

Anomalous diffusion and the first passage time problem

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We study the distribution of the first passage time (FPT) in Levy type anomalous diffusion. Using the recently formulated fractional Fokker-Planck equation we obtain three results. (1) We derive an explicit expression for the FPT distribution in terms of Fox or H functions when the diffusion has zero drift. (2) For the nonzero drift case we obtain an analytical expression for the Laplace transform of the FPT distribution. (3) We express the FPT distribution in terms of a power series for the case of two absorbing barriers. The known results for ordinary diffusion (Brownian motion) are obtained as special cases of our more general results.

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I. INTRODUCTION

For a stochastic process, the first passage time (FPT) is defined as the time T when the process, starting from a given point, reaches a predetermined level for the first time, and is a random variable [1–4]. In this paper, we consider the distribution of the FPT in the context of anomalous diffusion. By anomalous diffusion we mean a process where the mean square displacement of the diffusive variable $X(t)$ scales with time as $\langle X^2(t) \rangle \sim t^\gamma$ with $0 < \gamma < 2$. If $\gamma = 1$, we obtain ordinary diffusion. There are different mechanisms for generating anomalous diffusion. Our focus will be on the continuous time random walk (CTRW) [5,6], where the waiting time is a Levy type variable obeying certain power law distribution. We subsequently refer to the process as Levy type anomalous diffusion. Recent work shows that in the generalized diffusive limit the probability density function of the CTRW is described by a fractional Fokker-Planck equation (FFPE) [7,8]. Using this equation, together with appropriate initial and boundary value condition, we derive an exact solution for the FPT density function in terms of Fox or H functions [9,10], when the anomalous diffusion has zero drift. For the nonzero drift case we derive an expression for the Laplace transform of the FPT density function. This Laplace transform is then used to obtain the mean and variance of the FPT. Finally, we derive an explicit expression for the FPT density function for Levy type anomalous diffusion with absorbing barriers at finite distances from the origin.

II. LEVY TYPE ANOMALOUS DIFFUSION

For an ordinary diffusive process, the mean square displacement scales with t as $\langle X^2(t) \rangle \sim t$ in the large t limit. If $\langle X^2(t) \rangle \sim t^\gamma$, we have anomalous diffusion, with $0 < \gamma < 1$ and $1 < \gamma < 2$ corresponding to subdiffusive and superdiffu-

sive cases, respectively. Anomalous diffusion with drift $X_\mu(t)$ is defined by

$$X_\mu(t) = \mu t + X(t). \quad (2.1)$$

For further discussions and examples of anomalous diffusions in physical, chemical, and biological systems, see Refs. [5,6]. For completeness we give in what follows a brief introduction to CTRW and the limiting process leading to the establishment of the FFPE.

A. Details of the process

We start with a one-dimensional continuous time random walk described by the following Langevin equation:

$$\frac{dX}{dt} = \sum_{i=1}^{\infty} Y_i \delta(t - t_i). \quad (2.2)$$

Here the random walker starts at $x=0$ at time $t_0=0$. Subsequently, the random walker waits at a given location x_i for time $t_i - t_{i-1}$ before taking a jump Y_i which could depend on the waiting time. The waiting time $u > 0$ and the jump size y ($-\infty < y < \infty$) are drawn from the joint probability density function $\phi(y, u)$. The waiting time distribution $\psi(u)$ is given by

$$\psi(u) = \int_{-\infty}^{\infty} dy \phi(y, u). \quad (2.3)$$

The process is non-Markovian if $\psi(u)$ is a nonexponential distribution, since the probability for the next jump to occur depends on how long the random walker has been waiting since the previous jump. But the CTRW is non-Markovian in a special way, since it does not depend on the history of the process prior to the previous jump.

It can be shown [5] that the probability distribution $W(x, t)$ for the CTRW is related to $\phi(y, u)$ and $\psi(u)$. This relation is simpler to write down in the Fourier-Laplace transform space. Denoting the Fourier-Laplace transform of $W(x, t)$ and $\phi(y, u)$ by $\tilde{W}(k, s)$ and $\tilde{\phi}(k, s)$, respectively

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(where k is the Fourier transform of the space variable, and s the Laplace transform of the time variable), we have [5]

$$\tilde{W}(k,s) = \frac{1}{s} \frac{1 - \tilde{\psi}(s)}{1 - \tilde{\phi}(k,s)}. \quad (2.4)$$

Here $\tilde{\psi}(s)$ is the Laplace transform of $\psi(u)$.

It can be further shown, depending on the specific form of $\phi(y,u)$, that the CTRW can produce both subdiffusive ($0 < \gamma < 1$) and superdiffusive processes ($1 < \gamma < 2$) as well as ordinary diffusion ($\gamma = 1$) [5,11]. For example, consider

$$\phi(y,u) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp[-y^2/2\sigma^2] \frac{(\alpha-1)/\tau}{(1+u/\tau)^\alpha}, \quad (2.5)$$

where y and u are decoupled with y being a Gaussian variable with zero mean. For $1 < \alpha < 2$, the corresponding CTRW is characterized by a subdiffusive process with $\gamma = \alpha - 1$, and for $\alpha \geq 2$, one obtains ordinary diffusion with $\gamma = 1$. This is demonstrated as follows.

The waiting time distribution $\psi(u)$ is given by [cf. Eqs. (2.5) and (2.3)]

$$\psi(u) = \frac{(\alpha-1)/\tau}{(1+u/\tau)^\alpha}. \quad (2.6)$$

Even though this is not a Levy stable distribution, it belongs to the domain of attraction [12] of a one-sided stable Levy law. It has an infinite mean for $1 < \alpha < 2$, the range we are interested in (it has a finite mean for $\alpha > 2$). We call u a ‘‘Levy type variable’’ for want of a better name. The Laplace transform $\tilde{\psi}(s)$ of $\psi(u)$ is [13]

$$\tilde{\psi}(s) = (\alpha-1)(\tau s)^{\alpha-1} \Gamma(1-\alpha, \tau s) e^{\tau s}. \quad (2.7)$$

The Fourier-Laplace transform $\tilde{\phi}(k,s)$ of $\phi(y,u)$ in Eq. (2.5) is given by [13]

$$\tilde{\phi}(k,s) = \exp(-\sigma^2 k^2/2) \tilde{\psi}(s). \quad (2.8)$$

To show that the CTRW characterized by Eq. (2.5) exhibits anomalous diffusion, we need to demonstrate that $\langle X^2(t) \rangle \sim t^\gamma$ for large t ($0 < \gamma < 1$). By the Tauberian theorem [14], this is equivalent to $\langle X^2(s) \rangle \sim 1/s^{1+\gamma}$ for small s ($0 < \gamma < 1$). But we have the result

$$\langle X^2(s) \rangle = - \left. \frac{\partial^2}{\partial k^2} \tilde{W}(k,s) \right|_{k=0}. \quad (2.9)$$

Thus we need the expression for $W(k,s)$ in the limit $s \rightarrow 0$. Since $W(k,s)$ is a function of $\tilde{\psi}(s)$ and $\tilde{\phi}(k,s)$ [cf. Eq. (2.4)], we first consider $\tilde{\psi}(s)$. We have [15]

$$\Gamma(1-\alpha, \tau s) = \Gamma(1-\alpha) - \sum_{n=0}^{\infty} \frac{(-1)^n (\tau s)^{1-\alpha+n}}{n!(1-\alpha+n)}. \quad (2.10)$$

As $s \rightarrow 0$,

$$\Gamma(1-\alpha, \tau s) \approx - \frac{\Gamma(2-\alpha)}{\alpha-1} + \frac{(\tau s)^{1-\alpha}}{\alpha-1} + \frac{(\tau s)^{2-\alpha}}{2-\alpha}. \quad (2.11)$$

Therefore $\tilde{\psi}(s)$, as $s \rightarrow 0$, is given by

$$\tilde{\psi}(s) \approx 1 - \Gamma(2-\alpha)(\tau s)^{\alpha-1}, \quad 1 < \alpha < 2, \quad (2.12)$$

$$\approx 1 - (2\alpha-3)\tau s/(\alpha-2), \quad \alpha > 2. \quad (2.13)$$

Substituting this into Eq. (2.4) we have [cf. Eq. (2.8)]

$$\tilde{W}(k,s) \approx \frac{1}{s} \frac{\Gamma(2-\alpha)(\tau s)^{\alpha-1}}{1 - [1 - \Gamma(2-\alpha)(\tau s)^{\alpha-1}] \exp(-\sigma^2 k^2/2)}, \quad (2.14)$$

$$\approx \frac{1}{s} \frac{\alpha \tau s / (\alpha-2)}{1 - [1 - \alpha \tau s / (\alpha-2)] \exp(-\sigma^2 k^2/2)}, \quad (2.15)$$

Using this in Eq. (2.9) and evaluating the second derivative at $k=0$, in the limit $s \rightarrow 0$ we obtain

$$\langle X^2(s) \rangle \sim \frac{\sigma^2}{\Gamma(2-\alpha)\tau^{\alpha-1}} \frac{1}{s^\alpha}, \quad 1 < \alpha < 2, \quad (2.16)$$

$$\sim \frac{(\alpha-2)\sigma^2}{\alpha\tau} \frac{1}{s^2}, \quad \alpha > 2. \quad (2.17)$$

Thus we have shown that the CTRW characterized by Eq. (2.5) is a subdiffusive process for $1 < \alpha < 2$ with $\gamma = \alpha - 1$, and, for $\alpha > 2$, one obtains ordinary diffusion with $\gamma = 1$. For $\alpha = 2$, by taking proper limits, one can show that we again obtain ordinary diffusion.

We verify the above result numerically by simulating the CTRW process. For the sake of numerical efficiency, we replace the waiting time distribution $\psi(u)$ in Eq. (2.6) by the Pareto distribution [16]

$$\psi(u) = 0, \quad u < \tau, \quad (2.18)$$

$$= \frac{(\alpha-1)\tau^{\alpha-1}}{u^\alpha}, \quad u \geq \tau. \quad (2.19)$$

This approximation is well justified for small values of τ . A numerically obtained mean square displacement is compared with the theoretical prediction in Fig. 1 for $\alpha = 1.5$ (i.e., $\gamma = 0.5$), $a = 1.0$, $\tau = 10^{-4}$, and $\sigma^2 = 3.5 \times 10^{-3}$. We note that the numerical simulation is in excellent agreement with the theoretical prediction.

If, on the other hand, $\phi(y,u)$ is given by the coupled distribution [5]

$$\phi(y,u) = \frac{1}{2} \delta(u/\tau - |y|/\sigma) \frac{(\beta-1)/\tau}{(1+u/\tau)^\beta}, \quad (2.20)$$

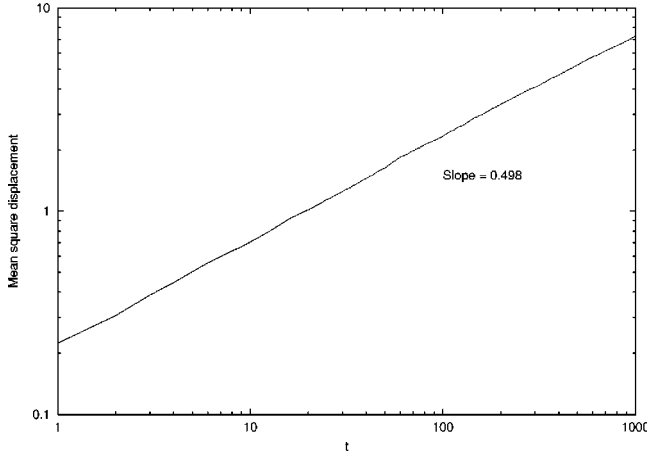


FIG. 1. A log-log plot of the mean squared displacement obtained by numerically simulating the underlying CTRW process for a Levy type anomalous diffusion with $\gamma=0.5$.

where $2 < \beta < 3$ and $\delta(\cdot)$ is the Dirac delta function, the CTRW describes a superdiffusive process with $\gamma = \beta - 1$. This can be seen as follows.

Proceeding as before, the waiting time distribution $\psi(u)$ is given by [cf. Eqs. (2.20) and (2.3)]

$$\psi(u) = \frac{(\beta-1)/\tau}{(1+u/\tau)^\beta}. \quad (2.21)$$

It has a finite mean but an infinite variance for $2 < \beta < 3$. Its Laplace transform in the limit $s \rightarrow 0$ is given by

$$\tilde{\psi}(s) \approx 1 - (2\beta-3)\tau s / (\beta-2). \quad (2.22)$$

The Fourier-Laplace transform $\tilde{\phi}(k,s)$ of $\phi(y,u)$ in Eq. (2.20) is given by (in the limit $s \rightarrow 0$ and $k \ll s$)

$$\tilde{\phi}(k,s) \approx \tilde{\psi}(s) - \frac{(\beta-1)\Gamma(3-\beta)}{2} k^2 \sigma^2 (\tau s)^{\beta-3}. \quad (2.23)$$

Substituting $\tilde{\psi}(s)$ and $\tilde{\phi}(k,s)$ into Eq. (2.4) we obtain

$$\tilde{W}(k,s) \approx \left[s + \frac{(\beta-1)(\beta-2)\Gamma(3-\beta)}{2(2\beta-3)} k^2 \sigma^2 (\tau s)^{\beta-3} \right]^{-1}. \quad (2.24)$$

Using this in Eq. (2.9) and evaluating the second derivative at $k=0$, in the limit $s \rightarrow 0$ we obtain

$$\langle X^2(s) \rangle \approx \frac{(\beta-1)(\beta-2)\Gamma(3-\beta)}{(2\beta-3)} \frac{1}{s^{5-\beta}}. \quad (2.25)$$

By the Tauberian theorem [14], this is equivalent to $\langle X^2(t) \rangle \sim t^{4-\beta}$. Thus the CTRW characterized by Eq. (2.20) is a superdiffusive process for $2 < \beta < 3$, with $\gamma = 4 - \beta$ ($1 < \gamma < 2$).

Note that there are several other possible forms for $\phi(y,u)$, which also give rise to subdiffusive and superdiffusive behaviors. See Ref. [5] for a detailed discussion.

B. Fractional Fokker-Planck equation for Levy type anomalous diffusion

In Sec. II A, we described CTRW processes that give rise to Levy type anomalous diffusion. However, it is difficult to derive analytical results directly from the process. It is more convenient to work in the general framework of Fokker-Planck equations [1]. One can go from the CTRW process to a fractional Fokker-Planck equation [8] by taking the generalized diffusion limit. This limit is analogous to the regular diffusion limit that one considers to derive the regular Fokker-Planck equation [1] from a random walk with $\langle X^2(t) \rangle \sim t$ for large t . In the regular diffusion limit, one lets $\sigma, \tau \rightarrow 0$, such that σ^2/τ is maintained a constant. For a CTRW where $\langle X^2(t) \rangle \sim t^\gamma$ ($0 < \gamma < 2$), the generalized diffusion limit is obtained by taking the limit $\sigma, \tau \rightarrow 0$ such that σ^2/τ^γ is maintained a constant.

Thus to obtain a FFPE from the CTRW process, we need to take the limit $\sigma, \tau \rightarrow 0$. We will take this limit for the Fourier-Laplace transform $\tilde{W}(k,s)$ of $W(x,t)$, and then invert the transform to obtain the FFPE. First consider the subdiffusive CTRW characterized by Eq. (2.5). In Sec. II A, we already derived an expression for $\tilde{W}(k,s)$ in the limit $s \rightarrow 0$ (which is equivalent to the limit $\tau \rightarrow 0$ that we now require):

$$\tilde{W}(k,s) \approx \frac{1}{s} \frac{\Gamma(1-\gamma)(\tau s)^\gamma}{1 - [1 - \Gamma(1-\gamma)(\tau s)^\gamma] \exp(-\sigma^2 k^2/2)}. \quad (2.26)$$

Here we have used $\gamma = \alpha - 1$ ($0 < \gamma < 1$) instead of α , since it is the physically relevant quantity. Now we take the further limit $\sigma \rightarrow 0$ such that $\sigma^2/2\Gamma(1-\gamma)\tau^\gamma = K$ is a constant. K is called the generalized diffusion constant. We then obtain

$$\tilde{W}(k,s) = \frac{1}{s + K k^2 s^{1-\gamma}}. \quad (2.27)$$

This can be rewritten as

$$\tilde{W}(k,s) - \frac{1}{s} = -K k^2 s^{-\gamma} \tilde{W}(k,s). \quad (2.28)$$

To take the inverse Fourier-Laplace transform of the above equation, we need the inverse Laplace transform of $s^{-\gamma} \tilde{W}(k,s)$. This is given by the Riemann-Liouville fractional integral ${}_0D_t^{-\gamma} W(k,t)$, which is defined as [17,18]

$${}_0D_t^{-\gamma} W(k,t) = \frac{1}{\Gamma(\gamma)} \int_0^t dt' (t-t')^{\gamma-1} W(k,t'), \quad \gamma > 0. \quad (2.29)$$

This result enables us to take the inverse Fourier-Laplace transform of Eq. (2.28), giving [7,8]

$$W(x,t) - W(x,0) = K {}_0D_t^{-\gamma} \frac{\partial^2}{\partial x^2} W(x,t), \quad 0 < \gamma < 1. \quad (2.30)$$

Here we have incorporated the initial condition $W(x,0) = \delta(x)$.

Next we consider the superdiffusive CTRW process characterized by Eq. (2.20). We have already derived an expression for $\tilde{W}(k,s)$ in the limit $k,s \rightarrow 0$ (which is equivalent to the limit $\sigma, \tau \rightarrow 0$ that we now require):

$$\tilde{W}(k,s) \approx \left[s + \frac{(3-\gamma)(2-\gamma)\Gamma(\gamma-1)}{2(5-2\gamma)} k^2 \sigma^2 (\tau s)^{1-\gamma} \right]^{-1}. \quad (2.31)$$

This expression is valid in the regime $\sigma \ll \tau$. Taking the generalized diffusion limit, we again obtain Eq. (2.28), but now $K = (3-\gamma)(2-\gamma)\Gamma(\gamma-1)\sigma^2/2(5-2\gamma)\tau^\gamma$ and $1 < \gamma < 2$. Therefore, this superdiffusive CTRW process also gives Eq. (2.30) with the above K and $1 < \gamma < 2$.

To summarize, a class of Levy type anomalous diffusion can be described by the following FFPE in the generalized diffusion limit:

$$W(x,t) - W(x,0) = K {}_0D_t^{-\gamma} \frac{\partial^2}{\partial x^2} W(x,t), \quad 0 < \gamma < 2. \quad (2.32)$$

Here K has different expressions for $0 < \gamma < 1$ and $1 < \gamma < 2$, as described above. We note that there are other CTRW processes which may give rise to different FFPE's. In this paper, we consider only the FFPE given in Eq. (2.32). The above FFPE describes Levy type anomalous diffusion with zero drift. For anomalous diffusion with drift μ , the above FFPE can be generalized to give [7]

$$W(x,t) - W(x,0) = K {}_0D_t^{-\gamma} \frac{\partial^2}{\partial x^2} W(x,t) - \mu {}_0D_t^{-1} \frac{\partial}{\partial x} W(x,t), \quad (2.33)$$

where $0 < \gamma < 2$. We also note that for $\gamma = 1$, the above FFPE reduces to the regular Fokker-Planck equation describing Brownian motion.

We now show that this FFPE gives the correct moments. The natural boundary conditions for the FFPE are

$$W(-\infty, t) = W(\infty, t) = 0, \quad W(x, 0) = \delta(x). \quad (2.34)$$

First we compute $\langle X_\mu \rangle$. Multiplying the FFPE given in Eq. (2.33) by x , and integrating from $x = -\infty$ to $x = \infty$, we obtain

$$\langle X_\mu \rangle = \mu {}_0D_t^{-1} \int_{-\infty}^{\infty} dx W(x,t) - K {}_0D_t^{-\gamma} \int_{-\infty}^{\infty} dx x \frac{\partial W(x,t)}{\partial x}, \quad (2.35)$$

where we have performed integration by parts and assumed that $xW(x,t) = 0$ and $x[\partial W(x,t)/\partial x] = 0$ at $x = \pm\infty$. Evaluating the remaining integrals using the natural boundary conditions and the normalization integral $\int_{-\infty}^{\infty} dx W(x,t) = 1$, we obtain

$$\langle X_\mu \rangle = \mu {}_0D_t^{-1}(1) = \mu t. \quad (2.36)$$

This is the expected result.

Next we compute $\text{Var}[X_\mu]$. Multiplying the FFPE in Eq. (2.33) by x^2 , and integrating, we obtain

$$\begin{aligned} \langle X_\mu^2 \rangle &= 2\mu {}_0D_t^{-1} \int_{-\infty}^{\infty} dx x^2 W(x,t) \\ &\quad - 2K {}_0D_t^{-\gamma} \int_{-\infty}^{\infty} dx x^2 \frac{\partial W(x,t)}{\partial x}, \end{aligned} \quad (2.37)$$

where we have again used integration by parts and assumed that $x^2W(x,t) = 0$ and $x^2[\partial W(x,t)/\partial x] = 0$ at $x = \pm\infty$. Evaluating the remaining integrals using the fact that $\int_{-\infty}^{\infty} dx x^2 W(x,t) = \langle X_\mu^2 \rangle = \mu t^2$ and the boundary and normalization conditions, we obtain

$$\langle X_\mu^2 \rangle = 2\mu^2 {}_0D_t^{-1}(t) + 2K {}_0D_t^{-\gamma}(1). \quad (2.38)$$

But ${}_0D_t^{-1}(t) = t^2/2$ and ${}_0D_t^{-\gamma}(1) = t^\gamma/\Gamma(\gamma+1)$ [18]. Therefore,

$$\langle X_\mu^2 \rangle = \mu^2 t^2 + \frac{2Kt^\gamma}{\Gamma(\gamma+1)}. \quad (2.39)$$

The variance $\text{Var}[X_\mu]$ is given by $\langle X_\mu^2 \rangle - \langle X_\mu \rangle^2$. Hence

$$\text{Var}[X_\mu] = \frac{2Kt^\gamma}{\Gamma(\gamma+1)}. \quad (2.40)$$

Thus we see that our FFPE gives the correct moments.

III. FIRST PASSAGE TIME PROBLEM FOR LEVY TYPE ANOMALOUS DIFFUSION

We now formulate the first passage time problem for the FFPE given in Eq. (2.33) describing Levy type anomalous diffusion with drift. Consider a stochastic process $X(t)$ with $X(0) = 0$. The first passage time (FPT) T to the point $X = a$ is defined as [19]

$$T = \inf\{t: X(t) = a\}. \quad (3.1)$$

We would like to obtain the probability density function for T . This is the first passage time problem.

For a process described by Fokker-Planck equations, the problem of obtaining the FPT density function can be recast as a boundary value problem with absorbing boundaries [1]. In our case, to obtain the FPT density function, we first need to solve Eq. (2.33) with absorbing boundaries at $x = -\infty$ and $x = a$, where a is the predetermined level of crossing, with the initial condition $W(x,0) = \delta(x)$ [1]. An equivalent formulation, due to symmetry, is to solve Eq. (2.33), with the boundary and initial conditions

$$W(0,t) = 0, \quad W(\infty,t) = 0, \quad W(x,0) = \delta(x-a), \quad (3.2)$$

where $x = a$ is the new starting point of the CTRW, containing the initial concentration of the distribution. The equivalence is easily seen by making the change of variables $x \rightarrow a - x$ in Eq. (2.33). The only change is in the interpretation of μ . Now $\mu < 0$ corresponds to a drift toward the barrier. This latter formulation makes the subsequent derivation less cumbersome. Once we solve for $W(x,t)$, the first passage time density $f(t)$ is given by [1]

$$f(t) = -\frac{d}{dt} \int_0^\infty dx W(x,t). \quad (3.3)$$

In the following subsections, we obtain the FPT density function for Levy type anomalous diffusion under different conditions.

A. Zero drift case

In this section, we obtain an explicit solution for the FPT density for a zero drift Levy type anomalous diffusion in terms of H functions [9,10,20]. Asymptotic expressions for the FPT density in various limits are obtained. Numerical simulations are performed to confirm the above results.

Setting $\mu=0$ in Eq. (2.33), we obtain

$$W(x,t) - W(x,0) = K {}_0D_t^{-\gamma} \frac{\partial^2}{\partial x^2} W(x,t). \quad (3.4)$$

Taking into account the boundary and initial conditions [cf. Eq. (3.2)], we are led to the following expansion for $W(x,t)$ [21]:

$$W(x,t) = \frac{2}{\pi} \int_0^\infty dk \sin kx \sin ka A(k,t), \quad (3.5)$$

with $A(k,0)=1$. To determine the unknown function $A(k,t)$, we substitute the above expansion for $W(x,t)$ in Eq. (3.4) and, after straightforward algebra, obtain $A(k,t) - 1 = -Kk^2 {}_0D_t^{-\gamma} A(k,t)$. Taking the Laplace transform with respect to t , we have

$$A(k,s) = \frac{1}{s + k^2 K s^{1-\gamma}}, \quad (3.6)$$

where $A(k,s)$ is the Laplace transform of $A(k,t)$. Here we have applied the result [18] that the Laplace transform of ${}_0D_t^{-\gamma} A(k,t)$ is $A(k,s)/s^\gamma$.

Inverse Laplace transform of Eq. (3.6) yields [22]

$$A(k,t) = E_\gamma(-k^2 K t^\gamma), \quad (3.7)$$

where $E_\gamma(z)$ is the Mittag-Leffler function [22]. The Mittag-Leffler function can be defined by the following power series expansion:

$$E_\gamma(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(n\gamma+1)}. \quad (3.8)$$

When $\gamma=1$, the Mittag-Leffler function reduces to the usual exponential function e^z . Substituting Eq. (3.7) into Eq. (3.5), we obtain

$$W(x,t) = \frac{2}{\pi} \int_0^\infty dk \sin kx \sin ka E_\gamma(-k^2 K t^\gamma). \quad (3.9)$$

To proceed further, we introduce the Fox or H function [9,10,20] which has the following alternating power series expansion:

$$\begin{aligned} H_{p,q}^{m,n} \left(z \left| \begin{array}{l} (a_j, A_j)_{j=1, \dots, p} \\ (b_j, B_j)_{j=1, \dots, q} \end{array} \right. \right) \\ = \sum_{l=1}^m \sum_{k=0}^{\infty} \frac{(-1)^k z^{s_{lk}}}{k! B_l} \\ \times \frac{\prod_{j=1, j \neq l}^m \Gamma(b_j - B_j s_{lk}) \prod_{r=1}^n \Gamma(1 - a_r + A_r s_{lk})}{\prod_{u=m+1}^q \Gamma(1 - b_u + B_u s_{lk}) \prod_{v=n+1}^p \Gamma(a_v - A_v s_{lk})}, \end{aligned} \quad (3.10)$$

where $s_{lk} = (b_l + k)/B_l$ and an empty product is interpreted as unity. Further, m, n, p , and q are non-negative integers such that $0 \leq n \leq p$ and $1 \leq m \leq q$; A_j and B_j are positive numbers; a_j and b_j can be complex numbers. We will denote the H function by $H_{p,q}^{m,n}(z)$ for the sake of notational simplicity wherever this does not lead to any confusion. The H function has several remarkable properties, some of which are listed in the Appendix.

Returning to our problem, by comparing the series expansion [cf. Eq. (3.8)] of the Mittag-Leffler function $E_\gamma(z)$ with that of the H function [cf. Eq. (3.10)], we see that

$$E_\gamma(-z) = H_{1,2}^{1,1} \left(z \left| \begin{array}{l} (0,1) \\ (0,1), (0,\gamma) \end{array} \right. \right). \quad (3.11)$$

Substituting this into Eq. (3.9), we obtain

$$W(x,t) = \frac{2}{\pi} \int_0^\infty dk \sin kx \sin ka H_{1,2}^{1,1} \left(k^2 K t^\gamma \left| \begin{array}{l} (0,1) \\ (0,1), (0,\gamma) \end{array} \right. \right). \quad (3.12)$$

Letting $k' = k(Kt^\gamma)^{1/2}$, the above equation becomes

$$\begin{aligned} W(x,t) &= \frac{2}{\pi(Kt^\gamma)^{1/2}} \\ &\times \int_0^\infty dk' \sin k'x \sin k'a \\ &\times H_{1,2}^{1,1} \left((k')^2 \left| \begin{array}{l} (0,1) \\ (0,1), (0,\gamma) \end{array} \right. \right). \end{aligned} \quad (3.13)$$

Using property 5 [Eq. (A4)] of the H functions to replace $(k')^2$ by k' , we obtain

$$\begin{aligned} W(x,t) &= \frac{1}{\pi(Kt^\gamma)^{1/2}} \\ &\times \int_0^\infty dk' \sin k'x \sin k'a \\ &\times H_{1,2}^{1,1} \left(k' \left| \begin{array}{l} (0,1/2) \\ (0,1/2), (0,\gamma/2) \end{array} \right. \right). \end{aligned} \quad (3.14)$$

The above equation can be rewritten as follows, making use of the standard trigonometric identity $2 \sin k'x \sin k'a = \cos k'(x-a) - \cos k'(x+a)$:

$$W(x,t) = \frac{1}{2\pi(Kt^\gamma)^{1/2}} \int_0^\infty dk' [\cos k'(x-a) - \cos k'(x+a)] H_{1,2}^{1,1} \left(k' \left| \begin{matrix} (0,1/2) \\ (0,1/2), (0,\gamma/2) \end{matrix} \right. \right). \quad (3.15)$$

The above Fourier cosine transforms can be solved by successive applications of a Laplace and an inverse Laplace transform (a technique pioneered by Fox [23] for solving a wide variety of integral transforms) to give [20]

$$W(x,t) = \frac{1}{2|x-a|} \times H_{3,3}^{2,1} \left(\frac{|x-a|}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1,1/2), (1,\gamma/2), (1,1/2) \\ (1,1), (1,1/2), (1,1/2) \end{matrix} \right. \right) - \frac{1}{2(x+a)} \times H_{3,3}^{2,1} \left(\frac{x+a}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1,1/2), (1,\gamma/2), (1,1/2) \\ (1,1), (1,1/2), (1,1/2) \end{matrix} \right. \right). \quad (3.16)$$

Now, applying property 2 [cf. Eq. (A1)] of the H functions to reduce the order of our H function, we obtain

$$W(x,t) = \frac{1}{2|x-a|} H_{2,2}^{2,0} \left(\frac{|x-a|}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1,\gamma/2), (1,1/2) \\ (1,1), (1,1/2) \end{matrix} \right. \right) - \frac{1}{2(x+a)} H_{2,2}^{2,0} \left(\frac{x+a}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1,\gamma/2), (1,1/2) \\ (1,1), (1,1/2) \end{matrix} \right. \right). \quad (3.17)$$

Applying properties 1 and 3 [cf. Eq. (A2)] of the H functions, we can further reduce the order of our H function:

$$W(x,t) = \frac{1}{2|x-a|} H_{1,1}^{1,0} \left(\frac{|x-a|}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1,\gamma/2) \\ (1,1) \end{matrix} \right. \right) - \frac{1}{2(x+a)} H_{1,1}^{1,0} \left(\frac{x+a}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1,\gamma/2) \\ (1,1) \end{matrix} \right. \right). \quad (3.18)$$

Applying property 6 [cf. Eq. (A5)] of the H functions with $z=|x-a|$ (or $z=x+a$) and $\rho=-1$, we finally obtain

$$W(x,t) = \frac{1}{2(Kt^\gamma)^{1/2}} \left[H_{1,1}^{1,0} \left(\frac{|x-a|}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1-\gamma/2,\gamma/2) \\ (0,1) \end{matrix} \right. \right) - H_{1,1}^{1,0} \left(\frac{x+a}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1-\gamma/2,\gamma/2) \\ (0,1) \end{matrix} \right. \right) \right]. \quad (3.19)$$

Substituting Eq. (3.19) into Eq. (3.3), we have

$$f(t) = -\frac{d}{dt} \left[\frac{1}{2(Kt^\gamma)^{1/2}} \times \int_0^\infty dx H_{1,1}^{1,0} \left(\frac{|x-a|}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1-\gamma/2,\gamma/2) \\ (0,1) \end{matrix} \right. \right) \right] + \frac{d}{dT} \left[\frac{1}{2(Kt^\gamma)^{1/2}} \times \int_0^\infty dx H_{1,1}^{1,0} \left(\frac{x+a}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1-\gamma/2,\gamma/2) \\ (0,1) \end{matrix} \right. \right) \right]. \quad (3.20)$$

Defining $z=(x-a)/(Kt^\gamma)^{1/2}$ and $z'=(x+a)/(Kt^\gamma)^{1/2}$, we obtain

$$f(t) = -\frac{d}{dt} \int_{-a/(Kt^\gamma)^{1/2}}^\infty dz H_{1,1}^{1,0} \left(|z| \left| \begin{matrix} (1-\gamma/2,\gamma/2) \\ (0,1) \end{matrix} \right. \right) + \frac{d}{dt} \int_{a/(Kt^\gamma)^{1/2}}^\infty dz' H_{1,1}^{1,0} \left(z' \left| \begin{matrix} (1-\gamma/2,\gamma/2) \\ (0,1) \end{matrix} \right. \right). \quad (3.21)$$

Evaluating the above equation (which is easily done since the only t dependence is in the limits of the integrals), we obtain the following expression for the first passage time density

$$f(t) = \frac{a\gamma}{2K^{1/2}t^{(2+\gamma)/2}} H_{1,1}^{1,0} \left(\frac{a}{(Kt^\gamma)^{1/2}} \left| \begin{matrix} (1-\gamma/2,\gamma/2) \\ (0,1) \end{matrix} \right. \right). \quad (3.22)$$

We mention that this result appeared earlier in a short communication [24]. It should be noted that H functions were first used in the context of probability distributions by Schneider [25]. They have also been used to express solutions of fractional diffusion equations [26]. The series expansion of the H function in Eq. (3.22) [cf. Eq. (3.10)] is

$$f(t) = \frac{a\gamma}{2K^{1/2}t^{(2+\gamma)/2}} \sum_{k=0}^{\infty} \frac{[-a/(Kt^\gamma)^{1/2}]^k}{k! \Gamma(1-\gamma/2-k\gamma/2)}. \quad (3.23)$$

This also turns out to be the series expansion of Maitland's generalized hypergeometric function or the Wright function ${}_0\psi_1$ [22]. Thus an alternative expression for $f(t)$ is

$$f(t) = \frac{a\gamma}{2K^{1/2}t^{(2+\gamma)/2}} {}_0\psi_1 \left(-; -\frac{a}{(Kt^\gamma)^{1/2}} \right). \quad (3.24)$$

It is difficult to work with the series expansion of $f(t)$ given in Eq. (3.23) due to the presence of the γ function with large negative arguments. We get around this as follows. From the properties of the γ function [15], we have

$$\Gamma(1 - \gamma/2 - k\gamma/2) = -\frac{(k+1)\gamma}{2} \Gamma[-(k+1)\gamma/2]. \quad \Gamma(-z) = \frac{-\pi}{\sin(\pi z)\Gamma(z+1)}, \quad (3.26)$$

Using the relation [15]

Eq. (3.25) can be rewritten as

$$\begin{aligned} \Gamma(1 - \gamma/2 - k\gamma/2) &= \frac{\pi(k+1)\gamma}{2} \frac{1}{\sin[(k+1)\pi\gamma/2]\Gamma[1+(k+1)\gamma/2]} \\ &= \frac{\pi}{\sin[(k+1)\pi\gamma/2]\Gamma[(k+1)\gamma/2]}. \end{aligned} \quad (3.27)$$

Substituting this into Eq. (3.23), we obtain

$$f(t) = \frac{a\gamma}{2\pi K^{1/2} t^{(2+\gamma)/2}} \sum_{k=0}^{\infty} \frac{[-a/(Kt^\gamma)^{1/2}]^k \sin[(k+1)\pi\gamma/2] \Gamma[(k+1)\gamma/2]}{\Gamma(k+1)}. \quad (3.28)$$

Note that for regular Brownian motion ($\gamma=1$), the above expression for $f(t)$ reduces to

$$f(t) = \frac{a}{2\pi\sqrt{Kt^3}} \sum_{k=0}^{\infty} \frac{(-a/\sqrt{Kt})^k \sin[(k+1)\pi/2] \Gamma[(k+1)/2]}{\Gamma(k+1)}. \quad (3.29)$$

However [15],

$$\Gamma(k+1) = \frac{4^{k/2} \Gamma[(k+1)/2] \Gamma(1+k/2)}{\sqrt{\pi}}. \quad (3.30)$$

Further,

$$\begin{aligned} \sin[(k+1)\pi/2] &= 0, \quad k \text{ odd}, \\ &= (-1)^{k/2}, \quad k \text{ even}. \end{aligned} \quad (3.31)$$

Substituting these relations into Eq. (3.29), and letting $n = k/2$, we obtain

$$f(t) = \frac{a}{2\pi\sqrt{Kt^3}} \sum_{n=0}^{\infty} \frac{(-a/\sqrt{Kt})^{2n} \Gamma[(2n+1)/2] (-1)^n}{(4)^n \Gamma[(2n+1)/2] \Gamma(n+1)}. \quad (3.32)$$

Simplifying this, we finally obtain

$$\begin{aligned} f(t) &= \frac{a}{\sqrt{4\pi Kt^3}} \sum_{n=0}^{\infty} \frac{(-a^2/4\sqrt{Kt})^n}{n!} \\ &= \frac{a}{\sqrt{4\pi Kt^3}} \exp[-a^2/4Kt]. \end{aligned} \quad (3.33)$$

This is the expected inverse Gaussian distribution for the FPT density function of the ordinary Brownian motion with zero drift [19].

Next we consider the asymptotic behavior of the FPT distribution for large values of t . Refer to Eq. (3.22). Let $z = a/(Kt^\gamma)^{1/2}$. It is known that [10,27], for small z , $H_{1,1}^{1,0}(z)$

$\sim |z|^{b_1/B_1} = 1$, since $b_1=0$ and $B_1=1$. Therefore, the FPT distribution $f(t)$, for large t , is characterized by the power law relation

$$f(t) \sim t^{-1-\gamma/2}, \quad (3.34)$$

which becomes the well known $-3/2$ scaling law for the ordinary Brownian motion. We make two comments. First, the above power law behavior was observed earlier by Balakrishnan [28] for subdiffusive processes ($0 < \gamma < 1$) using a different method. Using our method the same scaling law is shown also to be applicable to superdiffusive processes. Second, from Eq. (3.34), we see that the mean first passage time and all higher moments of the FPT distribution are undefined for $0 < \gamma < 2$.

Next we consider the asymptotic behavior of $f(t)$ for small t [i.e., large z where $z = a/(Kt^\gamma)^{1/2}$]. It is known [10,27] that, for large z ,

$$H_{1,1}^{1,0}(z) \sim Bz^{\alpha/\mu} \exp[-\mu C^{1/\mu} z^{1/\mu}], \quad (3.35)$$

where

$$\alpha = \sum_{j=1}^q b_j - \sum_{j=1}^p a_j + (p-q+1)/2,$$

$$C = \prod_{j=1}^p (A_j)^{A_j} \prod_{j=1}^q (B_j)^{B_j},$$

$$\mu = \sum_{j=1}^q B_j - \sum_{j=1}^p A_j,$$

$$B = (2\pi)^{(q-p-1)/2} C^{\alpha/\mu} \mu^{-1/2} \prod_{j=1}^p (A_j)^{-a_j+0.5} \prod_{l=1}^q (B_l)^{b_l-0.5}.$$

In our case, $p=1$, $q=1$, $a_1=1-\gamma/2$, $A_1=\gamma/2$, $b_1=0$, and $B_1=1$. Therefore, for large z ,

$$\begin{aligned} H_{1,1}^{1,0} \left(\frac{a}{(Kt)^\gamma} \middle| \begin{matrix} (1-\gamma/2, \gamma/2) \\ (0,1) \end{matrix} \right) \\ \sim \frac{1}{\sqrt{(2-\gamma)\pi}} \left(\frac{\gamma}{2} \right)^{(\gamma-1)/(2-\gamma)} z^{(\gamma-1)/(2-\gamma)} \\ \times \exp \left[-\frac{2-\gamma}{2} \left(\frac{\gamma}{2} \right)^{\gamma/(2-\gamma)} z^{2/(2-\gamma)} \right]. \end{aligned} \quad (3.36)$$

Substituting this into the expression for $f(t)$ [cf. Eq. (3.22)], for small t we obtain

$$f(t) \sim \frac{r}{t^{(4-\gamma)/(4-2\gamma)}} \exp \left[-\frac{d}{t^{\gamma/(2-\gamma)}} \right], \quad (3.37)$$

where

$$\begin{aligned} r &= \frac{a\gamma}{\sqrt{4K\pi(2-\gamma)}} \left(\frac{a\gamma}{2\sqrt{K}} \right)^{(\gamma-1)/(2-\gamma)}, \\ d &= \frac{2-\gamma}{2} \left(\frac{\gamma}{2} \right)^{\gamma/(2-\gamma)} \left(\frac{a}{\sqrt{K}} \right)^{2/(2-\gamma)}. \end{aligned}$$

For $0 < \gamma < 2$, both r and d are greater than zero. Therefore, $f(t)$ is exponentially decaying for small t . Note that for $\gamma=1$ (ordinary Brownian motion), the above expression reduces to

$$f(t) \sim \frac{a}{\sqrt{4\pi K t^3}} \exp[-a^2/4Kt]. \quad (3.38)$$

In this case, the asymptotic expression turns out to be the exact expression.

We can determine the t value where $f(t)$ attains its maximum value from the above expression. We obtain

$$t_{\max} = \left(\frac{2d\gamma}{4-\gamma} \right)^{(2-\gamma)/\gamma}. \quad (3.39)$$

For ordinary Brownian motion ($\gamma=1$),

$$t_{\max} = \frac{2d}{3} = \frac{a^2}{6K}. \quad (3.40)$$

The theoretical prediction for the full FPT density function given in Eq. (3.22) is verified by numerically simulating the underlying CTRW process characterized by the probability density function $\phi(y,u)$ [cf. Eq. (2.5)]. For the sake of numerical efficiency, we replace the waiting time distribution $(\alpha-1)/\tau(1+u/\tau)^\alpha$ in $\phi(y,u)$ by the Pareto density function [16] [which is equal to zero for $u < \tau$ and $(\alpha-1)\tau^{\alpha-1}/u^\alpha$ for $u \geq \tau$]. The parameter values are chosen as follows: $\gamma=0.5$, $a=1.0$, and $K=0.1$. In Fig. 2, the FPT den-

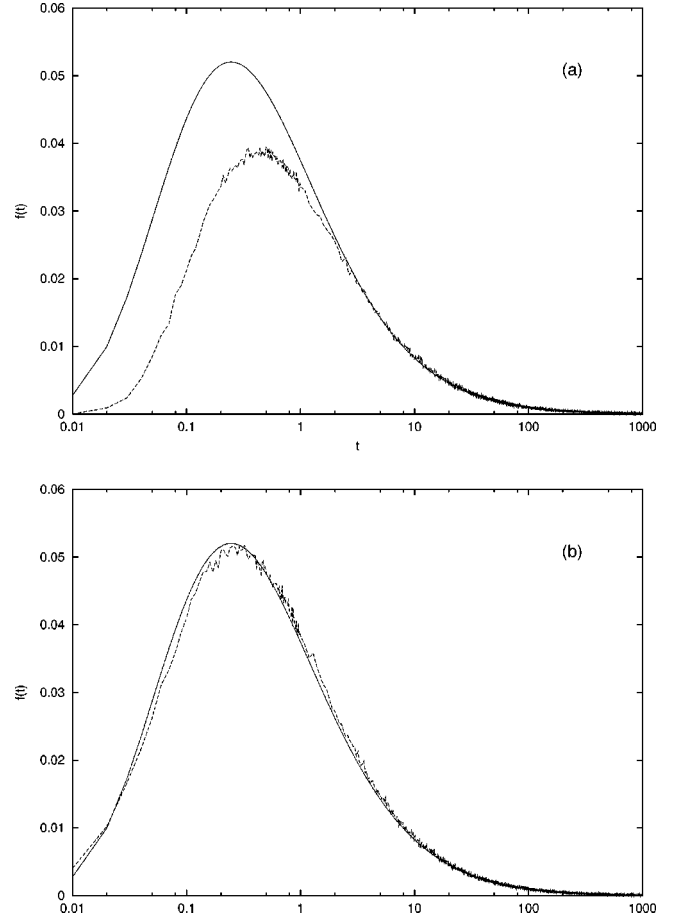


FIG. 2. (a) Comparison of the theoretical FPT distribution (solid line) with the distribution (dashed line) obtained by numerically simulating the underlying CTRW process for a Levy type anomalous diffusion (with $\gamma=0.5$) that is not close to the generalized diffusion limit ($\tau=10^{-2}$). (b) Same comparison as above, but closer to the generalized diffusion limit ($\tau=10^{-4}$).

sity function obtained theoretically from Eq. (3.22) is compared with the FPT density function obtained numerically using ten million realizations of the underlying stochastic process. If we take a large value for τ ($=0.01$), the agreement is not that good [see Fig. 2(a)], since we are not yet close to the generalized diffusion limit. If, however, we take τ to be 10^{-4} , the numerical simulation is in excellent agreement with the theoretical prediction [see Fig. 2(b)]. The agreement becomes better as τ and σ become smaller, approaching the generalized diffusion limit.

The above statement can be quantified as follows. Consider the Kullback-Leibler information criterion [29,30], which gives a quantitative measure of how “far apart” a given approximate density function $f_1(t)$ is from the exact density function $f(t)$. The Kullback-Leibler information criterion is defined as

$$KL(f, f_1) = \int_0^\infty dt f(t) \log \frac{f(t)}{f_1(t)}. \quad (3.41)$$

This is always greater than or equal to zero, and is equal to zero if and only if $f_1(t)$ agrees exactly with $f(t)$. The deviation away from zero quantifies the disagreement between the two density functions.

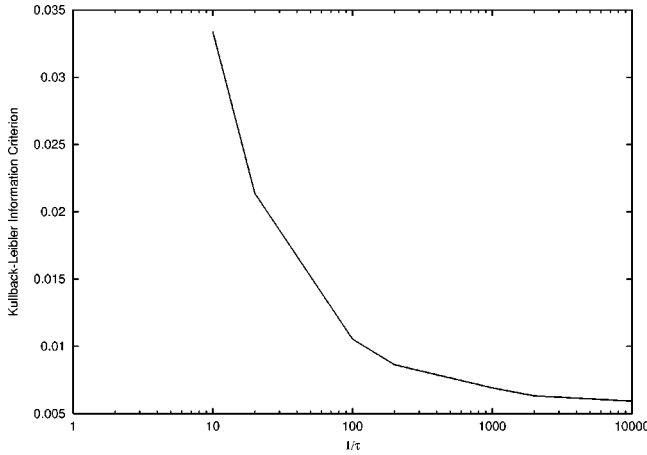


FIG. 3. Plot of the Kullback-Leibler information criterion against $1/\tau$.

In our case, we take $f_1(t)$ to be the approximate numerically simulated FPT density function for various values of τ (the value of σ is correspondingly varied to keep K constant). The plot of the Kullback-Leibler information criterion for different values of $1/\tau$ is given in Fig. 3. As τ decreases (i.e., as the generalized diffusion limit is approached), the Kullback-Leibler information criterion also decreases.

B. Nonzero drift case

In this section, we consider the first passage time problem for Levy type anomalous diffusion with drift. An explicit solution for the FPT density function is not possible in this case. We obtain the Laplace transform of the FPT density function (the so-called ‘‘moment generating function’’ [31]). Using this, we obtain the mean and variance of the first passage time distribution. For regular Brownian motion ($\gamma = 1$), the inverse Laplace transform of the moment generating function can be explicitly carried out to give the standard results.

Taking the Laplace transform of Eq. (2.33), we obtain

$$q(x,s) - \frac{W(x,0)}{s} = \frac{K}{s^\gamma} \frac{\partial^2}{\partial x^2} q(x,s) - \frac{\mu}{s} \frac{\partial}{\partial x} q(x,s), \quad (3.42)$$

where $q(x,s)$ is the Laplace transform of $W(x,t)$. Here we have again applied the result [18] that the Laplace transform of ${}_0D_t^{-\gamma} W(x,t)$ is $q(x,s)/s^\gamma$. The above equation can be rewritten as

$$\frac{\partial^2}{\partial x^2} q(x,s) + A \frac{\partial}{\partial x} q(x,s) + B q(x,s) = -\frac{s^{\gamma-1}}{K} \delta(x-a), \quad (3.43)$$

where

$$A = -\frac{\mu s^{\gamma-1}}{K}, \quad B = -\frac{s^\gamma}{K}. \quad (3.44)$$

Since $s, K > 0$, we have

$$\lambda^2 \equiv A^2 - 4B = \frac{\mu^2 s^{2\gamma-2}}{K^2} + 4\frac{s^\gamma}{K} > 0. \quad (3.45)$$

Therefore, two independent solutions of the homogeneous equation corresponding to Eq. (3.43) are given by [32]

$$q_1(x,s) = \exp[x(\lambda - A)/2], \quad q_2(x,s) = \exp[x(-\lambda - A)/2]. \quad (3.46)$$

Consequently, the general solution of Eq. (3.43), satisfying all the boundary and initial conditions [cf. Eq. (3.2)], is given by

$$q(x,s) = \frac{s^{\gamma-1}}{K\lambda} e^{-A(x-a)/2} [e^{-\lambda|x-a|/2} - e^{-\lambda(x+a)/2}]. \quad (3.47)$$

To obtain the Laplace transform of the FPT density function, we take the Laplace transform of Eq. (3.3) to obtain

$$F(s) = -s \int_0^\infty dx q(x,s) + \int_0^\infty dx W(x,0). \quad (3.48)$$

Here we have used the fact that Laplace transform of $dW(x,t)/dt$ is given by [13] $s q(x,s) - W(x,0)$. Since $W(x,0) = \delta(x-a)$ [cf. Eq. (3.2)], we obtain

$$F(s) = 1 - s \int_0^\infty dx q(x,s). \quad (3.49)$$

Substituting for $q(x,s)$ from Eq. (3.47), we obtain

$$F(s) = 1 - \frac{s^\gamma}{K\lambda} \left[\int_0^a dx e^{-A(x-a)/2} e^{-\lambda(a-x)/2} - \int_a^\infty dx e^{-A(x-a)/2} e^{-\lambda(x-a)/2} \right] + \frac{s^\gamma}{K\lambda} \int_0^\infty dx e^{-A(x-a)/2} e^{-\lambda(x+a)/2}.$$

The integrals can be easily evaluated, to finally give [upon using Eq. (3.44)]

$$F(s) = \exp \left[-\frac{a\mu s^{\gamma-1}}{2K} - a \sqrt{\frac{\mu^2 s^{2\gamma-2}}{4K^2} + \frac{s^\gamma}{K}} \right]. \quad (3.50)$$

For $0 < \gamma < 1$, $F(s)$ is not a completely monotone function [14]. That is, it does not satisfy the following conditions:

$$(-1)^n \frac{dF^n(s)}{ds^n} \geq 0, \quad \text{for } s \geq 0, \quad F(0) = 1. \quad (3.51)$$

Hence $F(s)$ is not a Laplace transform of a probability density function. The physical reason for this is not yet understood. For $1 \leq \gamma < 2$, we have not been able to prove rigorously that $F_{\gamma,\mu}(s)$ is a completely monotonic function. However, we have calculated the first hundred derivatives of $F_{\gamma,\mu}(s)$ using the symbolic manipulation program MATHEMATICA, and found that all of them satisfy Eq. (3.51).

Hence we conjecture that $F(s)$ is the Laplace transform of a probability density function for $1 \leq \gamma < 2$. Henceforth, we restrict ourselves to this parameter range.

First consider the case where the drift is toward the barrier. This implies that $\mu < 0$, since in our formulation the diffusive process starts at $x = a > 0$ and the barrier is at $x = 0$. In this case, the FPT density function can be written as [cf. Eq. (3.50)]

$$F(s) = e^{ag(s)}, \quad (3.52)$$

where

$$g(s) = \frac{|\mu|s^{\gamma-1}}{2K} - \frac{|\mu|s^{\gamma-1}}{2K} \sqrt{1 + \frac{4Ks^{2-\gamma}}{\mu^2}}. \quad (3.53)$$

The mean first passage time is given by

$$\langle T \rangle = - \left. \frac{dF(s)}{ds} \right|_{s=0}. \quad (3.54)$$

From Eqs. (3.52) and (3.53), we have

$$\begin{aligned} \frac{dF(s)}{ds} = & \left[\frac{|\mu|(\gamma-1)s^{\gamma-2}a}{2K} \left(1 - \sqrt{1 + \frac{4Ks^{2-\gamma}}{\mu^2}} \right) \right. \\ & \left. - \frac{(2-\gamma)a \left(1 + \frac{4Ks^{2-\gamma}}{\mu^2} \right)^{-1/2}}{|\mu|} \right] e^{ag(s)}. \end{aligned} \quad (3.55)$$

We need to find the limiting value of the above expression as $s \rightarrow 0$. First consider $e^{ag(s)}$. As $s \rightarrow 0$, we can expand the square root in Eq. (3.53) to give

$$g(s) = - \frac{s}{|\mu|} + \frac{Ks^{3-\gamma}}{|\mu|^3} - \dots. \quad (3.56)$$

Hence $g(s) \rightarrow 0$ as $s \rightarrow 0$. Consequently, $e^{ag(s)} \rightarrow 1$ as $s \rightarrow 0$. Performing similar expansions for the other terms in Eq. (3.55), we finally obtain [cf. Eq. (3.54)]

$$\langle T \rangle = \frac{a}{|\mu|}. \quad (3.57)$$

Note that the mean first passage time is independent of γ .

The variance is obtained as follows:

$$\text{Var}(T) = \langle T^2 \rangle - \langle T \rangle^2. \quad (3.58)$$

Therefore, we need to evaluate $\langle T^2 \rangle$. This is given by

$$\langle T^2 \rangle = \left. \frac{d^2F(s)}{ds^2} \right|_{s=0}. \quad (3.59)$$

Now

$$\frac{d^2F(s)}{ds^2} = \left[a \frac{d^2g(s)}{ds^2} + \left(a \frac{dg(s)}{ds} \right)^2 \right] e^{ag(s)}. \quad (3.60)$$

Consider the first term. The second derivative of $g(s)$ is given by

$$\begin{aligned} \frac{d^2g(s)}{ds^2} = & \frac{|\mu|(\gamma-1)(\gamma-2)s^{\gamma-3}}{2K} \left(1 - \sqrt{1 + \frac{4Ks^{2-\gamma}}{\mu^2}} \right) \\ & - \frac{(\gamma-1)(2-\gamma)}{|\mu|s} \left(1 + \frac{4Ks^{2-\gamma}}{\mu^2} \right)^{-1/2} \\ & + \frac{2K(2-\gamma)^2s^{1-\gamma}}{|\mu|^3} \left(1 + \frac{4Ks^{2-\gamma}}{\mu^2} \right)^{-3/2}. \end{aligned}$$

Expanding all terms, we obtain

$$\begin{aligned} \frac{d^2g(s)}{ds^2} = & - \frac{|\mu|(\gamma-1)(\gamma-2)s^{\gamma-3}}{2K} \\ & \times \sum_{n=2}^{\infty} \frac{(-1)^{n-1} 1 \cdot 3 \cdots (2n-3)}{2^n n!} \left(\frac{4Ks^{2-\gamma}}{\mu^2} \right)^n \\ & - \frac{(\gamma-1)(2-\gamma)}{|\mu|s} \sum_{n=1}^{\infty} \frac{(-1)^n 1 \cdot 3 \cdots (2n-1)}{2^n n!} \\ & \times \left(\frac{4Ks^{2-\gamma}}{\mu^2} \right)^n + \frac{2K(2-\gamma)^2s^{1-\gamma}}{|\mu|^3} \\ & \times \sum_{n=0}^{\infty} \frac{(-1)^n 1 \cdot 3 \cdots (2n+1)}{2^n n!} \left(\frac{4Ks^{2-\gamma}}{\mu^2} \right)^n. \end{aligned}$$

After considerable manipulation, this can be rewritten as

$$\begin{aligned} \frac{d^2g(s)}{ds^2} = & \frac{2K(2-\gamma)s^{1-\gamma}}{|\mu|^3} \\ & \times \sum_{n=0}^{\infty} \left[\frac{n(2-\gamma) + (3-\gamma)}{(n+2)} \right] \frac{(-1)^n 1 \cdot 3 \cdots (2n+1)}{2^n n!} \\ & \times \left(\frac{4Ks^{2-\gamma}}{\mu^2} \right)^n. \end{aligned}$$

Thus the first term in Eq. (3.60) is given by

$$\begin{aligned} a \frac{d^2g(s)}{ds^2} e^{ag(s)} = & \frac{2Ka(2-\gamma)s^{1-\gamma}}{|\mu|^3} e^{ag(s)} \\ & \times \sum_{n=0}^{\infty} \left[\frac{n(2-\gamma) + (3-\gamma)}{(n+2)} \right] \\ & \times \frac{(-1)^n 1 \cdot 3 \cdots (2n+1)}{2^n n!} \left(\frac{4Ks^{2-\gamma}}{\mu^2} \right)^n. \end{aligned} \quad (3.61)$$

For $\gamma = 1$, the case of ordinary Brownian motion, from the above equation we obtain

$$a \frac{d^2 g(s)}{ds^2} e^{ag(s)} \Big|_{s=0} = \frac{\sigma^2 a}{|\mu|^3}. \quad (3.62)$$

Here we have also used the fact that $K = \sigma^2/2$ for $\gamma = 1$. On the other hand, for $1 < \gamma < 2$, as $s \rightarrow 0$, the prefactor multiplying the sum in Eq. (3.61) diverges, whereas the sum itself is finite and bounded away from zero. Consequently, for $1 < \gamma < 2$ the first term in Eq. (3.60) diverges as $s \rightarrow 0$.

Next we consider the second term in Eq. (3.60). We already know the limiting behavior of this term for $1 \leq \gamma < 2$, as $s \rightarrow 0$, from our earlier analysis for mean first passage time, namely,

$$\left(\frac{dg(s)}{ds} \right)^2 e^{ag(s)} \Big|_{s=0} = \frac{a^2}{\mu^2}. \quad (3.63)$$

Substituting the above results into Eq. (3.59), for $\gamma = 1$ we obtain

$$\langle T^2 \rangle = \frac{\sigma^2 a}{|\mu|^3} + \frac{a^2}{\mu^2}. \quad (3.64)$$

Therefore [cf. Eq. (3.58)],

$$\text{Var}(T) = \sigma^2 a / |\mu|^3 \quad (3.65)$$

for $\gamma = 1$. For $1 < \gamma < 2$, the first term in Eq. (3.60) diverges as $s \rightarrow 0$, whereas the second term is finite. Therefore, $\langle T^2 \rangle$ diverges. Hence the variance also diverges.

Next consider the case where the drift is away from the barrier. This implies that $\mu > 0$ in our formulation. Now the FPT density function can be written as in Eq. (3.52), where

$$g(s) = -\frac{|\mu|s^{\gamma-1}}{2K} - \frac{|\mu|s^{\gamma-1}}{2K} \sqrt{1 + \frac{4Ks^{2-\gamma}}{\mu^2}}. \quad (3.66)$$

Performing the same analysis as above, it is easily seen that the mean and variance diverge for $1 \leq \gamma < 2$.

For $\gamma = 1$, the Laplace transform of the first passage time density function reduces to [cf. Eq. (3.50)]

$$F(s) = \exp \left[-\frac{a}{2K} (\mu + \sqrt{\mu^2 + 4Ks}) \right]. \quad (3.67)$$

Now the inverse Laplace transform of $\exp(-\alpha\sqrt{s})$, $\alpha \geq 0$, is [13]

$$\frac{\alpha}{2\sqrt{\pi t^3}} \exp(-\alpha^2/4t). \quad (3.68)$$

Using this result, we can easily perform the inverse Laplace transform of Eq. (3.67), to obtain

$$f(t) = \frac{a}{\sqrt{4\pi K t^3}} \exp \left[-\frac{(a + \mu t)^2}{4Kt} \right], \quad a > 0, \quad t > 0. \quad (3.69)$$

We comment that, if the starting point of the diffusion is chosen at $x(0) = 0$, a negative μ will be used in the above

equation, and we recover the expected inverse Gaussian density [19] for the FPT density function of Brownian motion with drift.

C. Absorbing barriers at $x = -b$ and $x = a$

In this section, we consider the first passage time problem for Levy type anomalous diffusion with zero drift and absorbing barriers placed at $x = -b$ and $x = a$. We obtain an explicit solution for the first passage time density.

The FFPE to be solved is given in Eq. (3.4). The boundary and initial conditions become

$$W(-b, t) = W(a, t) = 0, \quad W(x, 0) = \delta(x). \quad (3.70)$$

We solve the FFPE using the method of separation of variables [21]. Let $W(x, t) = X(x)T(t)$. Substituting in Eq. (3.4), we obtain

$$X(x)T(t) - X(x) = {}_0D_t^{-\gamma} T(t) K X''(x), \quad (3.71)$$

where $X''(x)$ denotes the second derivative of $X(x)$ with respect to x . Separating out the variables and introducing the separation constant λ , we obtain

$$K X''(x) = \lambda X(x) \quad (3.72)$$

and

$$T(t) - 1 = \lambda {}_0D_t^{-\gamma} T(t). \quad (3.73)$$

The solution of Eq. (3.72), with the given boundary conditions is given by

$$X_n(x) = A_n \sin \left[\frac{n\pi(b+x)}{(a+b)} \right], \quad (3.74)$$

with

$$\lambda_n = -\frac{n^2 \pi^2}{(a+b)^2} K, \quad n = 1, 2, \dots \quad (3.75)$$

To solve Eq. (3.73), we take its Laplace transform to obtain (introducing the subscript n coming from λ_n)

$$T_n(s) - \frac{1}{s} = \frac{\lambda_n}{s^\gamma} T_n(s). \quad (3.76)$$

Here we have used the fact that the Laplace transform of ${}_0D_t^{-\gamma} T(t)$ is $T(s)/s^\gamma$. Solving for $T_n(s)$, we obtain

$$T_n(s) = \frac{1}{s - \lambda_n s^{1-\gamma}}. \quad (3.77)$$

Taking the inverse Laplace transform [22], we finally obtain

$$T_n(t) = E_\gamma \left[-\frac{n^2 \pi^2}{(a+b)^2} K t^\gamma \right], \quad (3.78)$$

where $E_\gamma(z)$ is the Mittag-Leffler function introduced earlier [cf. Eq. (3.8)].

Combining the solutions for space and time parts, we obtain

$$W(x,t) = \sum_{n=1}^{\infty} A_n \sin\left[\frac{n\pi(b+x)}{(a+b)}\right] E_{\gamma}\left[-\frac{n^2\pi^2}{(a+b)^2} Kt^{\gamma}\right]. \quad (3.79)$$

The coefficients A_n are determined by imposing the initial condition $W(x,0) = \delta(x)$. This gives us

$$A_n = \frac{2}{a+b} \sin\left[\frac{n\pi b}{(a+b)}\right]. \quad (3.80)$$

Hence

$$W(x,t) = \sum_{n=1}^{\infty} \frac{2}{a+b} \sin\left[\frac{n\pi b}{(a+b)}\right] \sin\left[\frac{n\pi(b+x)}{(a+b)}\right] \times E_{\gamma}\left[-\frac{n^2\pi^2}{(a+b)^2} Kt^{\gamma}\right]. \quad (3.81)$$

From Eq. (3.3), the FPT density function is given by

$$f(t) = -\frac{d}{dt} \int_{-b}^a dx W(x,t). \quad (3.82)$$

Substituting for $W(x,t)$ in this equation, we obtain

$$f(t) = -\frac{d}{dt} \left\{ 4 \sum_{n=0}^{\infty} \frac{1}{(2n+1)\pi} \sin\left[\frac{(2n+1)\pi b}{(a+b)}\right] \times E_{\gamma}\left[-\frac{(2n+1)^2\pi^2}{(a+b)^2} Kt^{\gamma}\right] \right\}. \quad (3.83)$$

Here we have used the fact that

$$\int_{-b}^a \sin\left[\frac{n\pi(b+x)}{(a+b)}\right] dx = \frac{2(a+b)}{n\pi} \quad \text{if } n \text{ is odd,} \\ = 0 \quad \text{if } n \text{ is even.}$$

To evaluate the derivative in Eq. (3.83), we write the Mittag-Leffler function in terms of the H function using Eq. (3.11):

$$f(t) = -\frac{4}{\pi} \sum_{n=0}^{\infty} \frac{1}{2n+1} \sin\left[\frac{(2n+1)\pi b}{(a+b)}\right] \frac{d}{dt} \times H_{1,2}^{1,1}\left(\frac{(2n+1)^2\pi^2}{(a+b)^2} Kt^{\gamma}\right) \begin{matrix} (0,1) \\ (0,1), (0,\gamma) \end{matrix}. \quad (3.84)$$

However [10]

$$\frac{d}{dt} H_{1,2}^{1,1}\left(\frac{(2n+1)^2\pi^2}{(a+b)^2} Kt^{\gamma}\right) \begin{matrix} (0,1) \\ (0,1), (0,\gamma) \end{matrix} \\ = \frac{1}{t} H_{2,3}^{1,2}\left(\frac{(2n+1)^2\pi^2}{(a+b)^2} Kt^{\gamma}\right) \begin{matrix} (0,\gamma), (0,1) \\ (0,1), (0,\gamma), (1,\gamma) \end{matrix} \\ = \frac{1}{t} H_{1,2}^{1,1}\left(\frac{(2n+1)^2\pi^2}{(a+b)^2} Kt^{\gamma}\right) \begin{matrix} (0,1) \\ (0,1), (1,\gamma) \end{matrix}.$$

In the last step, we have used properties 1 and 2 of H functions [cf. the Appendix]. From the series expansion of the H function given in Eq. (3.10), it can be shown after some manipulation that

$$H_{1,2}^{1,1}\left(z \begin{matrix} (0,1) \\ (0,1), (1,\gamma) \end{matrix}\right) = -z E_{\gamma,\gamma}(-z), \quad (3.85)$$

where $E_{\alpha,\beta}(z)$ is the generalized Mittag-Leffler function [22]

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\beta+k\alpha)}, \quad \alpha, \beta > 0. \quad (3.86)$$

Using this in the expression for $f(t)$, we obtain

$$f(t) = \frac{4\pi K t^{\gamma-1}}{(a+b)^2} \sum_{n=0}^{\infty} (2n+1) \sin\left[\frac{(2n+1)\pi b}{(a+b)}\right] \times E_{\gamma,\gamma}\left[-\frac{(2n+1)^2\pi^2}{(a+b)^2} Kt^{\gamma}\right]. \quad (3.87)$$

For a regular Brownian motion ($\gamma=1$), we obtain

$$f(t) = \frac{4\pi K}{(a+b)^2} \sum_{n=0}^{\infty} (2n+1) \sin\left[\frac{(2n+1)\pi b}{(a+b)}\right] \times \exp\left[-\frac{(2n+1)^2\pi^2}{(a+b)^2} Kt\right]. \quad (3.88)$$

IV. CONCLUSIONS

We studied the first passage time (FPT) problem for Levy type anomalous diffusion. We obtained the FPT distribution using the recently formulated fractional Fokker-Planck equation. We derived an explicit expression for the FPT distribution in terms of Fox or H functions when the diffusion has zero drift. The theoretical result was verified by numerically simulating the underlying continuous time random walk. When the drift is nonzero, we obtained an analytic expression for the Laplace transform of the FPT distribution. This was used to calculate the mean and variance of the FPT distribution. Finally, for the case of two absorbing barriers at finite distances from the origin, we expressed the FPT distribution in terms of a power series. In all of the above situations, the known results for ordinary diffusion (Brownian motion) were obtained as special cases of our more general results.

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APPENDIX: PROPERTIES OF H FUNCTIONS

The H function has the following remarkable properties [10] which we will use later.

Property 1. The H function is symmetric in the pairs $(a_1, A_1), \dots, (a_n, A_n)$, likewise $(a_{n+1}, A_{n+1}), \dots, (a_p, A_p)$; in $(b_1, B_1), \dots, (b_m, B_m)$ and in $(b_{m+1}, B_{m+1}), \dots, (b_q, B_q)$.

Property 2. Provided $n \geq 1$ and $q > m$,

$$\begin{aligned} H_{p,q}^{m,n} \left(z \left| \begin{matrix} (a_1, A_1), & (a_2, A_2), & \cdots, & (a_p, A_p) \\ (b_1, B_1), & \cdots, & (b_{q-1}, B_{q-1}), & (a_1, A_1) \end{matrix} \right. \right) \\ = H_{p-1,q-1}^{m,n-1} \left(z \left| \begin{matrix} (a_2, A_2), & \cdots, & (a_p, A_p) \\ (b_1, B_1), & \cdots, & (b_{q-1}, B_{q-1}) \end{matrix} \right. \right). \end{aligned} \quad (\text{A1})$$

Property 3. Provided $m \geq 2$ and $p > n$,

$$H_{p,q}^{m,n} \left(z \left| \begin{matrix} (a_1, A_1), & \cdots, & (a_{p-1}, A_{p-1}), & (b_1, B_1) \\ (b_1, B_1), & (b_2, B_2), & \cdots, & (b_q, B_q) \end{matrix} \right. \right)$$

$$= H_{p-1,q-1}^{m-1,n} \left(z \left| \begin{matrix} (a_1, A_1), & \cdots, & (a_{p-1}, A_{p-1}) \\ (b_2, B_2), & \cdots, & (b_q, B_q) \end{matrix} \right. \right). \quad (\text{A2})$$

Property 4.

$$H_{p,q}^{m,n} \left(z \left| \begin{matrix} (a_j, A_j)_{j=1, \dots, p} \\ (b_j, B_j)_{j=1, \dots, q} \end{matrix} \right. \right) = H_{q,p}^{n,m} \left(\frac{1}{z} \left| \begin{matrix} (1-b_j, B_j)_{j=1, \dots, q} \\ (1-a_j, A_j)_{j=1, \dots, p} \end{matrix} \right. \right). \quad (\text{A3})$$

Property 5. For $k > 0$,

$$\frac{1}{k} H_{p,q}^{m,n} \left(z \left| \begin{matrix} (a_j, A_j)_{j=1, \dots, p} \\ (b_j, B_j)_{j=1, \dots, q} \end{matrix} \right. \right) = H_{p,q}^{m,n} \left(z^k \left| \begin{matrix} (a_j, kA_j)_{j=1, \dots, p} \\ (b_j, kB_j)_{j=1, \dots, q} \end{matrix} \right. \right). \quad (\text{A4})$$

Property 6.

$$\begin{aligned} z^\rho H_{p,q}^{m,n} \left(z \left| \begin{matrix} (a_j, A_j)_{j=1, \dots, p} \\ (b_j, B_j)_{j=1, \dots, q} \end{matrix} \right. \right) \\ = H_{p,q}^{m,n} \left(z \left| \begin{matrix} (a_j + \rho A_j, A_j)_{j=1, \dots, p} \\ (b_j + \rho B_j, B_j)_{j=1, \dots, q} \end{matrix} \right. \right). \end{aligned} \quad (\text{A5})$$

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