTRW is of current interest.

Time averages are closely related to functionals, which are defined as $A = \int_0^t U[x(\tau)]d\tau$ and have many applications in physics, mathematics, and other fields [22]. Denote by $G(x,A,t)$ the joint probability density function (PDF) of finding, at time t, the particle at x and the functional at A. The Feynman-Kac equation states that for a free Brownian particle [23],

$$\frac{\partial}{\partial t} G(x,p,t) = K_1 \frac{\partial^2}{\partial x^2} G(x,p,t) - pU(x)G(x,p,t), \tag{3}$$

where $G(x,p,t)$ is the Laplace transform $A \to p$ of $G(x,A,t)$ and K_1 is the diffusion coefficient. Recently, we developed a *fractional* Feynman-Kac equation for anomalous diffusion of free particles [24,25]. As time averages are in fact scaled functionals, $\overline{U} = A/t$, a generalized Feynman-Kac equation for anomalous functionals in a binding field would be invaluable for the study of weak ergodicity breaking. Currently, no such equation exists, and weak ergodicity breaking has been investigated only in the $t \to \infty$ limit or using functional- and potential-specific methods [7–10].

In this paper, we obtain an equation for functionals of anomalous diffusion in a force field $F(x)$. The equation takes the following form (reported without derivation in Ref. [24]):

$$\frac{\partial}{\partial t}G(x,p,t) = K_\alpha\left[\frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x}\frac{F(x)}{k_B T}\right]\mathcal{D}_t^{1-\alpha}G(x,p,t) - pU(x)G(x,p,t). \quad (4)$$

The symbol $\mathcal{D}_t^{1-\alpha}$ is a *fractional substantial derivative*, equal in Laplace $t \to s$ space to $[s + pU(x)]^{1-\alpha}$ [26,27], and K_α is a generalized diffusion coefficient. Solving Eq. (4) for $G(x,p,t)$, inverting $p \to A$, and integrating over all x yields $G(A,t)$, the PDF of A at time t. Changing variables $A \to A/t = \overline{U}$, one finally comes by $G(\overline{U},t)$, the (time-dependent) PDF of $\overline{U}$. Weak ergodicity breaking can then be determined by looking at the long-times properties of $G(\overline{U},t)$: if $\overline{U}$ is not identically equal to $\langle U\rangle_{\text{th}}$ for $t \to \infty$, ergodicity is broken. Moreover, if $G(\overline{U},t)$ or the moments of $\overline{U}$ can be found also for $t < \infty$, the kinetics of weak ergodicity breaking can be uncovered.

In the rest of the paper, we derive Eq. (4) as well as a backward equation and an equation for time-dependent forces. We then apply our equation to the two examples given above: the occupation fraction (in a box) and the time-averaged position (in a harmonic potential). In both cases, we calculate the long-times limit of $G(\overline{U},t)$ and the fluctuations $\langle(\Delta\overline{U})^2\rangle_t = \langle\overline{U}^2\rangle_t - \langle\overline{U}\rangle_t^2$ (the subscript t indicates the time). We demonstrate that for subdiffusion, both systems exhibit weak ergodicity breaking, and that the fluctuations decay as $t^{-\alpha}$ to their asymptotic limit. Part of the results for the fluctuations of the time-averaged position were briefly reported in Ref. [24].

II. DERIVATION OF THE FRACTIONAL EQUATIONS

A. The forward equation

1. Continuous-time random walk

In the continuous-time random walk model, a particle is placed on a one-dimensional lattice with spacing a and is allowed to jump to its nearest neighbors only. The probabilities of jumping left $L(x)$ and right $R(x)$ depend on $F(x)$, the force at x (see the next subsection for a derivation of these probabilities). If $F(x) = 0$, then $R(x) = L(x) = 1/2$. Waiting times between jump events are independent identically distributed random variables with PDF $\psi(\tau)$, and are independent of the external force. The initial position of the particle, x_0, is distributed according to $G_0(x)$. The particle waits in 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. We assume that the waiting time PDF scales as

$$\psi(\tau) \sim \frac{B_\alpha}{|\Gamma(-\alpha)|}\tau^{-(1+\alpha)}, \quad (5)$$

with $0 < \alpha < 1$. With this PDF, the mean waiting time diverges and the process is subdiffusive: for $F(x) = 0$, $x_0 = 0$, and an infinite open system, $\langle x^2\rangle \sim t^\alpha$ [28]. We also consider a finite mean waiting time, e.g., an exponential distribution $\psi(\tau) = e^{-\tau/\langle\tau\rangle}/\langle\tau\rangle$. This leads to normal diffusion $\langle x^2\rangle \sim t$, and we therefore refer to this case as $\alpha = 1$. For a discussion on the effect of an exponential cutoff on Eq. (5), see [29]. Below, we derive the differential equation that describes the distribution of functionals in the continuum limit of this model.

2. Derivation of the equation

Define $A = \int_0^t U[x(\tau)]d\tau$ and define $G(x,A,t)$ as 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 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

$$G(x,A,t) = \int_0^t W(\tau)\chi[x, A - \tau U(x), t - \tau]d\tau, \quad (6)$$

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, note that to *arrive at* (x,A) at time t, the particle must have arrived at either $[x - a, A - \tau U(x - a)]$ or $[x + a, A - \tau U(x + a)]$ at time $t - \tau$ when the previous jump was made. Therefore,

$$\chi(x,A,t) = G_0(x)\delta(A)\delta(t) + \int_0^t \psi(\tau)L(x + a)\chi[x + a, A - \tau U(x + a), t - \tau]d\tau + \int_0^t \psi(\tau)R(x - a)\chi\,[x - a, A - \tau U(x - a), t - \tau]d\tau. \quad (7)$$

The term $G_0(x)\delta(A)\delta(t)$ corresponds to the initial condition, namely that at $t = 0$, $A = 0$ and the particle's position is distributed as $G_0(x)$.

Assume that $U(x) \geqslant 0$ for all x and thus $A \geqslant 0$ (an assumption we will relax in Sec. II A 3). Let $\chi(x,p,t) = \int_0^\infty e^{-pA}\chi(x,A,t)dA$ be the Laplace transform $A \to p$ of $\chi(x,A,t)$ (throughout this work, we use the convention that the variables in parentheses define the space in which we are working). Laplace transforming Eq. (7) from A to p, we find

$$\chi(x,p,t) = G_0(x)\delta(t) + L(x + a)\int_0^t \psi(\tau)e^{-p\tau U(x+a)}\chi(x + a, p, t - \tau)d\tau + R(x - a)\int_0^t \psi(\tau)e^{-p\tau U(x-a)}\chi(x - a, p, t - \tau)d\tau. \quad (8)$$

Laplace transforming Eq. (8) from t to s using the convolution theorem,

$$\chi(x,p,s) = G_0(x) + L(x + a)\hat{\psi}[s + pU(x + a)]\chi(x + a, p, s) + R(x - a)\hat{\psi}[s + pU(x - a)]\chi(x - a, p, s), \quad (9)$$

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 $x \to k$ of χ. Fourier transforming Eq. (9) and changing variables $x \pm a \to x$,

$$\chi(k,p,s) = \hat{G}_0(k) + e^{-ika}\int_{-\infty}^\infty e^{ikx}L(x)\hat{\psi}[s + pU(x)]\chi(x,p,s)dx + e^{ika}\int_{-\infty}^\infty e^{ikx}R(x)\hat{\psi}[s + pU(x)]\chi(x,p,s)dx, \quad (10)$$

where $\hat{G}_0(k)$ is the Fourier transform of the initial condition.

We now express $L(x)$ and $R(x)$ in terms of the potential $V(x)$. Assuming the system is coupled to a heat bath at temperature T and assuming detailed balance, we have [10,28]

$$L(x)\exp\left[-\frac{V(x)}{k_BT}\right]=R(x-a)\exp\left[-\frac{V(x-a)}{k_BT}\right]. \quad (11)$$

If the lattice spacing a is small, we can expand

$$\exp\left[-\frac{V(x-a)}{k_BT}\right]\approx\exp\left[-\frac{V(x)}{k_BT}\right]\left[1-\frac{aF(x)}{k_BT}+O(a^2)\right], \quad (12)$$

where we used $F(x)=-V'(x)$. Expanding $R(x)$ and $L(x)$ for $\frac{aF(x)}{k_BT}\ll 1$, using the fact that $R(x)=L(x)=1/2$ for $F(x)=0$,

$$R(x)\approx\frac{1}{2}\left[1+c\frac{aF(x)}{k_BT}\right]=1-L(x), \quad (13)$$

where c is a constant to be determined. Substituting Eqs. (12) and (13) in Eq. (11), we have, up to first order in a,

$$1-c\frac{aF(x)}{k_BT}\approx\left[1-\frac{aF(x)}{k_BT}\right]\left[1+c\frac{aF(x)}{k_BT}\right].$$

This gives, again up to first order in a, $c=1/2$. We can thus write

$$R(x)\approx\frac{1}{2}\left[1+\frac{aF(x)}{2k_BT}\right],\quad L(x)\approx\frac{1}{2}\left[1-\frac{aF(x)}{2k_BT}\right]. \quad (14)$$

Substituting Eq. (14) in Eq. (10), we obtain

$$\begin{aligned}\chi(k,p,s)\approx{}&\hat{G}_0(k)\\&+\frac{1}{2}e^{-ika}\int_{-\infty}^{\infty}e^{ikx}\hat{\psi}[s+pU(x)]\chi(x,p,s)dx\\&-\frac{1}{2}e^{-ika}\int_{-\infty}^{\infty}e^{ikx}\frac{aF(x)}{2k_BT}\hat{\psi}[s+pU(x)]\chi(x,p,s)dx\\&+\frac{1}{2}e^{ika}\int_{-\infty}^{\infty}e^{ikx}\hat{\psi}[s+pU(x)]\chi(x,p,s)dx\\&+\frac{1}{2}e^{ika}\int_{-\infty}^{\infty}e^{ikx}\frac{aF(x)}{2k_BT}\hat{\psi}[s+pU(x)]\chi(x,p,s)dx.\end{aligned}$$

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

$$\chi(k,p,s)\approx\hat{G}_0(k)+\left[\cos(ka)+i\sin(ka)\frac{aF\left(-i\frac{\partial}{\partial k}\right)}{2k_BT}\right]\times\hat{\psi}\left[s+pU\left(-i\frac{\partial}{\partial k}\right)\right]\chi(k,p,s). \quad (15)$$

The symbols $F(-i\frac{\partial}{\partial k})$ and $U(-i\frac{\partial}{\partial k})$ represent the original functions $F(x)$ and $U(x)$, but with $-i\frac{\partial}{\partial k}$ as their argument. 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. (15) is

$$\chi(k,p,s)\approx\left\{1-\left[\cos(ka)+i\sin(ka)\frac{aF\left(-i\frac{\partial}{\partial k}\right)}{2k_BT}\right]\times\hat{\psi}\left[s+pU\left(-i\frac{\partial}{\partial k}\right)\right]\right\}^{-1}\hat{G}_0(k). \quad (16)$$

We next use our expression for χ to calculate $G(x,A,t)$. Transforming Eq. (6) $(x,A,t)\to(k,p,s)$,

$$G(k,p,s)=\frac{1-\hat{\psi}\left[s+pU\left(-i\frac{\partial}{\partial k}\right)\right]}{s+pU\left(-i\frac{\partial}{\partial k}\right)}\chi(k,p,s), \quad (17)$$

where we used the fact that $\hat{W}(s)=[1-\hat{\psi}(s)]/s$. Substituting Eq. (16) into (17), we have

$$\begin{aligned}G(k,p,s)\approx{}&\frac{1-\hat{\psi}\left[s+pU\left(-i\frac{\partial}{\partial k}\right)\right]}{s+pU\left(-i\frac{\partial}{\partial k}\right)}\\&\times\left\{1-\left[\cos(ka)+i\sin(ka)\frac{aF\left(-i\frac{\partial}{\partial k}\right)}{2k_BT}\right]\right.\\&\left.\times\hat{\psi}\left[s+pU\left(-i\frac{\partial}{\partial k}\right)\right]\right\}^{-1}\hat{G}_0(k). \quad (18)\end{aligned}$$

To derive a differential equation for $G(x,p,t)$, we take the small s and k limit of Eq. (18). For $0<\alpha<1$, the waiting time PDF is $\psi(\tau)\sim B_\alpha\tau^{-(1+\alpha)}/|\Gamma(-\alpha)|$ [Eq. (5)], which, for small s, has the Laplace transform [3]

$$\hat{\psi}(s)\approx 1-B_\alpha s^\alpha. \quad (19)$$

The case $\alpha=1$ is also described by Eq. (19) if we identify B_1 with the mean waiting time $\langle\tau\rangle$. Substituting Eq. (19) in Eq. (18), expanding $\cos(ka)\approx 1-k^2a^2/2$ and $\sin(ka)\approx ka$, and neglecting high-order terms, Eq. (18) becomes

$$\begin{aligned}G(k,p,s)\approx{}&\left[s+pU\left(-i\frac{\partial}{\partial k}\right)\right]^{\alpha-1}\\&\times\left\{K_\alpha\left[k^2-ik\frac{F\left(-i\frac{\partial}{\partial k}\right)}{k_BT}\right]+\left[s+pU\left(-i\frac{\partial}{\partial k}\right)\right]^\alpha\right\}^{-1}\hat{G}_0(k). \quad (20)\end{aligned}$$

In the preceding equation, we used the generalized diffusion coefficient [28]

$$K_\alpha\equiv\lim_{a^2,B_\alpha\to 0}\frac{a^2}{2B_\alpha}, \quad (21)$$

with units m^2/s^α. Rearranging Eq. (20),

$$\begin{aligned}sG(k,p,s)-\hat{G}_0(k)={}&-pU\left(-i\frac{\partial}{\partial k}\right)G(k,p,s)\\&-K_\alpha\left[k^2-ik\frac{F\left(-i\frac{\partial}{\partial k}\right)}{k_BT}\right]\left[s+pU\left(-i\frac{\partial}{\partial k}\right)\right]^{1-\alpha}G(k,p,s).\end{aligned}$$

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

$$\frac{\partial}{\partial t}G(x,p,t)=K_\alpha\mathcal{L}_{\rm FP}\mathcal{D}_t^{1-\alpha}G(x,p,t)-pU(x)G(x,p,t). \quad (22)$$

The symbol $\mathcal{L}_{\rm FP}$ represents the Fokker-Planck operator,

$$\mathcal{L}_{\rm FP}=\frac{\partial^2}{\partial x^2}-\frac{\partial}{\partial x}\frac{F(x)}{k_BT}, \quad (23)$$

and the initial condition is $G(x,A,t=0)=G_0(x)\delta(A)$, or $G(x,p,t=0)=G_0(x)$. The symbol $\mathcal{D}_t^{1-\alpha}$ represents the fractional substantial derivative operator introduced in Refs. [26,30]:

$$\mathcal{L}\left\{\mathcal{D}_t^{1-\alpha}G(x,p,t)\right\} = [s + pU(x)]^{1-\alpha}G(x,p,s), \quad (24)$$

where $\mathcal{L}\{f(t)\} = \int_0^\infty e^{-st}f(t)dt$ is the Laplace transform $t \to s$. In t space,

$$\mathcal{D}_t^{1-\alpha}G(x,p,t) = \frac{1}{\Gamma(\alpha)}\left[\frac{\partial}{\partial t} + pU(x)\right]\int_0^t \frac{e^{-(t-\tau)pU(x)}}{(t-\tau)^{1-\alpha}}G(x,p,\tau)d\tau. \quad (25)$$

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

3. Special cases and extensions

(a) Normal diffusion. For $\alpha = 1$, or normal diffusion, the fractional substantial derivative equals unity and we have

$$\frac{\partial}{\partial t}G(x,p,t) = K_1\mathcal{L}_{\rm FP}G(x,p,t) - pU(x)G(x,p,t). \quad (26)$$

This is simply the (integer) Feynman-Kac equation (3), extended to a general force field $F(x)$.

(b) 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. (22) reduces to the fractional Fokker-Planck equation [28,31,32]:

$$\frac{\partial}{\partial t}G(x,t) = K_\alpha\mathcal{L}_{\rm FP}\mathcal{D}_{{\rm RL},t}^{1-\alpha}G(x,t), \quad (27)$$

where $\mathcal{D}_{{\rm RL},t}^{1-\alpha} = \mathcal{D}_t^{1-\alpha}|_{p=0}$ is the Riemann-Liouville fractional derivative operator. In Laplace s space, $\mathcal{D}_{{\rm RL},t}^{1-\alpha}G(x,s) = s^{1-\alpha}G(x,s)$.

(c) Free particle. For $F(x) = 0$, $\mathcal{L}_{\rm FP} = \frac{\partial^2}{\partial x^2}$. Several applications of this special case were treated in Ref. [25].

(d) A general functional. When the functional is not necessarily positive, the Laplace transform $A \to p$ is replaced by a Fourier transform $G(x,p,t) = \int_{-\infty}^\infty e^{ipA}G(x,A,t)dA$. The fractional Feynman-Kac equation looks like (22), but with p replaced by $-ip$,

$$\frac{\partial}{\partial t}G(x,p,t) = K_\alpha\mathcal{L}_{\rm FP}\mathcal{D}_t^{1-\alpha}G(x,p,t) + ipU(x)G(x,p,t), \quad (28)$$

where $\mathcal{D}_t^{1-\alpha} \to [s - ipU(x)]^{1-\alpha}$ in Laplace s space. The derivation of Eq. (28) is similar to that of Eq. (22) (see [25] for more details).

(e) Time-dependent force. Anomalous diffusion with a time-dependent force is of recent interest [33–37]. In a corresponding CTRW model, the probabilities of jumping left and right are determined by the force at the end of the waiting period [33,36]. As we show in Appendix A, the equation for $G(x,p,t)$ is similar to Eq. (22):

$$\frac{\partial}{\partial t}G(x,p,t) = K_\alpha\mathcal{L}_{\rm FP}^{(\rm t)}\mathcal{D}_t^{1-\alpha}G(x,p,t) - pU(x)G(x,p,t), \quad (29)$$

but where

$$\mathcal{L}_{\rm FP}^{(\rm t)} = \frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x}\frac{F(x,t)}{k_BT}$$

is the time-dependent Fokker-Planck operator. For $p = 0$, Eq. (29) reduces to the recently derived equation for the PDF of x [36].

B. The backward equation

The forward equation describes $G(x,A,t)$, the joint PDF of x and A. Consequently, if we are interested only in the distribution of A, we must integrate G over all x, which could be inconvenient. We therefore develop below an equation for $G_{x_0}(A,t)$—the PDF of A at time t, given that the process has started at x_0. This equation, which is called the backward equation, turns out to be very useful in practical applications (see, e.g., [22,25] and Sec. IV A).

According to the CTRW model, the particle starts at $x = x_0$ and jumps at time τ to either $x_0 + a$ or $x_0 - a$. Alternatively, the particle does not move at all during the measurement time $[0,t]$. Hence,

$$G_{x_0}(A,t) = W(t)\delta[A - tU(x_0)] + \int_0^t \psi(\tau)R(x_0)G_{x_0+a}[A - \tau U(x_0),t-\tau]d\tau + \int_0^t \psi(\tau)L(x_0)G_{x_0-a}[A - \tau U(x_0),t-\tau]d\tau. \quad (30)$$

Here, $\tau U(x_0)$ is the contribution to A from the pausing time at x_0 in the interval $[0,\tau]$. The first term on the right-hand side (rhs) of Eq. (30) describes a motionless particle, for which $A(t) = tU(x_0)$. We now transform Eq. (30) $(x_0,A,t) \to (k_0,p,s)$, using techniques similar to those used in Sec. II A 2. In the continuum limit, $a \to 0$, this leads to

$$G_{k_0}(p,s) \approx \frac{1 - \hat{\psi}\left[s + pU\left(-i\frac{\partial}{\partial k_0}\right)\right]}{s + pU\left(-i\frac{\partial}{\partial k_0}\right)}\delta(k_0) + \hat{\psi}\left[s + pU\left(-i\frac{\partial}{\partial k_0}\right)\right] \times \left[\cos(k_0a) - \frac{aF\left(-i\frac{\partial}{\partial k_0}\right)}{2k_BT}i\sin(k_0a)\right]G_{k_0}(p,s).$$

We then expand $\hat{\psi}(s) \approx 1 - B_\alpha s^\alpha$, $\cos(k_0a) \approx 1 - k_0^2a^2/2$, and $\sin(k_0a) \approx k_0a$. After some rearrangements,

$$sG_{k_0}(p,s) - \delta(k_0) = -pU\left(-i\frac{\partial}{\partial k_0}\right)G_{k_0}(p,s) - K_\alpha\left[s + pU\left(-i\frac{\partial}{\partial k_0}\right)\right]^{1-\alpha} \times \left[{k_0}^2 + \frac{F\left(-i\frac{\partial}{\partial k_0}\right)}{k_BT}ik_0\right]G_{k_0}(p,s).$$

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

$$\frac{\partial}{\partial t}G_{x_0}(p,t) = K_\alpha\mathcal{D}_t^{1-\alpha}\mathcal{L}_{\rm FP}^{(\rm B)}G_{x_0}(p,t) - pU(x_0)G_{x_0}(p,t), \quad (31)$$

where

$$\mathcal{L}_{\mathrm{FP}}^{(\mathrm{B})} = \frac{\partial^2}{\partial x_0^2} + \frac{F(x_0)}{k_B T}\frac{\partial}{\partial x_0} \tag{32}$$

is the *backward* Fokker-Planck operator. The initial condition is $G_{x_0}(A,t=0)=\delta(A)$, or $G_{x_0}(p,t=0)=1$. Note the (+) sign in $\mathcal{L}_{\mathrm{FP}}^{(\mathrm{B})}$ and the order of the operators in its second term, which are opposite to those of $\mathcal{L}_{\mathrm{FP}}$ [Eq. (23)]. Here, $\mathcal{D}_t^{1-\alpha}$ equals in Laplace $t \to s$ space to $[s+pU(x_0)]^{1-\alpha}$. In Eq. (22), the operators depend on x while in Eq. (31) they depend on x_0. Therefore, Eq. (22) is a forward equation while Eq. (31) is a backward equation. Notice also that in Eq. (31), the fractional derivative operator appears to the left of the Fokker-Planck operator, in contrast to the forward equation (22).

III. THE PDF OF $\overline{U}$ FOR LONG TIMES

Consider a general time average:

$$\overline{U} = \frac{\int_0^t U[x(\tau)]d\tau}{t} = \frac{A}{t}.$$

For $t \to \infty$, the PDF of $\overline{U}$ becomes time-independent, and can be obtained from the fractional Feynman-Kac equation. Let us first write the forward equation (22) in Laplace (p,s) space:

$$[s+pU(x)]G(x,p,s) - G_0(x) \\ = K_\alpha\left[\frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x}\frac{F(x)}{k_B T}\right][s+pU(x)]^{1-\alpha}G(x,p,s). \tag{33}$$

For long times, CTRW functionals scale linearly with the time, $A \sim t$, and therefore, as shown in Ref. [38], $G(p,s) = g(p/s)/s$, where g is a scaling function. In the $t \to \infty$ limit, we take s and p to be small, with their ratio finite, and we therefore expect $G(x,p,s) \sim s^{-1}$ [indeed, see Eq. (36) below]. Consequently, both terms on the left-hand side (lhs) of Eq. (33) scale as s^0. However, the rhs of Eq. (33) scales as $s^{-\alpha}$, and therefore for small s the lhs is negligible. The forward equation thus reduces to

$$K_\alpha\left[\frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x}\frac{F(x)}{k_B T}\right][s+pU(x)]^{1-\alpha}G(x,p,s) = 0.$$

The solution of the last equation is

$$G(x,p,s) = C(p,s)[s+pU(x)]^{\alpha-1}\exp\left[-\frac{V(x)}{k_B T}\right], \tag{34}$$

where $C(p,s)$ is independent of x. To find C, we integrate Eq. (33) over all x:

$$\int_{-\infty}^{\infty}[s+pU(x)]\,G(x,p,s)dx - 1 = 0, \tag{35}$$

which is true, because for a binding field, $G(x,p,s)$ and its derivative vanish for large $|x|$. Substituting G from Eq. (34) into Eq. (35) gives

$$C(p,s) = \left\{\int_{-\infty}^{\infty}[s+pU(x)]^{\alpha}\exp\left[-\frac{V(x)}{k_B T}\right]dx\right\}^{-1}.$$

Therefore,

$$G(x,p,s) = \frac{[s+pU(x)]^{\alpha-1}\exp\left[-\frac{V(x)}{k_B T}\right]}{\int_{-\infty}^{\infty}[s+pU(x)]^{\alpha}\exp\left[-\frac{V(x)}{k_B T}\right]dx}. \tag{36}$$

Integrating Eq. (36) over all x,

$$G(p,s) = \frac{\int_{-\infty}^{\infty}[s+pU(x)]^{\alpha-1}\exp\left[-\frac{V(x)}{k_B T}\right]dx}{\int_{-\infty}^{\infty}[s+pU(x)]^{\alpha}\exp\left[-\frac{V(x)}{k_B T}\right]dx}, \tag{37}$$

where $G(p,s)$ is the double Laplace transform of $G(A,t)$, the PDF of A at time t. The last equation is the continuous version of the result derived using a different approach in Refs. [9,10]. As in Refs. [9,10], Eq. (37) can be inverted, using the method of Ref. [38], to give the equilibrium PDF of $\overline{U} = A/t$,

$$G(\overline{U}) = \frac{\sin(\pi\alpha)}{\pi} \\ \times \frac{I_{\alpha-1}^{<}(\overline{U})I_{\alpha}^{>}(\overline{U}) + I_{\alpha-1}^{>}(\overline{U})I_{\alpha}^{<}(\overline{U})}{[I_{\alpha}^{>}(\overline{U})]^2 + [I_{\alpha}^{<}(\overline{U})]^2 + 2\cos(\pi\alpha)I_{\alpha}^{>}(\overline{U})I_{\alpha}^{<}(\overline{U})}, \tag{38}$$

where

$$I_{\alpha}^{<}(\overline{U}) = \int_{\overline{U}<U(x)}\exp\left[-\frac{V(x)}{k_B T}\right][U(x)-\overline{U}]^{\alpha}dx$$

and

$$I_{\alpha}^{>}(\overline{U}) = \int_{\overline{U}>U(x)}\exp\left[-\frac{V(x)}{k_B T}\right][\overline{U}-U(x)]^{\alpha}dx.$$

For normal diffusion, $\alpha = 1$, the PDF is a delta function, $G(\overline{U}) = \delta[\overline{U} - \langle U\rangle_{\mathrm{th}}]$ [Eq. (37) and [9,10]]. For anomalous subdiffusion, $\alpha < 1$, $\overline{U}$ is a random variable, different from the ensemble average. This behavior of the time average results from the weak ergodicity breaking of the subdiffusing system. Similar results hold when $U(x)$ is not necessarily positive: the Laplace transform $A \to p$ is replaced by a Fourier transform, and in Eq. (37) p is replaced by $-ip$.

IV. APPLICATIONS: WEAK ERGODICITY BREAKING

In this section, we present two applications of the fractional Feynman-Kac equation: the occupation fraction in a box and the time-averaged position in a harmonic potential. We demonstrate weak ergodicity breaking in both cases and investigate the convergence to the asymptotic limits.

A. The occupation fraction in the positive half of a box

We study the problem of the occupation time in $x > 0$ for a subdiffusing particle moving freely in the box extending between $[-\frac{L}{2},\frac{L}{2}]$ [7,8,10].

1. The distribution

Define the occupation time in $x > 0$ as $T_+(t) = \int_0^t \Theta[x(\tau)]d\tau$ [namely $U(x) = \Theta(x)$]. To find the PDF of T_+, we write the backward fractional Feynman-Kac equation (31) in Laplace s space:

$$sG_{x_0}(p,s) - 1 = \begin{cases} K_\alpha s^{1-\alpha} \frac{\partial^2}{\partial x_0^2} G_{x_0}(p,s), & x_0 < 0, \\ K_\alpha (s+p)^{1-\alpha} \frac{\partial^2}{\partial x_0^2} G_{x_0}(p,s) - pG_{x_0}(p,s), & x_0 > 0. \end{cases} \tag{39}$$

Equation (39) is subject to the following boundary conditions:

$$\frac{\partial}{\partial x_0} G_{x_0}(p,s)\Big|_{x_0=\pm\frac{L}{2}} = 0.$$

The solution of the preceding equation is

$$G_{x_0}(p,s) = \begin{cases} C_0 \cosh\left[\left(\frac{L}{2} + x_0\right)\frac{s^{\alpha/2}}{\sqrt{K_\alpha}}\right] + \frac{1}{s}, & x_0 < 0, \\ C_1 \cosh\left[\left(\frac{L}{2} - x_0\right)\frac{(s+p)^{\alpha/2}}{\sqrt{K_\alpha}}\right] + \frac{1}{s+p}, & x_0 > 0. \end{cases} \tag{40}$$

Matching G and its derivative at $x_0 = 0$ yields the following equations:

$$C_0 \cosh\left(\frac{Ls^{\alpha/2}}{2\sqrt{K_\alpha}}\right) + \frac{1}{s} = C_1 \cosh\left[\frac{L(s+p)^{\alpha/2}}{2\sqrt{K_\alpha}}\right] + \frac{1}{s+p},$$
$$C_0 s^{\alpha/2} \sinh\left(\frac{Ls^{\alpha/2}}{2\sqrt{K_\alpha}}\right) = -C_1 (s+p)^{\alpha/2} \sinh\left[\frac{L(s+p)^{\alpha/2}}{2\sqrt{K_\alpha}}\right].$$

Solving these equations for C_0 and C_1 and substituting $x_0 = 0$ in Eq. (40) yields, after some algebra,

$$G_0(p,s) = \frac{s^{\alpha/2-1}\tanh[(s\tau)^{\alpha/2}] + (s+p)^{\alpha/2-1}\tanh\{[\tau(s+p)]^{\alpha/2}\}}{s^{\alpha/2}\tanh[(s\tau)^{\alpha/2}] + (s+p)^{\alpha/2}\tanh\{[\tau(s+p)]^{\alpha/2}\}}, \tag{41}$$

where we defined $\tau^\alpha \equiv L^2/(4K_\alpha)$. This equation was previously derived in Ref. [8] using a different method. Equation (41) describes the PDF of T_+ for all times, but cannot be directly inverted. For long times, or $(s\tau)^{\alpha/2} \ll 1$,

$$G_0(p,s) \approx \frac{s^{\alpha-1} + (s+p)^{\alpha-1}}{s^\alpha + (s+p)^\alpha}. \tag{42}$$

This can be inverted to give the equilibrium PDF of $\lambda \equiv T_+/t$, or the occupation fraction [8,38],

$$G(\lambda) = \frac{\sin(\pi\alpha)}{\pi} \frac{\lambda^{\alpha-1}(1-\lambda)^{\alpha-1}}{\lambda^{2\alpha} + (1-\lambda)^{2\alpha} + 2\cos(\pi\alpha)\lambda^\alpha(1-\lambda)^\alpha}. \tag{43}$$

Equation (43) is called Lamperti's PDF [39]. Note that Eqs. (42) and (43) can also be derived directly from the general long-times limit, Eqs. (37) and (38), respectively. Whereas the PDF of the occupation fraction for a free particle is also Lamperti's [8,25], in the free-particle case the exponent is $\alpha/2$, compared to α here. An equation for $G_{x_0}(p,s)$ for $x_0 \neq 0$ can be derived in exactly the same manner, leading, for long times, to Eqs. (42) and (43), as expected.

For $\alpha = 1$, it is easy to see from Eq. (42) that $G(T_+,t) = \delta(T_+ - t/2)$ or $\lambda = 1/2$. This is the expected result based on the ergodicity of normal diffusion. As α decreases below 1, the delta function spreads out to form a W shape. For even smaller

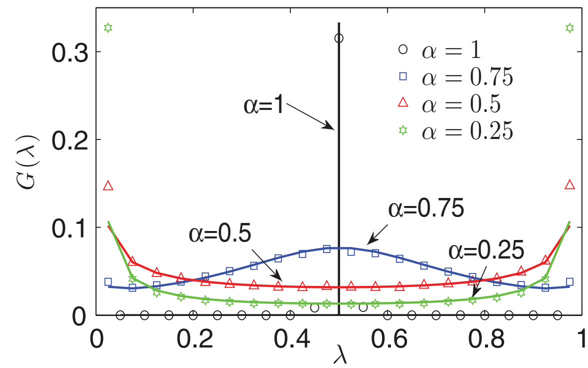

FIG. 1. (Color online) The PDF of the occupation fraction in half-space for a particle in the box [−1,1]. CTRW trajectories were generated as explained in Appendix B, with $x_0 = 0$. For each trajectory, the total time in $x > 0$, T_+, was recorded, and the occupation fraction, $\lambda = T_+/t$, was calculated. The figure shows the long-times PDF of the occupation fraction λ for $\alpha = 1$, 0.75, 0.5, and 0.25 (symbols). Lamperti's PDF, Eq. (43), is plotted as lines (for $\alpha = 1$, the PDF of both simulations and theory was scaled by 3 for visibility). While for $\alpha = 1$, λ is very narrowly distributed around 1/2, for $\alpha < 1$, the PDF becomes wider and even attains a U shape for small enough α.

values of α ($\lesssim 0.59$ [40]), the peak at $\lambda = 1/2$ disappears and the PDF attains a U shape, indicating that the particle spends almost its entire time in one side only. For $\alpha \to 0$, $G(\lambda) = \delta(\lambda)/2 + \delta(\lambda - 1)/2$, as expected. This behavior is demonstrated and compared to simulations in Fig. 1. Details on the simulation method are given in Appendix B.

For short times, $(t/\tau)^{\alpha/2} \ll 1$, we substitute in Eq. (41) the limit $(s\tau)^{\alpha/2} \gg 1$,

$$G_0(p,s) \approx \frac{s^{\alpha/2-1} + (s+p)^{\alpha/2-1}}{s^{\alpha/2} + (s+p)^{\alpha/2}}. \tag{44}$$

In t space, this gives again the Lamperti PDF, but now with index $\alpha/2$. This is exactly the PDF of the occupation fraction of a free particle, which is expected, because for short times the particle does not interact with the boundaries [8]. It can be shown that for short times, $G_{x_0>0}(T_+,t) = \delta(T_+ - t)$, and $G_{x_0<0}(T_+,t) = \delta(T_+)$, as expected.

2. An application of the occupation time functional—The first-passage time PDF

As a side note, we demonstrate how the fractional Feynman-Kac equation for the occupation time can be applied in an elegant manner to the problem of the first-passage time (FPT). The FPT in the box $[-\frac{L}{2},\frac{L}{2}]$ is defined as the time t_f it takes a particle starting at $x_0 = -b$ $(0 < b < L/2)$ to reach $x = 0$ for the first time [41]. A relation between the occupation time functional of the previous subsection and the FPT was proposed by Kac [42]:

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

where as in the previous subsection, $G_{x_0}(p,s)$ is the Laplace transform of the PDF of $T_+ = \int_0^t \Theta[x(\tau)]d\tau$. The last equation is true since $G_{x_0}(p,t) = \int_0^\infty e^{-pT_+}G_{x_0}(T_+,t)dT_+$, and thus, if the particle has never crossed $x = 0$, we have $T_+ = 0$ and $e^{-pT_+} = 1$, while otherwise $T_+ > 0$, and for $p \to \infty$, $e^{-pT_+} = 0$. Substituting $x_0 = -b$ and $p \to \infty$ in Eq. (40) of the previous subsection gives

$$\lim_{p\to\infty} G_{-b}(p,s) = \frac{1}{s}\left\{1 - \frac{\cosh\left[\left(\frac{L}{2} - b\right)\frac{s^{\alpha/2}}{\sqrt{K_\alpha}}\right]}{\cosh\left(\frac{Ls^{\alpha/2}}{2\sqrt{K_\alpha}}\right)}\right\}. \quad (45)$$

The first-passage time PDF satisfies $f(t) = \frac{\partial}{\partial t}[1 - \Pr\{t_f > t\}]$. We therefore have in Laplace space

$$f(s) = \frac{\cosh\left[\left(\frac{L}{2} - b\right)\frac{s^{\alpha/2}}{\sqrt{K_\alpha}}\right]}{\cosh\left(\frac{Ls^{\alpha/2}}{2\sqrt{K_\alpha}}\right)}.$$

For long times, the small-s limit yields

$$f(s) \approx 1 - \frac{b(L-b)}{2K_\alpha}s^\alpha.$$

For $0 < \alpha < 1$, inverting $s \to t$,

$$f(t_f) \approx \frac{b(L-b)}{2K_\alpha|\Gamma(-\alpha)|}t_f^{-(1+\alpha)}. \quad (46)$$

Therefore, $f(t_f) \sim t_f^{-(1+\alpha)}$ [compared to $f(t_f) \sim t_f^{-(1+\alpha/2)}$ for a free particle [25,32]], indicating that for $\alpha < 1$, $\langle t_f\rangle = \infty$. Equations (45) and (46) agree with previous work [8,43].

3. *The fluctuations*

Equation (41), giving $G_0(p,s)$ for the occupation time functional, cannot be directly inverted. It can nevertheless be used to calculate the first few moments using

$$\langle T_+^n\rangle_s = (-1)^n \left.\frac{\partial^n}{\partial p^n}G_0(p,s)\right|_{p=0},$$

where the subscript s indicates the equation is in Laplace space. The first moment (for $x_0 = 0$) is of course $\langle T_+\rangle = t/2$ or $\langle\lambda\rangle = 1/2$. For the second moment,

$$\langle T_+^2\rangle_s = \frac{4-\alpha}{4s^3} - \frac{\alpha(s\tau)^{\alpha/2}}{2s^3\sinh[2(s\tau)^{\alpha/2}]}. \quad (47)$$

For the long times, we take the limit of small s,

$$\langle T_+^2\rangle_s \approx \frac{2-\alpha}{2s^3} + \frac{\alpha\tau^\alpha}{6s^{3-\alpha}}.$$

Inverting and dividing by t^2, we obtain the fluctuations of the occupation fraction, $\langle(\Delta\lambda)^2\rangle_t = \langle\lambda^2\rangle_t - \langle\lambda\rangle_t^2$,

$$\langle(\Delta\lambda)^2\rangle_t \approx \frac{1-\alpha}{4} + \frac{\alpha}{6\Gamma(3-\alpha)}\left(\frac{t}{\tau}\right)^{-\alpha}. \quad (48)$$

For $\alpha < 1$ and $t \to \infty$, we see from Eq. (48) that $\langle(\Delta\lambda)^2\rangle = \frac{1-\alpha}{4} > 0$. For $\alpha = 1$, $\langle(\Delta\lambda)^2\rangle \to 0$ as $t \to \infty$. The convergence to the long-times limit exhibits a $t^{-\alpha}$ decay. For $x_0 \neq 0$, the first moment approaches $1/2$ as $\langle\lambda\rangle_t \approx 1/2 + \frac{x_0(L-|x_0|)}{4K_\alpha\Gamma(2-\alpha)}t^{-\alpha}$ and the fluctuations remain the same as in Eq. (48) up to order $t^{-\alpha}$.

For short times (and $x_0 = 0$), taking the limit $(s\tau)^{\alpha/2} \gg 1$ in Eq. (47) gives $\langle T_+^2\rangle_s \approx \frac{4-\alpha}{4s^3}$, from which

$$\langle(\Delta\lambda)^2\rangle_t \approx \frac{1-\alpha/2}{4}. \quad (49)$$

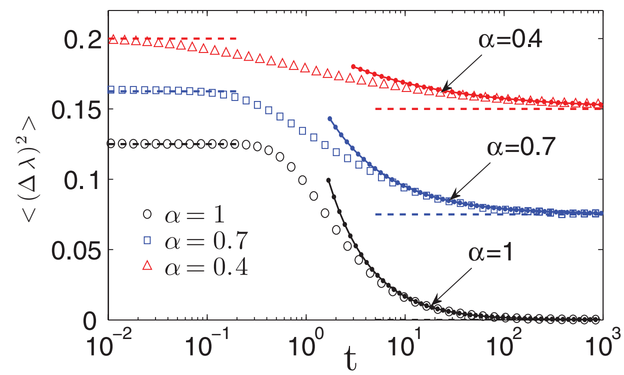

FIG. 2. (Color online) The fluctuations of the occupation fraction in half-box. CTRW trajectories were generated as explained in Appendix B (with $x_0 = 0$), and the occupation fraction in half-box, $\lambda = T_+/t$, was calculated. The figure shows the fluctuations $\langle(\Delta\lambda)^2\rangle$ vs t for $\alpha = 0.4, 0.7$, and 1 (symbols). Theory for long times, Eq. (48), is plotted as dotted lines. The fluctuations are initially equal to their free-particle counterpart, $(1 - \alpha/2)/4$ [Eq. (49), indicated as dashed lines], and then decay to their asymptotic value, $(1 - \alpha)/4$ (also indicated as dashed lines), as $t^{-\alpha}$. Only for $\alpha = 1$ do the fluctuations vanish for $t \to \infty$.

This is the expected result, since for short times the PDF is Lamperti's with index $\alpha/2$ [Eq. (44)].

The fluctuations $\langle(\Delta\lambda)^2\rangle$ are plotted versus t in Fig. 2 and agree well with Eq. (49) for short times and with Eq. (48) for long times. As expected, the approach to the asymptotic limit is slower as α becomes smaller.

B. The time-averaged position in a harmonic potential

We consider the time-averaged position, $\overline{x}(t) = \frac{1}{t}\int_0^t x(\tau)d\tau$, for a subdiffusing particle in a harmonic potential, $V(x) = m\omega^2x^2/2$ (fractional Ornstein-Uhlenbeck process [31,44]).

1. *The distribution*

We first study the PDF in the long-times limit using the general equation (38). Define the second moment in thermal equilibrium as $\langle x^2\rangle_{\rm th} = k_BT/(m\omega^2)$. Measuring $\overline{x}$ in units of $\sqrt{\langle x^2\rangle_{\rm th}}$, we have for $t \to \infty$,

$$G(\overline{x}) = \frac{1}{\sqrt{\langle x^2\rangle_{\rm th}}}g\left(\frac{\overline{x}}{\sqrt{\langle x^2\rangle_{\rm th}}}\right),$$

where

$$g(y) = \frac{\sin(\pi\alpha)}{\pi}\frac{I_{\alpha-1}^<(y)I_\alpha^>(y) + I_{\alpha-1}^>(y)I_\alpha^<(y)}{[I_\alpha^>(y)]^2 + [I_\alpha^<(y)]^2 + 2\cos(\pi\alpha)I_\alpha^>(y)I_\alpha^<(y)}, \quad (50)$$

with

$$I_\alpha^< = \int_y^\infty e^{-\frac{x^2}{2}}(x-y)^\alpha dx, \quad I_\alpha^> = \int_{-\infty}^y e^{-\frac{x^2}{2}}(y-x)^\alpha dx.$$

Using MATHEMATICA, we could express the solution of the integrals in Eq. (50) in terms of Kummer's functions. The full expression is given in Appendix C [Eq. (C1)]. It can be shown that for $\alpha = 1$, $G(\overline{x}) = \delta(\overline{x})$, as expected for an ergodic system [9,10]. For $\alpha < 1$, $G(\overline{x})$ has a nonzero width, and when

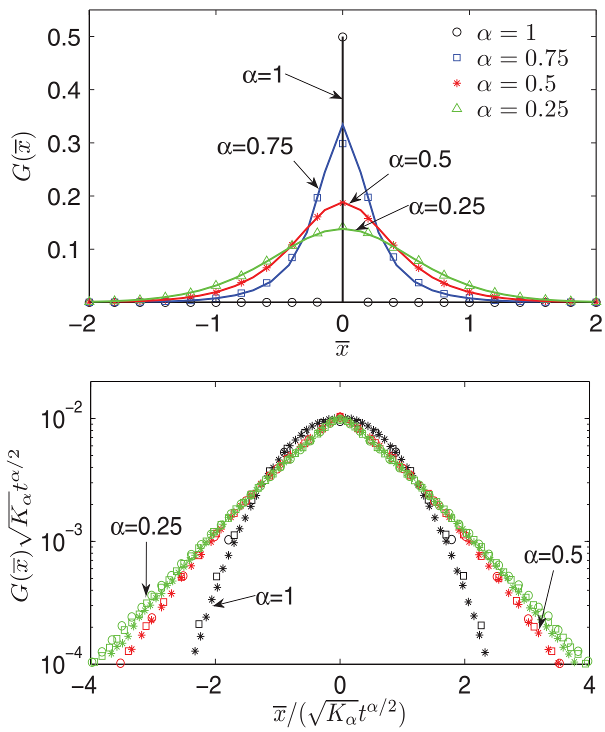

FIG. 3. (Color online) The PDF $G(\overline{x},t)$ for a particle in a binding harmonic field. CTRW trajectories were generated using the method described in Appendix B, with $x_0 = 0$. Top panel: Simulation results for long times for $\alpha = 0.25$, 0.5, 0.75, and 1 (symbols). Theory for $t \to \infty$, Eq. (50), is plotted as solid lines (for $\alpha = 1$, the PDF of both simulations and theory was scaled by 2 for visibility). For $\alpha = 1$, the distribution is a delta function, whereas for $\alpha < 1$, $\overline{x}$ is a random variable even for long times, indicating ergodicity breaking. Bottom panel: Simulation results for the PDF of $\overline{x}$ for a number of short times and for $\alpha = 0.25$, 0.5, and 1 (symbols). The plot illustrates the free-particle scaling form, Eq. (51).

$\alpha \to 0$, $G(\overline{x}) = \sqrt{\frac{m\omega^2}{2\pi k_B T}}\exp[-\frac{m\omega^2\overline{x}^2}{2k_BT}]$, which is the Boltzmann distribution, since for $\alpha \to 0$, $\overline{x} \to x$ [9,10]. For $\overline{x} \ll \sqrt{\langle x^2\rangle_{\rm th}}$ ($y \ll 1$), $g(y)$ has a Taylor expansion around $y = 0$ of the form $g(y) = \frac{\Gamma(\frac{\alpha}{2})\tan(\frac{\pi\alpha}{2})}{\sqrt{2\pi}\Gamma(\frac{1+\alpha}{2})} + O(y^2)$. For $\overline{x} \gg \sqrt{\langle x^2\rangle_{\rm th}}$ ($y \gg 1$), $g(y) \sim \frac{\Gamma(\alpha)\sin(\pi\alpha)}{\sqrt{2\pi^3}}y^{-2\alpha}e^{-y^2/2}$, which gives the expected results for $\alpha \to 0$ and $\alpha = 1$. Equation (50) is plotted and compared to simulations in the top panel of Fig. 3.

For *short* times, $t^\alpha \ll \langle x^2\rangle_{\rm th}/K_\alpha$, and for $x_0 = 0$, the particle is at the minimum of the potential and therefore behaves as a free particle. For the free-particle case, we have previously shown the scaling form [25]

$$G(\overline{x},t) = \frac{1}{\sqrt{K_\alpha}t^{\alpha/2}} h\left(\frac{\overline{x}}{\sqrt{K_\alpha}t^{\alpha/2}}\right), \tag{51}$$

where $h(y)$ is a dimensionless scaling function. This behavior is numerically demonstrated in the bottom panel of Fig. 3.

2. *The fluctuations*

The PDF of the time-averaged position was shown in the previous subsection to have a nontrivial limiting form for $t \to \infty$ [Eq. (50)] and $t \to 0$ [Eq. (51)]. However, the shape of the PDF for other times is unknown. In this subsection, we show that using the fractional Feynman-Kac equation, we can determine the width of the distribution for all times.

Let us write the forward equation in (p,s) space for the functional $A = \overline{x}t = \int_0^t x(\tau)d\tau$ and for $x_0 = 0$. Since A is not necessarily positive, p here is the Fourier pair of A and we use Eq. (28) of Sec. II A 3:

$$sG(x,p,s) - \delta(x) = ipxG(x,p,s) + K_\alpha\left[\frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial x}\frac{m\omega^2 x}{k_BT}\right][s - ipx]^{1-\alpha}G(x,p,s). \tag{52}$$

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

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

Operating on both sides of Eq. (52) with $-\frac{\partial^2}{\partial p^2}$, substituting $p = 0$, and integrating over all x, we obtain, in s space,

$$s\langle A^2\rangle_s = 2\,\langle Ax\rangle_s\,, \tag{53}$$

where we used the fact that the integral over the Fokker-Planck operator vanishes. Equation (53) can be intuitively understood by noting that $\frac{\partial}{\partial t}\langle A^2\rangle = 2\langle A\dot{A}\rangle$ and that $\dot{A} = x$. We next use Eq. (52) and

$$\langle Ax\rangle_s = -i\int_{-\infty}^{\infty} x\,\frac{\partial}{\partial p}G(x,p,s)\bigg|_{p=0}dx$$

to obtain

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

where we defined the relaxation time $\tau^\alpha = k_BT/(K_\alpha m\omega^2) = \langle x^2\rangle_{\rm th}/K_\alpha$. Thus,

$$s\,\langle A_x x\rangle_s = \frac{(1-\alpha) + (s\tau)^\alpha}{1 + (s\tau)^\alpha}\langle x^2\rangle_s. \tag{54}$$

Finally, to find $\langle x^2\rangle_s$, we use $\langle x^2\rangle_s = \int_{-\infty}^{\infty} x^2 G(x,p=0,s)dx$,

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

where we used the normalization condition $\int G(x,p = 0,s)dx = 1/s$. Thus,

$$s\langle x^2\rangle_s = \frac{2\langle x^2\rangle_{\rm th}}{2 + (s\tau)^\alpha}. \tag{55}$$

Combining Eqs. (53), (54), and (55), we find

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

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

$$\langle A^2\rangle_s = \frac{2\langle x^2\rangle_{\rm th}}{s^3}\left[(1-\alpha) + 2\alpha\frac{(s\tau)^\alpha}{1+(s\tau)^\alpha} - (1+\alpha)\frac{(s\tau)^\alpha}{2+(s\tau)^\alpha}\right]. \tag{56}$$

Inverting the last equation, we find

$$\langle A^2\rangle_t = \langle x^2\rangle_{\rm th}t^2 \times\{(1-\alpha) + 4\alpha E_{\alpha,3}[-(t/\tau)^\alpha] - 2(1+\alpha)E_{\alpha,3}[-2(t/\tau)^\alpha]\}, \tag{57}$$

where we used the Laplace transform relation [45]

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

and $E_{\alpha,3}(z)$ is the Mittag-Leffler function, defined as [45]

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

To obtain the fluctuations of the time-averaged position, $\langle(\Delta\overline{x})^2\rangle_t = \langle\overline{x}^2\rangle_t - \langle\overline{x}\rangle_t^2$, we use $\langle\overline{x}^2\rangle_t = \langle A^2\rangle/t^2$ and $\langle\overline{x}\rangle_t = 0$ (since $x_0 = 0$). This gives

$$\langle(\Delta\overline{x})^2\rangle_t = \langle x^2\rangle_{\rm th} \times \{(1-\alpha) + 4\alpha E_{\alpha,3}[-(t/\tau)^\alpha] - 2(1+\alpha)E_{\alpha,3}[-2(t/\tau)^\alpha]\}. \tag{58}$$

Equation (58) is compared to simulations in the top panel of Fig. 4.

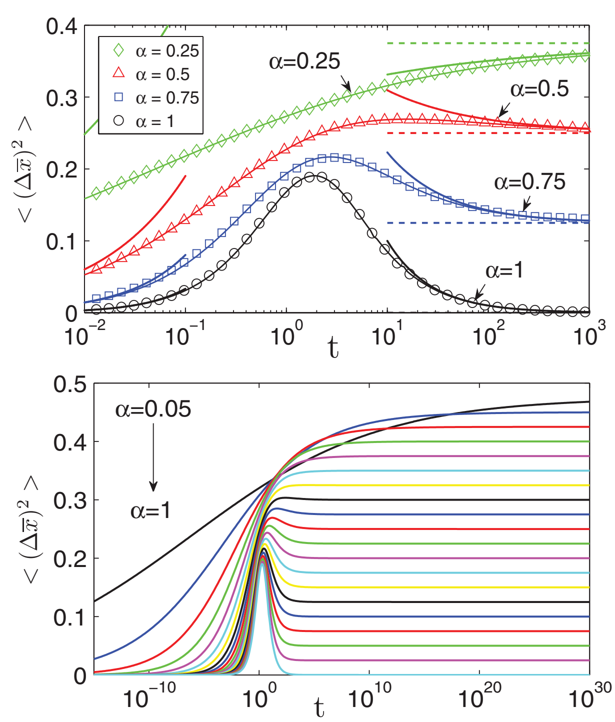

FIG. 4. (Color online) The fluctuations $\langle(\Delta\overline{x})^2\rangle_t$ for a particle in a harmonic potential. Top panel: CTRW trajectories were generated using the method described in Appendix B, with $x_0 = 0$. Symbols represent simulation results for $\alpha = 0.25$, 0.5, 0.75, and 1. Theory, Eq. (58), is plotted as solid lines (with the Mittag-Leffler functions computed using the program of Ref. [46]). The straight dashed lines are $\lim_{t\to\infty}\langle(\Delta\overline{x})^2\rangle_t = (1-\alpha)\langle x^2\rangle_{\rm th}$. Except for $\alpha = 1$, the fluctuations do not vanish when $t \to \infty$ and thus ergodicity is broken. The dotted lines represent the long-times and short-times approximations, Eqs. (59) and (60), respectively. Bottom panel: The fluctuations, Eq. (58), plotted for a wide time range $[10^{-15}, 10^{30}]$. Shown are 20 curves for $\alpha = 0.05, 0.1, 0.15, \ldots, 1$ (top to bottom). The fluctuations display a maximum when $\alpha > 1/3$ and a crossover when $\alpha \lesssim 0.15$. As expected, the fluctuations approach their asymptotic value slower for smaller values of α.

To find the long-times behavior of the fluctuations (58), we expand Eq. (56) for small s, invert, and divide by t^2,

$$\langle(\Delta\overline{x})^2\rangle_t \approx (1-\alpha)\langle x^2\rangle_{\rm th} + \frac{(3\alpha-1)\langle x^2\rangle_{\rm th}}{\Gamma(3-\alpha)} \left(\frac{t}{\tau}\right)^{-\alpha}. \tag{59}$$

Thus, for $\alpha < 1$ and $t \to \infty$, $\langle(\Delta\overline{x})^2\rangle = (1-\alpha)\langle x^2\rangle_{\rm th} > 0$ and ergodicity is broken. Only when $\alpha = 1$ do we have ergodic behavior $\langle(\Delta\overline{x})^2\rangle = 0$. As we observed for the occupation fraction [Eq. (48)], Eq. (59) also exhibits a $t^{-\alpha}$ convergence of the fluctuations to their asymptotic limit.

For short times,

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

Therefore,

$$\langle(\Delta\overline{x})^2\rangle_t \approx \frac{4\langle x^2\rangle_{\rm th}}{\Gamma(3+\alpha)} \left(\frac{t}{\tau}\right)^{\alpha}. \tag{60}$$

Noting that $\langle x^2\rangle_{\rm th}/\tau^\alpha = K_\alpha$, we can rewrite Eq. (60) as $\langle(\Delta\overline{x})^2\rangle_t \approx \frac{4K_\alpha}{\Gamma(3+\alpha)} t^\alpha$, which is, as expected, equal to the free-particle expression [25].

The bottom panel of Fig. 4 presents the fluctuations of the time average (for $x_0 = 0$) for a wide range of times and for $\alpha = 0.05, 0.1, 0.15, \ldots, 1$. As expected from Eqs. (59) and (60), the fluctuations increase from $\langle(\Delta\overline{x})^2\rangle = 0$ at $t \to 0$ to their asymptotic value at $t \to \infty$, $(1-\alpha)\langle x^2\rangle_{\rm th}$. However, as can be seen also in Eq. (59), for $\alpha > 1/3$ the fluctuations display a maximum and decay to their asymptotic limit from above. We found numerically that the value of the maximal fluctuations scales roughly as $\alpha^{-1/2}$ (not shown). It can also be seen that for almost all times and all values of α, the fluctuations $\langle(\Delta\overline{x})^2\rangle$ decrease as the diffusion becomes more "normal" (increasing α), as expected. However, this pattern surprisingly breaks down for $\alpha \lesssim 0.15$, for which there is a time window when the fluctuations increase with α.

It is straightforward to generalize our results to any initial condition with first moment $\langle x_0\rangle$ and second moment $\langle x_0^2\rangle$. The first moment of the time average is $\langle\overline{x}\rangle_t = \langle x_0\rangle E_{\alpha,2}[-(t/\tau)^\alpha]$, which decays for long times as $\langle\overline{x}\rangle_t \approx \frac{\langle x_0\rangle}{\Gamma(2-\alpha)}(\frac{t}{\tau})^{-\alpha}$. The second moment is

$$\langle\overline{x}^2\rangle_t = (1-\alpha)\langle x^2\rangle_{\rm th} + 2\alpha\left[2\langle x^2\rangle_{\rm th} - \langle x_0^2\rangle\right] E_{\alpha,3}\left[-(t/\tau)^\alpha\right] + 2(1+\alpha)\left[\langle x_0^2\rangle - \langle x^2\rangle_{\rm th}\right] E_{\alpha,3}\left[-2(t/\tau)^\alpha\right], \tag{61}$$

from which the fluctuations directly follow. For long times,

$$\langle(\Delta\overline{x})^2\rangle_t \approx (1-\alpha)\langle x^2\rangle_{\rm th} + \frac{(3\alpha-1)\langle x^2\rangle_{\rm th} + (1-\alpha)\langle x_0^2\rangle}{\Gamma(3-\alpha)} \left(\frac{t}{\tau}\right)^{-\alpha}.$$

For short times,

$$\langle(\Delta\overline{x})^2\rangle_t \approx \langle(\Delta x_0)^2\rangle - 2\left[\frac{\langle(\Delta x_0)^2\rangle}{\Gamma(2+\alpha)} - \frac{2\langle x^2\rangle_{\rm th}}{\Gamma(3+\alpha)}\right]\left(\frac{t}{\tau}\right)^{\alpha},$$

where $\langle(\Delta x_0)^2\rangle = \langle x_0^2\rangle - \langle x_0\rangle^2$. According to the last two equations, if the system is already in equilibrium at $t = 0$ such that $\langle x_0^2\rangle = \langle x^2\rangle_{\rm th}$, the fluctuations decay monotonically, for all α, from $\langle x^2\rangle_{\rm th}$ at $t = 0$ to $(1-\alpha)\langle x^2\rangle_{\rm th}$ at $t \to \infty$.

For $\alpha = 1$ (and $x_0 = 0$), we find the known result [47]:

$$\langle(\Delta\overline{x})^2\rangle_t = \langle x^2\rangle_{\rm th}\left(\frac{t}{\tau}\right)^{-2}\left(4e^{-t/\tau} - e^{-2t/\tau} + \frac{2t}{\tau} - 3\right) \quad (62)$$

To derive the preceding equation, we used Eq. (58) and the relation $E_{1,3}(z) = [e^z - z - 1]/z^2$. Since the ordinary ($\alpha = 1$) Ornstein-Uhlenbeck process is a Gaussian process [48], the PDF of $\overline{x}$ is a Gaussian too, with the variance indicated by Eq. (62).

3. Fractional Kramers equation

Finally, we remark on the connection between the fractional Feynman-Kac equation of this section and an important class of processes in which the *velocity* of the particle is the quantity undergoing subdiffusion. For example, consider a Rayleigh-like model in which a free, heavy test particle of mass M collides with light bath particles at random times, but where the times between collisions are distributed according to $\psi(\tau) \sim \tau^{-(1+\alpha)}$. The PDF of the velocity of the test particle, $G(v,t)$, satisfies the fractional Fokker-Planck equation [44]:

$$\frac{\partial}{\partial t}G(v,t) = \gamma_\alpha\left[\frac{k_B T}{M}\frac{\partial^2}{\partial v^2} + \frac{\partial}{\partial v}v\right]\mathcal{D}_{{\rm RL},t}^{1-\alpha}G(v,t),$$

where $\mathcal{D}_{{\rm RL},t}^{1-\alpha}$ is the Riemann-Liouville fractional derivative operator (see Sec. II A 3) and γ_α is the damping coefficient. Since in the collisions model $x(t) = \int_0^t v(\tau)d\tau$, x is a functional of $v(\tau)$, and therefore the joint PDF of v and x, $G(v,x,t)$, is described by our fractional Feynman-Kac equation. Denoting the Fourier transform $x \to p$ of $G(v,x,t)$ as $G(v,p,t)$, we have [see Eq. (28)]

$$\frac{\partial}{\partial t}G(v,p,t) = ipvG(v,p,t) + \gamma_\alpha\left[\frac{k_B T}{M}\frac{\partial^2}{\partial v^2} + \frac{\partial}{\partial v}v\right]\mathcal{D}_t^{1-\alpha}G(v,p,t), \quad (63)$$

where $\mathcal{D}_t^{1-\alpha}$ is the fractional substantial derivative, which here is equal in Laplace s space to $(s - ipv)^{1-\alpha}$. Within this model, for $0 < \alpha < 1$ the motion is ballistic, $\langle x^2\rangle \sim t^2$, while for $\alpha = 1$ it is diffusive, $\langle x^2\rangle \sim t$ [see Eq. (59)]. Equation (63) is exactly equal to the fractional Kramers equation derived by Friedrich and co-workers [26,27], and in that sense, our results generalize their pioneering work.

V. SUMMARY AND DISCUSSION

Time averages of subdiffusive continuous-time random walks (CTRW's) in binding fields are known to exhibit weak ergodicity breaking and were thus a subject of recent interest. In this paper, we developed a general equation for time averages of CTRW [Eq. (22)], which can be seen as a fractional generalization of the Feynman-Kac equation, and is good for all observables, potentials, and times. We also derived a backward equation (31), which is useful in practical problems.

We investigated two applications of our equations: the occupation fraction in the positive half of a box, and the time-averaged position in a harmonic potential. In both cases, we obtained expressions for the PDF for long times and short times and calculated the fluctuations. We found that the fluctuations decay as $t^{-\alpha}$ to their asymptotic limit, which is nonzero for anomalous diffusion, $\alpha < 1$. Our fractional Feynman-Kac equation thus provides a general tool for the study of the kinetics of weak ergodicity breaking.

Recently, the occupation time functional has been studied in the context of dynamical systems with an infinite (non-normalizable) invariant measure [49]. It remains to be seen whether a framework similar to that of the fractional Feynman-Kac equation could be developed for general functionals of these processes. We also note that while a derivation of the (integer) Feynman-Kac equation using path integrals is long known [22], a path integral approach to the fractional Feynman-Kac equation is only now emerging [50].

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APPENDIX A: TIME-DEPENDENT FORCE

In our model of CTRW with a time-dependent force, the jump probabilities are determined according to the force at the time of the jump. To derive an equation for $G(x,A,t)$ in that case, we rewrite Eq. (7) as follows:

$$\begin{aligned}\chi(x,A,t) &= G_0(x)\delta(A)\delta(t)\\ &+ \int_0^t \psi(\tau)L(x+a,t)\chi\,[x+a,A-\tau U(x+a),t-\tau]d\tau\\ &+ \int_0^t \psi(\tau)R(x-a,t)\chi\,[x-a,A-\tau U(x-a),t-\tau]d\tau.\end{aligned} \quad (A1)$$

Note that the jump probabilities are time-dependent (but have no memory). Laplace transforming $A \to p$ and $t \to s$, using the Laplace identity $\mathcal{L}\{tf(t)\} = -\frac{\partial}{\partial s}f(s)$,

$$\begin{aligned}\chi(x,p,s) &= G_0(x)\\ &+ L\left(x+a,-\frac{\partial}{\partial s}\right)\hat{\psi}\,[s+pU(x+a)]\chi(x+a,p,s)\\ &+ R\left(x-a,-\frac{\partial}{\partial s}\right)\hat{\psi}\,[s+pU(x-a)]\chi(x-a,p,s).\end{aligned}$$

Fourier transforming $x \to k$,

$$\chi(k,p,s) = \hat{G}_0(k) + \left[\cos(ka) + i\sin(ka)\frac{aF\left(-i\frac{\partial}{\partial k},-\frac{\partial}{\partial s}\right)}{2k_BT}\right] \times \hat{\psi}\left[s + pU\left(-i\frac{\partial}{\partial k}\right)\right]\chi(k,p,s).$$

Continuing as in Sec. II A 2, we find the formal solutions for $\chi(k,p,s)$ and $G(k,p,s)$ and then take the continuum limit. This gives

$$sG(k,p,s) - \hat{G}_0(k) = -pU\left(-i\frac{\partial}{\partial k}\right)G(k,p,s) - K_\alpha\left[k^2 - ik\frac{F\left(-i\frac{\partial}{\partial k}, -\frac{\partial}{\partial s}\right)}{k_B T}\right]\left[s + pU\left(-i\frac{\partial}{\partial k}\right)\right]^{1-\alpha} G(k,p,s).$$

Inverting $k \to x, s \to t$, we obtain the fractional Feynman-Kac equation for a time-dependent force:

$$\frac{\partial}{\partial t}G(x,p,t) = K_\alpha \mathcal{L}_{\mathrm{FP}}^{(\mathrm{t})}\mathcal{D}_t^{1-\alpha}G(x,p,t) - pU(x)G(x,p,t), \tag{A2}$$

where

$$\mathcal{L}_{\mathrm{FP}}^{(\mathrm{t})} = \frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x}\frac{F(x,t)}{k_B T}$$

is the time-dependent Fokker-Planck operator.

APPENDIX B: THE SIMULATION METHOD

The fractional Feynman-Kac equation describes the joint PDF of x and A in the continuum limit of CTRW. In this limit, $a \to 0$ and $B_\alpha \to 0$, but the generalized diffusion coefficient $K_\alpha = a^2/(2B_\alpha)$ [Eq. (21)] is kept finite [28]. We simulate trajectories of this process as follows [51]. We place a particle on a one-dimensional lattice in initial position x_0, where usually $x_0 = 0$. 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 uniformly distributed in [0,1]. For $\alpha < 1$, we set $\tau_0 = [B_\alpha/\Gamma(1-\alpha)]^{1/\alpha}$ and $\tau = \tau_0 u^{-1/\alpha}$, which corresponds to $\psi(\tau) = \frac{B_\alpha}{|\Gamma(-\alpha)|}\tau^{-(1+\alpha)}$ with $\tau \geqslant \tau_0$ [Eq. (5)]. After waiting time τ, we move the particle right or left with probabilities $R(x)$ or $L(x)$, respectively, as given by Eq. (14). For the harmonic potential, Eq. (14) gives $R(x) = [1 - ax/(2\langle x^2\rangle_{\mathrm{th}})]/2$ and $L(x) = [1 + ax/(2\langle x^2\rangle_{\mathrm{th}})]/2$. Since the typical x is of the order of $\sqrt{\langle x^2\rangle_{\mathrm{th}}}$, it is sufficient to choose $a \ll \sqrt{\langle x^2\rangle_{\mathrm{th}}}$ to guarantee that $0 < R(x), L(x) < 1$ (see discussion in Ref. [43]). For the box, $R(x) = L(x) = 1/2$ and we make the boundaries at $x = \pm\frac{L}{2}$ reflecting.

The parameters we used in the simulations were as follows. In all simulations, we used $a = 0.1$ or smaller, and each curve represents at least 10^4 trajectories. For the occupation time in a box, we set $L = 2$ and $K_\alpha = 1$, and the final simulation time in Fig. 1 was $t = 10^3$. For the time-averaged position in the harmonic potential, we set $K_\alpha = 1/2$ and $\langle x^2\rangle_{\mathrm{th}} = 1/2$ (or $\tau^\alpha = 1$). In Fig. 3, the final simulation times were as follows. For the long-times limit (top panel), we used $t = 10^7$, 10^4, 10^3, and 10^3 for $\alpha = 0.25$, 0.5, 0.75, and 1, respectively. For the short times (bottom panel), we used $t = 10^{-3}$, 10^{-2}, and 10^{-1} for $\alpha = 1$; $t = 10^{-5}$, 10^{-4}, and 10^{-3} for $\alpha = 0.5$; and $t = 10^{-6}$, 10^{-5}, and 10^{-4} for $\alpha = 0.25$.

APPENDIX C: THE $t \to \infty$ DISTRIBUTION OF THE TIME-AVERAGED POSITION IN A HARMONIC POTENTIAL

Consider the time-averaged position, $\overline{x} = \frac{1}{t}\int_0^t x(\tau)d\tau$, for a subdiffusing particle in a harmonic potential, $V(x) = m\omega^2 x^2/2$. Using the thermal second moment, $\langle x^2\rangle_{\mathrm{th}} = k_B T/(m\omega^2)$, and for $t \to \infty$, we have

$$G(\overline{x}) = \frac{1}{\sqrt{\langle x^2\rangle_{\mathrm{th}}}}\, g\left(\frac{\overline{x}}{\sqrt{\langle x^2\rangle_{\mathrm{th}}}}\right),$$

where

$$\begin{aligned} g(y) = \frac{\sin(\pi\alpha)}{\pi}&\left\{e^{y^2/2}y\Gamma\left(\frac{\alpha}{2}\right)\Gamma(1+\alpha)\left[\mathrm{M}\left(\frac{1-\alpha}{2},\frac{1}{2},-\frac{y^2}{2}\right)\mathrm{U}\left(1+\frac{\alpha}{2},\frac{3}{2},\frac{y^2}{2}\right) + 2\mathrm{M}\left(\frac{1-\alpha}{2},\frac{3}{2},-\frac{y^2}{2}\right)\mathrm{U}\left(\frac{\alpha}{2},\frac{1}{2},\frac{y^2}{2}\right)\right]\right.\\ &\left.+\sqrt{2}\Gamma(\alpha)\Gamma\left(\frac{1+\alpha}{2}\right)\left[y^2\alpha\mathrm{M}\left(\frac{1+\alpha}{2},\frac{3}{2},\frac{y^2}{2}\right)\mathrm{U}\left(1+\frac{\alpha}{2},\frac{3}{2},\frac{y^2}{2}\right) + 2\mathrm{M}\left(\frac{1+\alpha}{2},\frac{1}{2},\frac{y^2}{2}\right)\mathrm{U}\left(\frac{\alpha}{2},\frac{1}{2},\frac{y^2}{2}\right)\right]\right\}\\ &\times\left\{2^{2+\alpha}y^2\Gamma^2\left(1+\frac{\alpha}{2}\right)\left[e^{y^2}\mathrm{M}^2\left(\frac{1-\alpha}{2},\frac{3}{2},-\frac{y^2}{2}\right) - 2\cos(\pi\alpha)\mathrm{M}^2\left(1+\frac{\alpha}{2},\frac{3}{2},\frac{y^2}{2}\right)\right]\right.\\ &+4\sqrt{2}e^{y^2}\sqrt{\pi}y\Gamma(1+\alpha)\mathrm{M}\left(\frac{1-\alpha}{2},\frac{3}{2},-\frac{y^2}{2}\right)\mathrm{M}\left(-\frac{\alpha}{2},\frac{1}{2},-\frac{y^2}{2}\right)\\ &+2^{1+\alpha}\Gamma^2\left(\frac{1+\alpha}{2}\right)\left[e^{y^2}\mathrm{M}^2\left(-\frac{\alpha}{2},\frac{1}{2},-\frac{y^2}{2}\right) + 2\cos(\pi\alpha)\mathrm{M}^2\left(\frac{1+\alpha}{2},\frac{1}{2},\frac{y^2}{2}\right)\right]\\ &\left.+2^{-\alpha}y^2\Gamma^2(1+\alpha)\mathrm{U}^2\left(1+\frac{\alpha}{2},\frac{3}{2},\frac{y^2}{2}\right)\right\}^{-1}. \end{aligned} \tag{C1}$$

In the last equation, $\mathrm{M}(a,b,z)$ is the confluent hypergeometric (or Kummer's) function of the first kind and $\mathrm{U}(a,b,z)$ is the confluent hypergeometric (or Kummer's) function of the second kind [52]. Equation (C1) is valid for $y > 0$. Due to the symmetry of the potential, $g(-y) = g(y)$.

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