Target problem with evanescent subdiffusive traps

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We calculate the survival probability of a stationary target in one dimension surrounded by diffusive or subdiffusive traps of time-dependent density. The survival probability of a target in the presence of traps of constant density is known to go to zero as a stretched exponential whose specific power is determined by the exponent that characterizes the motion of the traps. A density of traps that grows in time always leads to an asymptotically vanishing survival probability. Trap evanescence leads to a survival probability of the target that may go to zero or to a finite value indicating a probability of eternal survival, depending on the way in which the traps disappear with time.

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I. INTRODUCTION

The traditional trapping problem involves diffusive (Brownian) particles (A) that wander in a medium doped with static traps (B) and disappear when they meet [1−4]. In the traditional target problem [5−7], on the other hand, one has static A particles and mobile traps. Both of these problems are described by the "reaction" A + B → B, but in one case the A’s move and the B’s stand still, while in the other the B’s move while the A’s are stationary. Both of these problems have a long and active history in the literature. They not only represent experimentally observable phenomena, but they have served as a testbed for theoretical and numerical studies and as a starting point for the formulation of models for more complex systems that have only recently been successfully solved analytically. For example, the survival probability of an A particle in a medium of B particles when both species are diffusive, first investigated numerically in the seminal work of Toussaint and Wilczek [8], was only partially solved analytically [9,10] until the recent full (asymptotic) solution in one dimension [11−14]. These results have also recently been generalized to subdiffusive species [15].

The survival probability of A particles in the reactions A+A → A and A+A → 0 in one dimension when A is mobile is also of relatively recent vintage in the history of such analytic solutions [4,16,17].

The purpose of this paper is to extend the one-dimensional target problem calculations for both diffusive and subdiffusive traps to the case of traps that themselves disappear in time according to some survival probability function of their own (e.g., exponential or power law). The decay of the moving traps with time of course increases the survival probability of the stationary target, and the interesting questions concern the interplay of the time dependences of the movement and decay of the traps. A related problem was considered in Ref. [18], where diffusive particles A and traps B and C undergoing the explicit reactions (a) A + B → B, B + C → C, and (b) A + B → B, B + C → 0 were considered using entirely different methods. Our methods are equally applicable to trap densities that increase with time, but this problem is less interesting because it necessarily leads to the eventual demise of the target.

A common characterization of the diffusive motion of a particle is through its mean square displacement for large t,

$$\langle x^2(t) \rangle = \frac{2K_x}{\Gamma(1 + \gamma)} t^\gamma. \quad (1)$$

Here \( K_x \) is the (generalized) diffusion constant, and \( \gamma \) is the exponent that characterizes normal (\( \gamma = 1 \)) or anomalous (\( \gamma \neq 1 \)) diffusion. In particular, the process is subdiffusive when \( 0 < \gamma < 1 \). Subdiffusive processes are ubiquitous in nature [19−24], and are particularly useful for understanding transport in complex systems [3,25].

The problem considered in this paper is a special case of a broad class of reaction-subdiffusion processes that have been studied over the past decades. One approach that has been used to study these processes is based on the continuous time random walk (CTRW) theory with waiting-time distributions between steps that have broad long-time tails and consequently infinite moments, \( \psi(t) \propto t^{\gamma-1} \) for \( t \to \infty \) with \( 0 < \gamma < 1 \). Another approach is based on the fractional diffusion equation, which describes the evolution of the probability density \( P(x,t) \) of finding the particle at position \( x \) at time \( t \) by means of the fractional partial differential equation (in one dimension) [7,19,26−29]

$$\frac{\partial}{\partial t} P(x,t) = K_\gamma \partial^{1-\gamma} \frac{\partial}{\partial x} P(x,t), \quad (2)$$

where \( \partial^{1-\gamma} \) is the Riemann-Liouville operator,

$$\partial^{1-\gamma} P(x,t) = \frac{1}{\Gamma(\gamma)} \frac{\partial}{\partial t} \int_0^t dt' P(x,t') \frac{t}{(t-t')^{1-\gamma}}. \quad (3)$$

In this paper we study the one-dimensional target problem for a static particle A subject to attack by diffusive or subdiffusive traps B that may die before reaching the target A [18]. For this purpose, we generalize the ideas of Bray and Blythe [11], and of our own work [15] based on a fractional diffusion equation approach. While recent work shows that a simple generalization of reaction-diffusion to reaction-subdiffusion equations in which the reaction and subdiffusion terms are assumed to enter additively is not valid in
some cases [30], this is not a difficulty in our particular application. The difficulties do not arise when the reaction process can be translated into a static boundary value problem, which is the case for the target (as well as the trapping) problem [28].

In some cases, asymptotic anomalous diffusion behavior can be found from corresponding results for normal diffusion via the simple replacement of $t$ by $t^\gamma$. This can be understood from a CTRW perspective because the average number of jumps $n$ made by a subdiffusive walker up to time $t$ scales as $\langle n \rangle \sim t^\gamma$ and, in many instances the number of jumps is the relevant factor that explains the behavior of the system. The simple replacement result is evidence of “subordination” (see Secs. 5 and 7.2 of Ref. [6]). However, there are other instances where the behavior of subdiffusive systems cannot be found in this way. A simple example is the survival probability of subdiffusive particles in the trapping problem (see Sec. 5 of Ref. [6]). In particular, for systems where competing processes (motion toward target and death) occur according to different temporal rules, such a replacement becomes ambiguous. This is the case for the problem considered here.

While our analytic results are based on the fractional diffusion equation formalism, our numerical simulations are based on a CTRW algorithm. These two renditions of the problem are expected to differ if trapping events are likely in a small number of steps, that is, if the initial density of traps is too high. On the other hand, if the initial trap density is too low, then the simulations to produce valid statistics would take inordinately long because trapping events are rare and because the system must be sufficiently large to include many particles. We note this as a caveat for our subsequent comparisons.

In Sec. II we present an integral equation for the survival probability, which we reduce to quadrature in Sec. III. The resulting integral is explicitly evaluated for exponentially decaying trap densities (including a stretched exponential decay), as well as for trap densities that decay as a power law. Not surprisingly, we find that a sufficiently rapid decay of the trap density leads to a finite asymptotic survival probability of the target. Comparisons of our results with numerical simulations are also shown in this section. A summary and some conclusions are presented in Sec. IV.

II. INTEGRAL EQUATION FOR THE SURVIVAL PROBABILITY

We consider a finite interval $L$ containing $N=pL$ mobile traps $B$ of constant density $\rho$ initially distributed at random, and a single immobile $A$ particle at the origin. Following the approach of Bray et al. [14] for diffusive traps and our generalization of this approach to the subdiffusive case [15], we write the survival probability of $A$ as $P(t) = \exp[-\mu_0(t)t]$, where $\mu_0(t)$ is to be determined. To find this function, one calculates in two ways the probability density to find a $B$ particle at the origin at time $t$,

$$\rho = \int_0^t dt^\gamma \mu_0(t') G(t-t').$$

(4)

That the left-hand side is this probability density is obvious. On the right-hand side one has the renewal theory expression

where $\mu_0(t')dt' = (-\dot{\rho}/\rho)dt'$ is the probability that a $B$ particle intersected $A$ in the time interval $(t', t'+dt')$ for the first time, and the propagator $G(t-t')$ is the probability density for this particular $B$ to be at the origin at time $t$. In one dimension it is given by [31,32]

$$G(t) = \frac{1}{\sqrt{4\pi K^\gamma t^\gamma}} H_{1,2}^{2,0} \left[ 0 \left( 1 - \frac{\gamma}{2}, \frac{\gamma}{2} \right), \left( 0, 1/(2, 1) \right) \right] = \frac{1}{\sqrt{4\pi K^\gamma t^\gamma}} \left( 1 - \frac{\gamma}{2} \right)^{1/2},$$

(5)

where $H_{1,2}^{2,0}$ is Fox’s $H$ function, whose value at the given arguments we have used to write the last equality. This formulation assumes that the initial random distribution of traps remains random (Poisson) at all times for both diffusion and subdiffusion. [This is easily established by noting that the integration of the distribution $P(x,t)$ over all the initial positions of the traps is independent of $x$ and of $t$, i.e., it remains uniform for all time.] In a different context than the target problem, Bray et al. [14] generalized their approach to a time-dependent density $\rho(t)$ of $B$. They argue that in place of Eq. (4) one now has

$$\rho(t) = \int_0^t dt' \frac{\rho(t)}{\rho(t')} \mu_0 G(t-t'),$$

(6)

that is,

$$1 = \int_0^t dt' \frac{\mu_0(t')}{\rho(t')} G(t-t').$$

(7)

This is the basic equation to be considered in this paper.

III. THE SURVIVAL PROBABILITY

To calculate the survival probability of particle $A$, we rewrite Eq. (7) explicitly as

$$\sqrt{4K^\gamma} = \frac{1}{\Gamma(1-\gamma/2)} \int_0^t dt' \frac{\Omega(t')}{(t-t')^{\gamma/2}},$$

(8)

where we have multiplied both sides by $\sqrt{4K^\gamma}$, and where we have introduced

$$\Omega(t) = \frac{\mu_0(t)}{\rho(t)}.$$  

(9)

Equation (8) is an equation of Abel of the first kind [33–35],

$$f(t) = \frac{1}{\Gamma(1-\gamma/2)} \int_0^t dt' \frac{\Omega(t')}{(t-t')^{\gamma/2}},$$

(10)

with $f(t) = \sqrt{4K^\gamma}$. The solution of this classic equation is well known [see Sec. 12 in Ref. [33] or Eqs. (2.5a) and (2.5b) in Ref. [34]],

$$\Omega(t) = eD^{1-\gamma/2}_t f(t) = \frac{1}{\Gamma(\gamma/2)} \int_0^t dt' \left( \frac{f(t')}{(t-t')^{1-\gamma/2}} + f(0) \right) \left( \frac{t'}{(t-t')^{\gamma/2}} \right).$$  

(11)

Here, as earlier, $eD^{1-\gamma/2}_t$ is the Riemann-Liouville fractional derivative. In our case $f(t) = \sqrt{4K^\gamma}$ is constant, so that
It then follows that

$$
\mu_0(t) = \frac{\sqrt{4 K_\gamma}}{\Gamma(\gamma/2)} \int_0^t dz \rho(z) z^{\gamma/2 - 1},
$$

(13)

which provides a general solution to our problem for any \( \rho(t) \). While Eq. (13) applies to trap densities that grow or that decrease or even oscillate in time, the case of evanescent traps is the more interesting and the one we choose to focus on.

As a reminder, we note that for traps of a constant density \( \rho(t) = \rho_0 \) the survival probability is given by

$$
P(t) = \exp\left(-\frac{\sqrt{4 K_\gamma} \rho_0 t^{\gamma/2}}{\Gamma(1 + \gamma/2)}\right).
$$

(14)

As a benchmark, we show in Fig. 1 a typical comparison of this result with simulation results. The agreement is clearly good, although a lower initial density run for a longer time would lead to even better agreement.

### A. Exponentially decaying trap density

Suppose that the traps have a finite lifetime \( \tau \) and decay exponentially, as in a unimolecular reaction, \( \rho(t) = \rho_0 \exp(-t/\tau) \). The integral in Eq. (13) immediately leads to the solution

$$
\mu_0(t) = \ell_\gamma \rho_0 \left( 1 - \frac{\Gamma(\gamma/2, t/\tau)}{\Gamma(\gamma/2)} \right),
$$

(15)

where \( \Gamma(b,x) \) is an incomplete gamma function, and

$$
\ell_\gamma = (4 K_\gamma \tau^2)^{1/2}.
$$

(16)

When \( \gamma = 1 \), i.e., when the traps are diffusive, this reduces to

$$
\mu_0(t) = \ell_1 \rho_0 \erf\left(\sqrt{t/\tau}\right).
$$

(17)

For arbitrary \( \gamma < 1 \), the survival probability of the target in the presence of the subdiffusive traps with finite lifetime thus is

$$
P(t) = \exp\left[-\ell_\gamma \rho_0 \left( 1 - \frac{\Gamma(\gamma/2, t/\tau)}{\Gamma(\gamma/2)} \right)\right].
$$

(18)

The interesting result here is that the function \( \mu_0(t) \) goes to the constant \( \mu_0(\infty) = \ell_\gamma \rho_0 \) and not to infinity as \( t \to \infty \). Therefore the survival probability does not vanish with increasing time,

$$
P(t) \to \exp\left[-\ell_\gamma \rho_0 \left( 1 - \frac{e^{-t/\tau}}{\Gamma(\gamma/2)(t/\tau)^{1-\gamma/2}} \right)\right].
$$

(19)

We note that \( \ell_\gamma \) is a characteristic distance that measures the root mean square displacement of the traps during their decay time \( \tau \). Therefore \( \mu_0(\infty) = \ell_\gamma \rho_0 \) is the ratio of this average displacement to the average initial distance \( \rho_0^{-1} \) between traps. This finite asymptotic survival probability reflects the fact that if the traps disappear sufficiently rapidly (which they do if they disappear exponentially while the traps move diffusively or subdiffusively), then many traps disappear before they can reach the particle, and there is a finite probability that the particle remains forever “safe.”

The next two figures show the comparison of simulation results with our analytic outcome. First, in Fig. 2 we illustrate our earlier caveat, that agreement cannot be expected if the initial density of traps is too high and the extinction rate of the traps is large, and that the agreement improves with lower initial density. The disagreement is clear and can be traced exactly to the early time trapping events that cumulatively affect the survival probability. Figure 3 shows typical
An interesting interplay of values are...
Analytic and simulation results for this case are shown in FIG. 4. (Color online) $\mu_0(t)=-\ln P(t)$ vs $t$ for power law evanescent traps with $\beta > \gamma/2$ (case 1). Parameter values are $\gamma=0.75$, $\beta=0.8$, $\rho_0=0.01$, $\tau=10^6$, and $K_\gamma=1/(2\sqrt{\pi})$. Asymptotic value, $\mu_0(\infty)=\ell_3 \rho_0 = 2.36549$. Solid line, Eq. (23). Symbols, simulation results.

$$\mu_0(t) \rightarrow \frac{\ell_3 \rho_0}{(\gamma/2 - \beta) \Gamma(\gamma/2)} \left( \frac{t}{\tau} \right)^{\gamma/2 - \beta} + \cdots.$$  \hspace{1cm} (29)

The survival probability vanishes at long times as a stretched exponential,

$$P(t) \rightarrow \exp \left( -\frac{\ell_3 \rho_0}{(\gamma/2 - \beta) \Gamma(\gamma/2)} (t/\tau)^{\gamma/2 - \beta} \right). \hspace{1cm} (30)$$

Analytic and simulation results for this case are shown in Fig. 5.

Case 3. $\beta=\gamma/2$. This is the marginal case, and the incomplete beta function (24) can be rewritten as a hypergeometric function,

$$P(t) \rightarrow \exp \left( -\frac{\ell_3 \rho_0}{(\gamma/2 - \beta) \Gamma(\gamma/2)} (t/\tau)^{\gamma/2 - \beta} \right).$$  \hspace{1cm} (31)

The survival probability thus decays as an inverse power,

$$P(t) \rightarrow (t/\tau)^{-\ell_3 \rho_0 / \Gamma(\gamma/2)}. \hspace{1cm} (32)$$

Results for the marginal case are shown in Fig. 6.

### IV. CONCLUSIONS

We have calculated the survival probability of a stationary target in a one-dimensional system in which diffusive or subdiffusive traps that eliminate the target upon encounter themselves disappear according to a survival probability. The root mean square displacement of the traps grows with time as $t^{\gamma/2}$, that is, diffusively when $\gamma=1$ and subdiffusively when $\gamma<1$. The survival probability of the target depends sensitively on the interplay of two temporal events, namely, the motion of the traps as characterized by the exponent $\gamma$ and their disappearance. When the motion of the traps is diffusive or subdiffusive and the traps do not decay in time, the survival probability goes to zero as a stretched exponential, Eq. (14). When the traps undergo exponential decay or stretched exponential decay, the target has an asymptotic safety margin, that is, a finite probability of surviving forever, cf. Eqs. (19) and (21). When the traps are diffusive or subdiffusive and disappear according to a power law survival probability $\sim t^\beta$, the survival of the target depends sensitively on the relation between $\gamma$ and $\beta$. If the traps move sufficiently rapidly relative to their disappearance, that is, if $\gamma/2 > \beta$, the target is trapped with certainty at long times, its survival probability going to zero again as a stretched exponential, cf. Eq. (30). If the traps move slowly, $\gamma/2 < \beta$, then the target has a chance of eternal survival, cf. Eq. (28). At the critical relation $\gamma/2 = \beta$ the survival probability goes to zero as an inverse power of time, cf. Eq. (32). In fact the trap
density increases with time, the survival probability of the target necessarily vanishes asymptotically.

In this paper we have calculated the survival probability of a target particle in the presence of evanescent subdiffusive traps of given time-dependent density. We could equally consider the inverse problem, namely, that of finding the time dependence of the density of traps to obtain a particular survival probability function. For this purpose we need only “invert” Eq. (12),

$$\rho(t) = -\frac{\Gamma(\gamma/2)}{4K^2} t^{1-\gamma/2} P(t).$$

An exponentially decaying survival probability of the form $P(t) = e^{-t^\beta}$ requires a density that decays as $\rho(t) \sim t^{1-\gamma/2}$. This is included in and consistent with case 2 in Sec. III B with $\gamma/2 - \beta = 1$. Similarly, for an inverse power decay of the form $P(t) \sim (t/\tau)^{-r}$ we require that $\rho(t) \sim t^{\gamma/2}$, which is consistent with case 3 in the same section.

This work has focused on the survival probability of a stationary target. The survival probability of a moving target, diffusive or subdiffusive, surrounded by nonevanescent diffusive or subdiffusive traps has been considered recently in a number of papers [11,15]. Extension of our work with evanescent traps to the case of a diffusive or subdiffusive target is in progress [38].

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