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Some exact results for the trapping of subdiffusive particles in one dimension

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Abstract

We study a generalization of the standard trapping problem of random walk theory in which particles move *subdiffusively* on a one-dimensional lattice. We consider the cases in which the lattice is filled with a one-sided and a two-sided random distribution of static absorbing traps with concentration c. The survival probability $\Phi(t)$ that the random walker is not trapped by time t is obtained exactly in both versions of the problem through a fractional diffusion approach. Comparison with simulation results is made.
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1. Introduction

The trapping of Brownian particles by static traps randomly distributed over either a Euclidean or a disordered substrate is a fundamental problem of non-equilibrium statistical mechanics and chemistry with a very wide range of applications [1–5]. This is also one of the oldest problems in random walk theory which was essentially formulated by Smoluchowski at the beginning of past century in his theory of coagulation of colloidal particles [1–3,5]. This model has proven useful in research areas such as the trapping of mobile defects in crystals with point sinks [6–8], the kinetics of luminescent organic materials [7], the kinetics of photosynthetic light energy to oxygen conversion

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[9], anchoring of polymers by chemically active sites [10], atomic diffusion in glasslike materials [11], and others [12]. Some generalizations of the basic model have also been considered recently. The case of a gated (ungated) random walker trapped by a distribution of ungated (gated) fixed traps has been proposed in connection with the kinetics of reactions between complex molecules whose active groups are screened as the molecules diffuse [13]. The trapping problem with many random walkers has also been studied in one dimension [14] and the corresponding trapping statistics have been found on Euclidean and fractal lattices [15–17]. The multiparticle predator–prey problems in which a single fixed trap, the "lamb", is captured by one of a set of N random walkers or "lions" initially placed at a given distance from the prey was also discussed by Krapivsky and Redner [18,19]. Another quite interesting and difficult variation of the standard trapping problem is that where the particle diffuses in a sea of *diffusive* traps [5,20].

Trapping reactions between molecules embedded in biological samples and disordered materials are usually handicapped by the porous and statistical fractal structure of these media [4]. In some cases this gives rise to subdiffusion of the particles, i.e., the mean square displacement $\langle r^2(t)\rangle$ of the particles from the original starting site is no longer linear on time, but verifies a generalized Fick's second law:

$$\langle r^2(t)\rangle \approx \frac{2K_\gamma}{\Gamma(1+\gamma)}\, t^\gamma \,, \tag{1}$$

where γ (with $0<\gamma<1$) is the (anomalous) diffusion exponent and K_γ is the diffusion coefficient. Of course, there are many other instances in which subdiffusion processes appear [21–25]. A useful approach for understanding subdiffusion processes is by means of the continuous time random walk (CTRW) model in which the random walker performs jumps with a waiting time distribution with a broad long-time tail: $\psi(t) \sim t^{-(1+\gamma)}$ for large t [1–3,21,26,27]. The long-time tail of this waiting time distribution incorporates, in a statistical sense, the effect of the bottlenecks and the dead-ends in the diffusion of the random walker embedded in the disordered structure, and the model is compatible with Eq. (1). For subdiffusive random walkers the continuum description given by the ordinary diffusion equation is replaced by the fractional diffusion equation [27]

$$\frac{\partial}{\partial t}\, W(x,t) = K_\gamma {}_0D_t^{1-\gamma}\, \frac{\partial^2}{\partial x^2}\, W(x,t) \,, \tag{2}$$

where ${}_0D_t^{1-\gamma}$ is the Riemann–Liouville fractional derivative of order $1-\gamma$ [27–29],

$${}_0D_t^{1-\gamma} W(x,t) = \frac{1}{\Gamma(\gamma)}\, \frac{\partial}{\partial t} \int_0^t \mathrm{d}\tau\, \frac{W(x,\tau)}{(t-\tau)^{1-\gamma}} \tag{3}$$

and $W(x,t)$ is the probability density that the particle that started at 0 at time 0 is at x at time t.

Our objective in this paper is to find analytical expressions for the survival probability $\Phi(t)$ defined as the probability that no trap site has been reached by the *subdiffusive*

random walker by time t. Two variations of the classical trapping problem (sometimes called Rosenstock's trapping problem) are considered: (i) the "one-sided" trapping problem [14] in which only *one half-line* of a one-dimensional lattice is filled with a random distribution of static traps (this process could mimic the excitation or production of defects on one side of a fiber by irradiation, the other side being shielded); and (ii) the "two-sided" trapping problem corresponding to the trapping of a single subdiffusive random walker placed initially at $x=0$ between *two half-lines* ($x<0$ and $x>0$) randomly filled with static traps. We find exact analytical solutions for both problems and compare them with simulations. As precedents of these results we would cite the work of Blumen et al. (see Refs. [12,30,31] and references therein) about the trapping of particles on Euclidean and fractal substrates for random walkers with waiting time distributions with broad long-time tails: $\psi(t) \sim t^{-1-\gamma}$, $0<\gamma<1$. Another recent related work is that of Sung et al. [32] in which the nonclassical dynamics of reactions occurring in disordered media is studied by means of a theory based on the fractional diffusion equation.

The paper is organized as follows. In Section 2, the exact solution of the one-sided trapping problem is obtained and compared with simulation results. In Section 3, we build the extended Rosenstock's approximation for the survival probability of the particle in the one-sided trapping problem by calculating an exact expression for the moments of the one-sided span (the number of distinct sites visited by the random walker in a given direction). In Section 4, we obtain the exact survival probability of the subdiffusive random walker for the two-sided case in integral form. This integral is evaluated in the asymptotic long-time and short-time limits in order to get simple closed expressions. The paper ends with some conclusions and remarks in Section 5.

2. The one-sided trapping problem

In the one-sided trapping model quenched traps are randomly distributed on, say, the right-hand side of a one-dimensional lattice ($x>0$) with concentration c. The random walker is placed initially upon site $x=0$ and performs jumps to its nearest neighbor sites with a waiting time distribution $\psi(t)$ until it reaches a trap site where it is absorbed. The survival probability is given by [1]:

$$\Phi(t) = \sum_{r=1}^{t} \mathrm{e}^{-\lambda r} P(t|r) \,, \tag{4}$$

where $\lambda = -\ln(1-c)$ and $P(t|r)$ is the probability that the span of the random walker in the positive direction (the largest distance reached by the random walker for $x>0$) is equal to r after t time steps. Now let $\Gamma(t|r)$ be the probability that the site $x=r$ has not been visited by the random walker by time t (the so-called fixed-trap survival probability). Because [33]

$$P(t|r) = \frac{\mathrm{d}\Gamma(t|r)}{\mathrm{d}r} \,, \tag{5}$$

Eq. (4) takes the following form in the continuous limit:

$$\Phi(t) = \int_0^\infty \mathrm{e}^{-\lambda r} \frac{\mathrm{d}\Gamma(t|r)}{\mathrm{d}r}\,\mathrm{d}r\,, \tag{6}$$

or, integrating by parts,

$$\Phi(t) = \lambda \int_0^\infty \mathrm{e}^{-\lambda r}\Gamma(t|r)\,\mathrm{d}r\,, \tag{7}$$

because $\Gamma(t|0) = 0$, $\Gamma(t|\infty) = 1$ and $\mathrm{e}^{-\lambda r} \to 0$ as $r \to \infty$. For subdiffusive particles, the function $\Gamma(t|r)$ can be written in terms of Fox's H function [34]:

$$\Gamma(t|r) = 1 - H_{11}^{10}\left[\frac{r}{\sqrt{K_\gamma}t^{\gamma/2}}\,\middle|\,\begin{matrix}(1,\gamma/2)\\(0,1)\end{matrix}\right]\,. \tag{8}$$

The time Laplace transform of $\Gamma(t|r)$ is [35] [1]

$$\tilde{\Gamma}(s|r) = \frac{1}{s}\left[1 - \exp\left(-r\sqrt{s^\gamma}\right)\right]\,. \tag{9}$$

Then the Laplace transform of $\Phi(t)$ is readily calculated from Eqs. (7) and (9):

$$\tilde{\Phi}(s) = \frac{1}{s + \lambda\sqrt{K_\gamma}s^{1-\gamma/2}} \tag{10}$$

so that [36]

$$\Phi(t) = E_{\gamma/2}(-\xi)\,, \tag{11}$$

where $\xi \equiv \lambda\sqrt{K_\gamma t^\gamma}$ and $E_\alpha(z)$ is the Mittag–Leffler function with parameter α [36,28]. For $\gamma = 1$, the Mitagg–Leffler function becomes [27,28]:

$$\Phi(t) = \mathrm{e}^{\xi^2}\,\mathrm{erfc}(\xi)\,, \tag{12}$$

with $\xi = \lambda\sqrt{Dt}$, ($K_1 \equiv D$), and we recover the result for the survival probability of a normal diffusive random walker in the one-sided trapping problem [4]. For very long times, the asymptotic expansion of the Mittag–Leffler function [28] allows us to write

$$\Phi(t) = \sum_{k=1}^{n} \frac{(-1)^{k+1}}{\Gamma(1-k\gamma/2)}\,\xi^{-k} + \mathcal{O}(\xi^{-1-n})\,. \tag{13}$$

Thus, an asymptotic time regime is reached for $t \gg 1/(K_\gamma\lambda^2)^{1/\gamma}$, where the survival probability exhibits a power-law decay

$$\Phi(t) \approx \frac{1}{\Gamma(1-\gamma/2)}\,\frac{1}{\lambda\sqrt{K_\gamma t^\gamma}}\,. \tag{14}$$

This is an *algebraic* fluctuation slowdown corresponding to the Donsker–Varadhan limit [1,2,37]. We compare in Fig. 1 the exact survival probability for a subdiffusive

[1] Equation (9) can be obtained by other approaches: see (Ref. [35]).

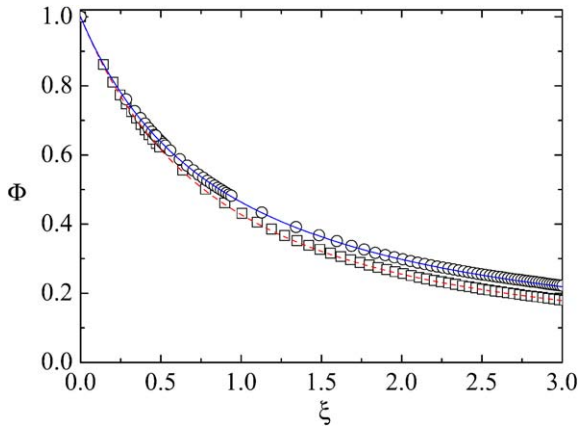

Fig. 1. Survival probability $\Phi(t)$ versus $\xi = \lambda\sqrt{K_\gamma t^\gamma}$. The circles are simulation results for subdiffusive walkers with $\gamma = \frac{1}{2}$. The squares are simulation results for normal diffusive walkers with $\psi(t) = \mathrm{e}^{-t}$. The lines are the corresponding exact results given by Eqs. (11) (solid line) and (12) (dashed line), respectively.

random walker with a waiting time distribution with the form of the Pareto law

$$\psi(t) = \frac{\gamma}{(1+t)^{1+\gamma}} \tag{15}$$

and $\gamma = \frac{1}{2}$. Taking the distance between nearest neighbor sites (jump length) as 1, the subdiffusion constant is $K_{1/2} = 1/[2\Gamma(\frac{1}{2})] = 1/\sqrt{4\pi}$. The concentration of traps used was $c = 0.01$.

3. The Rosenstock's approximation for the one-sided trapping problem

Let $S(t)$ be the number of distinct sites on the positive half-line visited up to time t by a random walker who started at $x = 0$ at time $t = 0$. Then, the survival probability of the random walker is given by $\Phi(t) = \langle (1-c)^{S(t)} \rangle = \langle \mathrm{e}^{-\lambda S(t)} \rangle$, the average being performed over all realizations of the random walker's exploration of the lattice from time 0 until time t. By means of the cumulant expansion technique [1,2] the following equivalent form (first expressed in this way by Zumofen and Blumen [38]) is derived:

$$\Phi(t) = \exp\left[\sum_{n=1}^{\infty} (-1)^n \frac{\kappa_n \lambda^n}{n!}\right], \tag{16}$$

where κ_n, $n = 1, 2, \ldots$ denote the cumulants of $S(t)$: $\kappa_1 = \langle S(t) \rangle$, $\kappa_2 = \langle S^2(t) \rangle - \langle S(t) \rangle^2 \equiv \sigma^2(t), \ldots$. If we keep the first $n+1$ terms of the sum in Eq. (16) we arrive at the nth-order Rosenstock approximation [1,2,30]. The error made by using this approximation is $\mathcal{O}(\kappa_{n+2}\lambda^{n+2})$. Thus, the condition $\kappa_{n+2} \ll 1/\lambda^{n+2}$ must be fulfilled for the nth-order Rosenstock approximation to be reasonable.

For the Rosenstock approximation to be useful for the subdiffusive case, it is necessary to know the cumulants or, equivalently, the moments of $S(t)$ for subdiffusive

particles. The next step is thus to derive exact expressions for the moments $\langle S^m(t)\rangle$, $m = 1, 2, \ldots$ of the one-sided span of a subdiffusive random walker, i.e., the territory explored in a given direction. The probability density of the one-sided span, $P(t|r)$, was given in Eq. (5) in terms of the survival probability. Hence

$$\langle S^m(t)\rangle = \int_0^\infty \frac{\mathrm{d}\Gamma(t|r)}{\mathrm{d}r}\, r^m\, \mathrm{d}r = -\int_0^\infty \frac{\mathrm{d}}{\mathrm{d}r}\,(1-\Gamma(t|r))r^m\, \mathrm{d}r \tag{17}$$

or, integrating by parts,

$$\langle S^m(t)\rangle = m\int_0^\infty [1-\Gamma(t|r)]r^{m-1}\, \mathrm{d}r\ , \tag{18}$$

where we have taken into account that $\Gamma(t|0) = 0$ and $\lim_{r\to\infty} r^m[1-\Gamma(t|r)] = 0$ as a consequence of the stretched exponential behavior of $1-\Gamma(t|r)$ as $r \to \infty$ for subdiffusive particles [34]. From Eq. (18) and the explicit expression of the survival probability in Eq. (8) we obtain

$$\langle S^m(t)\rangle = m s_m (K_\gamma t^\gamma)^{m/2}\ , \tag{19}$$

with

$$s_m = \int_0^\infty z^{m-1} H_{11}^{10}\left[z \left| \begin{matrix} (1, \frac{\gamma}{2}) \\ (0,1) \end{matrix} \right. \right] \mathrm{d}z\ . \tag{20}$$

In order to calculate the coefficients s_m, $m = 1, 2, \ldots$ we observe that the Laplace transform of the Fox H function appearing in the integrand in Eq. (20), $\tilde{H}(u)$, is a generating function of these coefficients

$$\tilde{H}(u) = \sum_{m=1}^{\infty} (-1)^{m-1} \frac{u^{m-1}}{(m-1)!}\, s_m\ . \tag{21}$$

Taking into account some properties of the Fox functions [39,40,27] we finally identify $\tilde{H}(u)$ with a two-parameter Mittag–Leffler function as follows:

$$\tilde{H}(u) = E_{\gamma/2, 1+\gamma/2}(-u)\ , \tag{22}$$

where, in the last identity, we have used the relation [27]

$$E_{\alpha\beta}(-u) = H_{12}^{11}\left[u \left| \begin{matrix} (0,1) \\ (0,1), (1-\beta, \alpha) \end{matrix} \right. \right] \tag{23}$$

between the two-parameter Mittag–Leffler functions and the Fox functions [27]. The function $E_{\alpha\beta}(u)$ admits the following series expansion [27,28]:

$$E_{\alpha\beta}(u) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \qquad \alpha > 0,\ \ \beta > 0\ . \tag{24}$$

From Eqs. (21), (22) and (24) we find

$$s_m = \frac{(m-1)!}{\Gamma(1+m\gamma/2)}, \quad m = 1, 2, \ldots , \tag{25}$$

so that from Eq. (19) we finally obtain

$$\langle S^m(t)\rangle = \frac{m!}{\Gamma(1+m\gamma/2)} (K_\gamma t^\gamma)^{m/2} . \tag{26}$$

Obviously, for $\gamma = 1$ we recover the exact result for the moments of the one-sided span of a diffusive random walker [14]:

$$\langle S^m(t)\rangle = \frac{\Gamma[(m+1)/2]}{\sqrt{\pi}} (4Dt)^{m/2} . \tag{27}$$

From Eq. (26) one can calculate the cumulants κ_n, $n = 1, 2, \ldots$ of the one-sided span distribution, and their direct substitution into Eq. (16) yields the general expression for the Rosenstock approximation for subdiffusive particles:

$$\Phi(t) = \exp\left\{\sum_{n=1}^{\infty} \frac{(-1)^n}{n!} a_n \xi^n\right\} . \tag{28}$$

The first three coefficients a_n are

$$\begin{aligned} a_1 &= \frac{1}{\Gamma(1+\gamma/2)} , \\ a_2 &= -\frac{1}{[\Gamma(1+\gamma/2)]^2} + \frac{2}{\Gamma(1+\gamma)} , \\ a_3 &= \frac{2}{[\Gamma(1+\gamma/2)]^3} - \frac{6}{\Gamma(1+\gamma/2)\Gamma(1+\gamma)} + \frac{6}{\Gamma(1+3\gamma/2)} . \end{aligned} \tag{29}$$

It is interesting to note that from Eqs. (11) and (28) we get the following identity:

$$\ln E_{\gamma/2}(\xi) = \sum_{n=1}^{\infty} \frac{a_n}{n!} \xi^n , \tag{30}$$

which provides a series expansion of the logarithm of the Mittag–Leffler function.

4. The two-sided trapping problem

In this section we calculate the exact survival probability of a single subdiffusive random walker placed initially between two half-lines populated with a random distribution of traps with concentration c. We will use parallel arguments to the standard ones for diffusive random walkers [2,41]. We must also mention that an alternative approach was proposed by Anlauf [42] to find the long-time behavior for the one-dimensional trapping problem with a diffusive particle.

As a starting point we evaluate the probability $W(x, t|x_0, t = 0)$ that a random walker starting from x_0 at $t = 0$ inside a box $0 \leqslant x \leqslant L$ with absorbing boundaries is at x at

time t. The function $W(x,t|x_0,t=0)$ satisfies the fractional partial differential equation (the subdiffusion equation):

$$\frac{\partial}{\partial t}\,W(x,t|x_0,0)=K_\gamma {}_0D_t^{1-\gamma}\,\frac{\partial^2}{\partial x^2}\,W(x,t|x_0,0)\,, \tag{31}$$

with the boundary conditions $W(0,t|x_0,0)=W(L,t|x_0,0)=0$, and the initial condition $W(x,0|x_0,0)=\delta(x-x_0)$ with $0<\gamma\leqslant 1$. Eq. (31) is straightforwardly solved by separation of variables [27]:

$$W(x,t|x_0,0)=\frac{2}{L}\sum_{n=1}^{\infty}\sin\left(\frac{n\pi x_0}{L}\right)\sin\left(\frac{n\pi x}{L}\right)E_\gamma\left(-K_\gamma\frac{n^2\pi^2}{L^2}\,t^\gamma\right)\,, \tag{32}$$

where we have taken into account that the solution of the fractional differential equation $\mathrm{d}T/\mathrm{d}t=-K_\gamma\lambda^2{}_0D_t^{1-\gamma}T$ is given by a Mittag–Leffler function $T(t)=E_\gamma(-K_\gamma\lambda^2t^\gamma)$. The survival probability of a subdiffusive random walker starting from $x_0\in(0,L)$ is given by $\int_0^L W(x,t|x_0,0)\,\mathrm{d}x$. Let $\Phi_L(t)$ be the survival probability of the random walker averaged over all configurations of traps which contain the origin inside a hole of length L. Then $\Phi_L(t)=\int_0^L\int_0^L W(x,t|x_0,0)\,\mathrm{d}x\,\mathrm{d}x_0$, and Eq. (32) yields

$$\Phi_L(t)=\frac{8}{\pi^2}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2}\,E_\gamma\left(-\frac{(2n+1)^2\pi^2}{L^2}\,\lambda^2K_\gamma t^\gamma\right)\,. \tag{33}$$

The survival probability of the subdiffusive random walker in the two-sided trapping problem is finally given by an average of $\Phi_L(t)$ over the distribution of hole lengths in the random trap configurations. This distribution is $\eta(L)=\lambda^2L\mathrm{e}^{-\lambda L}$ [2], and consequently we have

$$\begin{aligned}\Phi(t)&=\lambda^2\int_0^\infty L\mathrm{e}^{-\lambda L}\Phi_L(t)\,\mathrm{d}L\\&=\frac{8\lambda^2}{\pi^2}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2}\int_0^\infty L\mathrm{e}^{-\lambda L}E_\gamma\left(-\frac{\beta_n}{L^2}\right)\mathrm{d}L\end{aligned} \tag{34}$$

with $\beta_n=K_\gamma(2n+1)^2\pi^2t^\gamma$, $n=1,2,\ldots$. This is the exact integral representation of the survival probability of the subdiffusive particle in the two-sided trapping problem.

4.1. Long-time behavior of $\Phi(t)$

For $\gamma=1$ the Mittag-Leffler function reduces to an exponential and the integrals in Eq. (34) are estimated asymptotically for large times by means of the Laplace method [2]. However, this approach is not possible for $\gamma\neq 1$. In order to perform a long-time asymptotic evaluation of the integrals in Eq. (34), we use the following series expansion of the Mittag–Leffler function:

$$E_\gamma\left(-\frac{\beta_n}{L^2}\right)=\sum_{m=1}^{p}\frac{(-1)^{m+1}L^{2m}}{\beta_n^m\Gamma(1-\gamma m)}+O\left(\frac{L^2}{\beta_n}\right)^{1+p}\,, \tag{35}$$

which is valid for $\beta_n/L^2 \to \infty$ in the range $0<\gamma<2$ [28]. Inserting this series expansion into Eq. (34), integrating term by term, and after some rearrangements we find

$$\Phi(t) = \frac{2}{\pi^2}\sum_{m=1}^{p}\frac{(4-2^{-2m})\zeta(2m+2)\Gamma(2m+2)}{(-1)^{m+1}\Gamma(1-\gamma m)\pi^{2m}\xi^{2m}} + O(\xi^{-2p-2}) , \tag{36}$$

where we have taken into account that $\sum_{n=0}^{\infty} 1/(2n+1)^{2m+2} = (1-2^{-2m-2})\zeta(2m+2)$, $\zeta(s)$ being Riemann's zeta function. The dominant term is

$$\Phi(t) \sim \frac{1}{2\Gamma(1-\gamma)\lambda^2 K_\gamma}\, t^{-\gamma} , \tag{37}$$

which is valid for $\xi \gg 1$. Therefore we find an algebraic fluctuation slowdown of the survival probability corresponding to the Donsker–Varadhan [37] limit with an exponent two times greater than that of the one-sided long-time behavior in Eq. (14). The two-sided result $\Phi(t) \sim t^{-\gamma}$ is well known and has been interpreted as an "avoided crossing effect": trapping cannot be more efficient that the probability $\int_t^\infty \psi(t)\,\mathrm{d}t \sim t^{-\gamma}$ of remaining at the initial site (see Refs. [12,30,31] and references therein). However, note that this "avoided crossing effect" is absent for the one-sided trapping problem since the probability of trapping $\Phi(t) \sim t^{-\gamma/2}$ decays even more slowly than the probability of remaining at the initial site.

4.2. Short-time behavior of $\Phi(t)$

A simple analytical expression for the short-time behavior of $\Phi(t)$ can also be derived. To do so, we calculate the time derivative of $\Phi_L(t)$ in Eq. (33) obtaining

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\Phi_L(t) = -\frac{8}{L^2}\,K_{\gamma 0} D_t^{1-\gamma} J(\gamma) , \tag{38}$$

where we have taken into account that Mittag–Leffler functions are the solution of the fractional relaxation equation [27] and

$$J(\gamma) = \sum_{n=0}^{\infty} E_\gamma(-4a^2(n+1/2)^2) \tag{39}$$

with $a^2 = K_\gamma \pi^2 t^\gamma / L^2$. The major contribution to the sum defining $J(\gamma)$ in Eq. (39) when a is small comes from large n. Hence, to find the lowest-order term in the small-a behavior of $J(\gamma)$, we can approximate the sum by an integral:

$$J(\gamma) \sim \int_0^\infty E_\gamma[-4a^2x^2]\,\mathrm{d}x = \frac{1}{2a}\,\tilde{E}_\gamma(u=0) , \tag{40}$$

where $\tilde{E}_\gamma(u) = \int_0^\infty \mathrm{e}^{-uy} E_\gamma(y^2)\,\mathrm{d}y$ is the Laplace transform of $E_\gamma(y^2)$. To calculate $\tilde{E}_\gamma(u)$ we will exploit the relation between the Mittag–Leffler and the Fox H

functions [27,40]:

$$E_\gamma(-y^2) = \frac{1}{2} H_{12}^{11}\left[y \left| \begin{matrix} (0,1/2) \\ (0,1/2),(0,\gamma/2) \end{matrix} \right. \right] . \tag{41}$$

From Eq. (41) and the properties of Fox functions [39,40] we find

$$\tilde{E}_\gamma(s) = \frac{1}{2} H_{22}^{21}\left[s \left| \begin{matrix} (1/2,1/2),(1-\gamma/2,\gamma/2) \\ (0,1),(1/2,1/2) \end{matrix} \right. \right] . \tag{42}$$

Inserting the result in Eq. (42) into Eq. (40), we finally arrive at the following explicit expression for $J(\gamma)$:

$$J(\gamma) \sim \frac{1}{4a} \frac{\pi}{\Gamma(1-\gamma/2)} = \frac{1}{4\Gamma(1-\gamma/2)} \frac{L}{\sqrt{K_\gamma}} t^{-\gamma/2} , \tag{43}$$

where we have calculated the value of the Laplace transform for $s = 0$ by resorting to the general series expansion of Fox functions [27]. From Eqs. (38) and (43) we can also write

$$\frac{\mathrm{d}}{\mathrm{d}t} \Phi_L(t) \sim -\frac{2}{\Gamma(\gamma/2)} \frac{\sqrt{K_\gamma}}{L} t^{\gamma/2-1} , \tag{44}$$

where the fractional derivative has been performed according to the rule: ${}_0D_t^\nu t^\mu = \Gamma(1+\mu)t^{\mu-\nu}/\Gamma(1+\mu-\nu)$ which is valid for arbitrary real parameters μ and ν [27]. By integrating Eq. (44) with the initial condition $\Phi_L(t=0) = 1$ we find

$$\Phi_L(t) \sim 1 - \frac{4}{\gamma\Gamma(\gamma/2)} \frac{\sqrt{K_\gamma t^\gamma}}{L} , \tag{45}$$

and performing the average in Eq. (34) over trap configurations we finally obtain the short-time behavior of the survival probability of a subdiffusive random walker in the two-sided trapping problem

$$\Phi(t) \sim 1 - \frac{4\xi}{\gamma\Gamma(\gamma/2)} \tag{46}$$

or, for $\xi \ll 1$,

$$\Phi(t) \sim \exp\left(-\frac{2\xi}{\Gamma(1+\gamma/2)} \right) . \tag{47}$$

This expression is just the zeroth-order Rosenstock approximation $\Phi(t) = \exp[-\lambda \langle S_\leftrightarrow(t)\rangle]$ [see Eq. (16)] because the average two-sided span $\langle S_\leftrightarrow(t)\rangle$ is simply twice the average one-sided span $\langle S(t)\rangle$ and, by Eq. (26), $\langle S(t)\rangle = (K_\gamma t^\gamma)^{1/2}/\Gamma(1+\gamma/2)$. In Fig. 2 we compare simulation results for subdiffusive random walkers in the case $\gamma = \frac{1}{2}$ with the numerical integration of the exact integral representation of $\Phi(t)$ given by Eq. (34), the long-time behavior given in Eq. (36), and the Rosentock short-time behavior in Eq. (47).

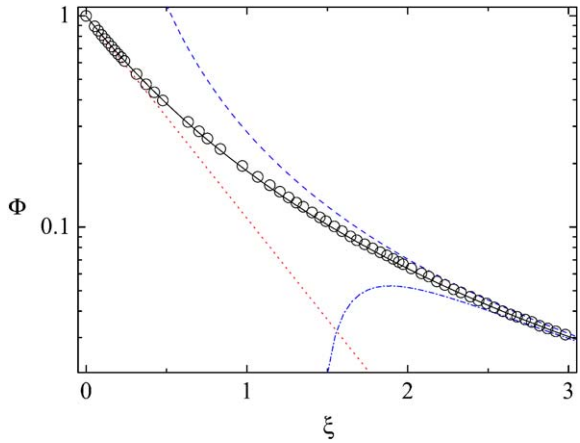

Fig. 2. Survival probability $\Phi(t)$ versus $\xi = \lambda\sqrt{K_\gamma t^\gamma}$ for subdiffusive random walkers with $\gamma = \frac{1}{2}$ for the two-sided trapping case. The symbols are simulation results for $c = 0.01$ and 5×10^4 trials. The solid line corresponds to the numerical integration of the exact expression (34). The dashed and dash–dotted line are the long-time behavior predictions obtained by keeping a single term and three terms in Eq. (36), respectively. The dotted line is the short-time behavior given by Eq. (47).

5. Conclusions and remarks

In this paper we considered the one-dimensional trapping problem for subdiffusive particles. In this problem a single subdiffusive random walker starting at $x = 0$ on a lattice randomly filled with absorbing static traps with a density c performs a random exploration until he encounters one of these traps. The quantity of main interest is the survival probability $\phi(t)$ of the particle. We have considered two versions of the problem: the one-sided case in which only one half-line is filled with traps, and the two-sided case corresponding to a random filling of both sides of the line $x > 0$ and $x < 0$. In the context of ordinary diffusive random walkers, this problem has a long tradition, and many applications to physics and chemistry have been discussed [1–4].

Great interest has also arisen recently around subdiffusive anomalous processes (for example, as a way of mimicking transport in disordered media), and a continuous fractional diffusion description has been put forward (see Ref. [27] and references therein). It thus seems convenient to extend the fruitful trapping model to the case of subdiffusive particles. We achieved this objective for the trapping of a single subdiffusive random walker in one dimension and, by means of the fractional diffusion formalism, exact analytical expressions were found in terms of the special functions characteristic of fractional calculus. There is a possibility for these results to be checked in diffusion experiments performed in constrained geometries and/or disordered materials [25]. From another point of view, the trapping problem could also be interpreted as a pseudo-first-order reaction of the form $A + T \to T$, where A is the random walker and T is the trap. There is also an increasing interest in reaction–subdiffusion processes [43,44], and our exact results apply to a special class of these processes.

The long-time behavior of the survival probability $\Phi(t)$ has been a subject of particular interest in the ordinary diffusive trapping problem [1,2,37,42]. In this regime an anomalous fluctuation slowdown, known as the Donsker–Varadhan limit, has been reported. In the one-sided and two-sided subdiffusive models we found the algebraic decays $\Phi(t) \sim t^{-\gamma/2}$ and $\Phi(t) \sim t^{-\gamma}$, respectively. For normal diffusive particles, the algebraic decay $\Phi(t) \sim t^{-1/2}$ was found in Ref. [14] for the one-sided trapping case and interpreted as due to the long explorations carried by the random walkers on the half-line free of traps [14]. A stretched exponential decay is the corresponding behavior for the long-time two-sided trapping of diffusive particles [42]. The two-sided subdiffusive result $\Phi(t) \sim t^{-\gamma}$ is well known and has been interpreted as an "avoided crossing effect" (see Refs. [12,30,31] and references therein). This effect is absent for the one-sided trapping problem since the probability of trapping $\Phi(t) \sim t^{-\gamma/2}$ for this case decays even more slowly than the probability of remaining at the initial site.

The present work can continue along several directions. First, the generalization of the subdiffusive trapping problem to the case of $N > 1$ independent subdiffusive random walkers could be analyzed as has already been done in the diffusive case [14]. Application of the same techniques to higher dimensional spaces is also an obvious approach, but we consider it unlikely to produce exact closed expressions for the relevant quantities. Trapping models of subdiffusive particles in which the trapping process is stochastically "gated" is also an interesting field. The effect of "gates" in diffusion-limited reactions has recently been considered in connection with reactions of complex molecules in biological media [13]. The chemically active groups of these molecules may be screened by the inactive parts, giving rise to effective reactivities described by Poisson processes. The media where these reactions takes place are usually disordered and reaction–subdiffusion models should provide a better description of these processes.

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