

Trapping reactions with subdiffusive traps and particles

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ABSTRACT

Reaction dynamics involving subdiffusive species is an interesting topic with only few known results, especially when the motion of different species is characterized by different anomalous diffusion exponents. Here we study the reaction dynamics of a (sub)diffusive particle surrounded by a sea of (sub)diffusive traps in one dimension. Under some reasonable assumptions we find rigorous results for the asymptotic survival probability of the particle in most cases, but have not succeeded in doing so for a particle that diffuses normally while the anomalous diffusion exponent of the traps is smaller than $2/3$.

Keywords: Subdiffusion, diffusion, reactions, mobile traps, survival probability

1. INTRODUCTION

In the traditional version of the trapping problem, a normal diffusive (Brownian) particle (A) wanders in a medium doped at random with *static* traps (B), and disappears when they meet, $A + B \rightarrow B$. The quantity of interest is the survival probability $P(t)$ of the particle A . This problem dates back to Smoluchowski's theory of reaction rates at the beginning of last century, and is one of the most widely investigated and applied problems of non-equilibrium statistical mechanics.¹⁻⁶ An important variation of the basic trapping problem, in which a diffusive particle wanders in a medium in which the traps are also *diffusive*, has been the subject of intense research since the seminal work of Toussaint and Wilczek.⁷

The principal quantity of interest in the trapping problem is the survival probability $P(t)$ of the A particles. From this survival probability one is able to calculate essentially all other quantities of practical interest. Yet this probability is usually difficult to calculate, and the few instances in which it has been obtained are considered landmark contributions. In 1988, Bramson and Lebowitz^{8,9} proved rigorously that the long-time survival probability $P(t)$ of a particle diffusing in a one-dimensional medium doped with diffusive traps decays as $P(t) \sim \exp(-\lambda t^{1/2})$, λ being an undetermined parameter. The evaluation of this constant proved elusive for many years, engendering much confusion and proposed solutions that were mutually contradictory. Finally, quite recently Bray and Blythe^{10,11} proved in a simple and elegant way, assuming the so-called "Pascal principle," that the survival probability $P(t)$ of a diffusing particle with diffusion coefficient D' in a d -dimensional medium with $d \leq 2$ in which the traps are also diffusive with diffusion coefficient D is *independent* of D' for long times, and coincides with the survival probability of an immobile target ($D' = 0$) in the presence of a density ρ of diffusive traps. In particular, in a one-dimensional medium $P(t) \sim \exp(-4\rho(Dt/\pi)^{1/2})$. Bray and Blythe obtained their results by calculating an upper and a lower bound for the survival probability that converge to one another asymptotically. Some (but not all) of the bounding results of Bray and Blythe have been extended by Oshanin et al.¹² to systems where the traps perform a compact exploration of the space, i. e., where the fractal dimension d_w of the trajectories of the traps is greater than the dimension d of the space.

The purpose of this work is to extend the procedure and results of Bray and Blythe,^{10,11} which are valid for a Brownian diffusive particle and Brownian diffusive traps, to situations in which the particle and traps exhibit

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anomalous diffusion, in particular, subdiffusion. The usual characterization of anomalous diffusion of a particle is through its mean squared displacement $x(t)$ for large t :

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

Here K_γ is the (generalized) diffusion constant and γ is the (anomalous) diffusion exponent. Ordinary Brownian diffusion ($\gamma = 1$, $K_1 \equiv D$) follows Fick's second law, $\langle x^2(t) \rangle \propto t$. The process is called subdiffusive when $0 < \gamma < 1$. Subdiffusive processes are ubiquitous in nature,¹³⁻²¹ and are particularly useful for understanding transport in complex systems.^{5, 22-24}

Two main approaches have been used to study subdiffusive processes. The older 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, $\psi(t) \sim t^{-1-\gamma}$ for $t \rightarrow \infty$ 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)^{13, 25}

$$\frac{\partial}{\partial t} P(x, t) = K_\gamma {}_0 D_t^{1-\gamma} \frac{\partial^2}{\partial x^2} P(x, t) \quad (2)$$

where K_γ is the generalized diffusion coefficient that appears in Eq. (1) and ${}_0 D_t^{1-\gamma}$ is the Riemann-Liouville operator,

$${}_0 D_t^{1-\gamma} P(x, t) = \frac{1}{\Gamma(\gamma)} \frac{\partial}{\partial t} \int_0^t d\tau \frac{P(x, \tau)}{(t-\tau)^{1-\gamma}}. \quad (3)$$

Here we implement the latter approach to study the one-dimensional trapping problem in the long-time regime for subdiffusive (or diffusive) particles that move among a distribution of *non-static* traps. The traps can be either subdiffusive or (Brownian) diffusive. For this purpose, we generalize the ideas of Bray and Blythe.^{10, 11}

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 using one or the other of the established formalisms. Using the CTRW formalism, Blumen et al.²⁶⁻²⁸ considered a variety of reactions including the trapping problem $A + T(\text{static}) \rightarrow T(\text{static})$, the target problem $A(\text{static}) + T \rightarrow T$, and the bimolecular reactions $A + A \rightarrow \emptyset$ and $A + B \rightarrow \emptyset$. The moving particles were modeled as continuous-time random walkers with long-tailed waiting-time densities. Quite recently, Sung and Silbey²⁹ have used the CTRW model to study the dynamics of particles that react at a boundary. A CTRW approach has also been applied by Seki et al.³⁰ to study the kinetics of the recombination reaction in subdiffusive media. However, Seki et al. went further and, from the CTRW model, derived a fractional reaction-diffusion equation for the geminate recombination problem. Sung et al.³¹ directly addressed this problem from a fractional diffusion equation approach, but some of their assumptions and results disagree with those of Seki et al. The fractional diffusion approach has recently been used to get exact solutions for two types of one-dimensional trapping problems: the so called one-sided problem, in which all the traps lie on one side of the particle, and the two-sided problem, in which the traps are located on both sides of the particle (this is the traditional or standard version of the trapping problem).³² These recent articles^{29, 32} share the simplifying characteristic that the reaction takes place between a static particle (or fixed boundary) and a subdiffusive particle. The present paper differs from these in that all the reacting particles (including traps) are (sub)diffusive and, moreover, the diffusion constant and the anomalous diffusion exponent of each species may be different. The fractional-diffusion approach has already been employed to study bimolecular reactions between subdiffusive particles. In particular, the annihilation $A + A \rightarrow \emptyset$ and coagulation $A + A \rightarrow A$ of subdiffusive particles was studied^{33, 34} by means of a fractional generalization of the interparticle distribution function method.⁶ The evolution of reaction-subdiffusion fronts for $A + B \rightarrow C$ reactions, where both A and B move subdiffusively, is also amenable to analysis by means of the fractional diffusion approach.³⁵ Other recent work on fractional diffusion and CTRW models of subdiffusive reacting particles can be found in a number of references.³⁶⁻³⁹

In some cases, asymptotic anomalous diffusion behavior can be found from corresponding results for normal diffusion with the simple replacement of t by t^γ wherever t appears. 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”.²⁸ Examples of this phenomenon are given in Secs. 5 and 7.2 of the preceding reference. 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 the preceding reference. In particular, for systems where each species has a different anomalous diffusion exponent, such a replacement becomes ambiguous. This is the case for the problem considered here.

Bray and Blythe obtained the asymptotic survival probability of a diffusing particle in a sea of diffusing traps by calculating an upper and lower bound that converge asymptotically. We follow their procedure for subdiffusive particle and traps, with partial success. While it is possible to obtain convergent bounds in most anomalous diffusion exponent regimes, this procedure does not work in all regimes. In particular, the bounding procedure encounters difficulties when the particle A diffuses normally and the traps are “too slow.” In Sec. 2 we calculate the upper bound of the survival probability, and in Sec. 3 the lower bound. The survival probability is established, when possible, in Sec. 4. Section 5 and the Appendix presents a compendary of results and some comments on open problems.

2. UPPER BOUND FOR THE SURVIVAL PROBABILITY

The “Pascal principle” of random walks says that the best survival strategy for a random walker A surrounded by a sea of trapping random walkers B is to stand still. This assumption was adopted in one dimension by Bray and Blythe,^{10,11} and proved by Bray, Majumdar and Blythe⁴⁰ for $d \leq 2$. Almost simultaneously, Moreau et al.⁴¹ proved the Pascal principle for a rather general class of random walks on d -dimensional lattices. Although the case in which both particle and traps perform subdiffusive random walks was not considered, the Pascal principle is an intuitively plausible (and most likely provable) result for this case as well, and we will simply assume that it is applicable.

The Pascal principle thus says that the survival probability $P_U(t)$ of a static particle A surrounded by a random (Poisson) distribution of randomly walking traps (the “target problem”) is an upper bound for the survival probability $P(t)$ of a (sub)diffusing particle A . We proceed to calculate this upper bound for the subdiffusive target problem. This problem has been considered²⁸ by means of the CTRW model and, for the three-dimensional case³¹ by means of a fractional diffusion approach. Here we calculate $P_U(t)$ by generalizing the approach of Bray and Blythe^{10,11} to the subdiffusive case.

Consider a target of size $2L$ centered at the origin, and let $Q_1(t|y)$ be the probability that the trap initially placed at $y > L$ has not reached the target A at $y = L$ by time t . Then,⁴² in terms of the Fox’s H function,

$$Q_1(t|y) = 1 - H_{11}^{10} \left[\frac{y-L}{\sqrt{K_\gamma t^\gamma}} \middle| \begin{matrix} (1, \gamma/2) \\ (0, 1) \end{matrix} \right] \equiv 1 - H \left[\frac{y-L}{\sqrt{K_\gamma t^\gamma}} \right]. \quad (4)$$

For $\gamma \rightarrow 1$ the Fox’s H function becomes the complementary error function (we set $K_1 \equiv D$), and the ordinary Brownian motion result is recovered,

$$Q_1(t|y) = 1 - \operatorname{erfc} \left(\frac{y-L}{\sqrt{4Dt}} \right), \quad \gamma = 1. \quad (5)$$

Next consider N independently diffusing traps that, at $t = 0$, are placed at random in the interval $L \leq y \leq L+R$. Here and henceforth $2R$ is the size of the system, which we will take to infinity at appropriate points in the calculations. The probability $Q_N(t)$ that the stationary target A has survived up to time t is

$$Q_N(t) = \prod_{i=1}^N \frac{1}{R} \int_L^{L+R} dy_i \left\{ 1 - H \left[\frac{y_i-L}{\sqrt{K_\gamma t^\gamma}} \right] \right\} = \left\{ 1 - \frac{1}{R} \int_L^{L+R} dy H \left[\frac{y-L}{\sqrt{K_\gamma t^\gamma}} \right] \right\}^N, \quad (6)$$

or, in terms of the density $\rho = N/R$ of traps,

$$Q_\infty(t) = \lim_{R \rightarrow \infty} \left\{ 1 - \frac{1}{R} \int_L^{L+R} dy H \left[\frac{y}{\sqrt{K_\gamma t^\gamma}} \right] \right\}^{\rho R} = \exp \left\{ -\rho \sqrt{K_\gamma t^\gamma} \int_0^\infty dz H[z] \right\}. \quad (7)$$

We need to evaluate the integral

$$I_\gamma = \int_0^\infty dz H_{11}^{10} \left[z \left| \begin{matrix} (1, \gamma/2) \\ (0, 1) \end{matrix} \right. \right], \quad (8)$$

which can be done from the properties of the Fox's H function.⁴³ One finds that

$$H_{11}^{10} \left[z \left| \begin{matrix} (1, \gamma/2) \\ (0, 1) \end{matrix} \right. \right] = \frac{d}{dz} H_{11}^{10} \left[z \left| \begin{matrix} (1 + \gamma/2, \gamma/2) \\ (0, 1) \end{matrix} \right. \right]. \quad (9)$$

But

$$H_{11}^{10} \left[\infty \left| \begin{matrix} (1 + \gamma/2, \gamma/2) \\ (0, 1) \end{matrix} \right. \right] = 0 \quad (10)$$

and

$$H_{11}^{10} \left[0 \left| \begin{matrix} (1 + \gamma/2, \gamma/2) \\ (0, 1) \end{matrix} \right. \right] = \frac{1}{\Gamma(1 + \gamma/2)}, \quad (11)$$

so that

$$I_\gamma = \frac{1}{\Gamma(1 + \gamma/2)}. \quad (12)$$

Therefore,

$$Q_\infty(t) = \exp \left[-\frac{\sqrt{\rho^2 K_\gamma t^\gamma}}{\Gamma(1 + \gamma/2)} \right]. \quad (13)$$

This is the survival probability of the target when all the traps are located to its right. When the traps are located on both sides of the target, the survival probability of the target is the square of Eq. (13):

$$P_U(t) = Q_\infty^2(t) = \exp \left[-\frac{2\sqrt{\rho^2 K_\gamma t^\gamma}}{\Gamma(1 + \gamma/2)} \right]. \quad (14)$$

This is the *upper bound* on the survival probability of the moving particle.

Incidentally, as is well known, the survival probability for the target problem is related to the distinct number of sites $S(t)$ visited by a trap up to time t :^{28, 44}

$$P_U(t) = e^{-\rho \langle S(t) \rangle}. \quad (15)$$

Comparing this expression with Eq. (14), one finds that the average value $\langle S(t) \rangle$ of the territory explored up to time t by a subdiffusive walker with generalized diffusion coefficient K_γ and anomalous diffusion exponent γ is

$$\langle S(t) \rangle \sim \frac{2\sqrt{K_\gamma t^\gamma}}{\Gamma(1 + \gamma/2)}. \quad (16)$$

This result agrees with that found by Yuste and Acedo³² using a different approach.

3. LOWER BOUND FOR THE SURVIVAL PROBABILITY

Let $P_L(t)$ be the probability that the particle A (which is now allowed to move) remains inside a box of size L and that all the traps remain outside this box until time t . When this happens, the particle A survives. It is clear that $P_L(t)$ is a lower bound for the survival probability $P(t)$ of interest here because there exist many other ways in which the particle A may survive. The probability $P_L(t)$ is itself the product of three probabilities:

1. The probability Q_1 that at $t = 0$ the box of size L contains no traps:

$$Q_1 = e^{-\rho L}. \quad (17)$$

2. The probability Q_2 that no traps enter the box of size L up to time t :

$$Q_2 = \exp \left[-\frac{2}{\Gamma(1 + \gamma/2)} \sqrt{\rho^2 K_\gamma t^\gamma} \right] = P_U(t). \quad (18)$$

3. The probability Q_3 that the particle has not left the box of size L up to time t . We proceed to evaluate this quantity.

Let $W(x, t)$ be the probability of finding the particle A at position x at time t if it was at position $x = 0$ at time $t = 0$ and there are absorbing boundaries at $x = -L/2$ and $x = L/2$. Solving the fractional diffusion equation by means of separation of variables¹³ one finds

$$W(x, t) = \frac{2}{L} \sum_{n=0}^{\infty} (-1)^n \sin \frac{(2n+1)\pi(x+L/2)}{L} E_{\gamma'} \left(-K'_{\gamma'} (2n+1)^2 \pi^2 t^{\gamma'} / L^2 \right), \quad (19)$$

where K' and γ' are the generalized diffusion constant and the anomalous diffusion exponent of the particle A . Therefore,

$$Q_3 = \int_{-L/2}^{L/2} W(x, t) dx = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} E_{\gamma'} \left[-K'_{\gamma'} (2n+1)^2 \pi^2 t^{\gamma'} / L^2 \right]. \quad (20)$$

Next we distinguish two cases in the handling of the sum in Eq. (20): first we deal with a subdiffusive particle, and subsequently with an ordinary diffusive particle. In the subdiffusive case, we note that for large arguments ($z \gg 1$) the Mittag-Leffler function has the expansion

$$E_{\gamma'}(-z) = \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{\Gamma(1 - \gamma' m)} z^{-m} \quad (21)$$

so that

$$Q_3 = \frac{4}{\pi} \sum_{m=1}^{\infty} \frac{(-1)^{m+1} L^{2m}}{\Gamma(1 - \gamma' m) \left[\pi^2 K'_{\gamma'} t^{\gamma'} \right]^m} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^{m+1}}. \quad (22)$$

Therefore, for $t \rightarrow \infty$ one finds

$$Q_3 = \frac{1}{8\Gamma(1 - \gamma')} \frac{L^2}{K'_{\gamma'} t^{\gamma'}} + O \left(\frac{L^2}{K'_{\gamma'} t^{\gamma'}} \right)^2. \quad (23)$$

Consequently, a lower bound on the survival probability of the particle A is

$$P_L(t) = Q_1 Q_2 Q_3 = e^{-\rho L} \exp \left[-\frac{2}{\Gamma(1 + \gamma/2)} \sqrt{\rho^2 K_\gamma t^\gamma} \right] \frac{1}{8\Gamma(1 - \gamma')} \frac{L^2}{K'_{\gamma'} t^{\gamma'}} \left[1 + O \left(\frac{L^2}{K'_{\gamma'} t^{\gamma'}} \right) \right]. \quad (24)$$

It can easily be ascertained that this expression is maximal when $L = L^* \equiv 2/\rho$, i.e., $P_L(t) \leq P_{L^*}(t)$ with

$$P_{L^*}(t) = \frac{e^{-2}}{8\Gamma(1-\gamma')} \left(\frac{2}{\rho}\right)^2 \frac{1}{K'_{\gamma'} t^{\gamma'}} \exp\left[-\frac{2}{\Gamma(1+\gamma/2)} \sqrt{\rho^2 K_{\gamma} t^{\gamma}}\right] \left[1 + O\left(\frac{1}{\rho^2 K'_{\gamma'} t^{\gamma'}}\right)\right]. \quad (25)$$

This is then our best lower bound for the survival probability $P(t)$ of a subdiffusive particle.

When the particle A diffuses normally, Eq. (20) becomes

$$Q_3 = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} \exp[-D'(2n+1)^2 \pi^2 t/L^2], \quad (26)$$

with $D' \equiv K'_1$. For long times^{10,11}

$$Q_3 \sim \frac{4}{\pi} \exp[-D' \pi^2 t/L^2], \quad t \gg 1 \quad (27)$$

so that

$$P_L(t) = Q_1 Q_2 Q_3 \sim \frac{4}{\pi} e^{-\rho L} \exp\left[-\frac{2}{\Gamma(1+\gamma/2)} \sqrt{\rho^2 K_{\gamma} t^{\gamma}}\right] \exp[-D' \pi^2 t/L^2] \quad (28)$$

for $t \gg 1$. This lower bound can be again be maximized by optimizing the value of L . The optimal value is^{10,11} $L^* = (2\pi^2 D' t/\rho)^{1/3}$, so that

$$P_L(t) \leq P_{L^*}(t) = \frac{4}{\pi} \exp\left[-\frac{2\sqrt{\rho^2 K_{\gamma} t^{\gamma}}}{\Gamma(1+\gamma/2)} - 3(\pi^2 \rho^2 D' t/4)^{1/3}\right]. \quad (29)$$

Note that the dominant term inside the bracket depends on the value of γ , the anomalous diffusion exponent for the traps. We distinguish three cases:

1. Traps with $2/3 < \gamma \leq 1$. In this case, for $t \gg 1$,

$$\frac{2\sqrt{\rho^2 K_{\gamma} t^{\gamma}}}{\Gamma(1+\gamma/2)} \gg 3(\pi^2 \rho^2 D' t/4)^{1/3} \quad (30)$$

so that

$$P_{L^*}(t) = \frac{4}{\pi} \exp\left[-\frac{2\sqrt{\rho^2 K_{\gamma} t^{\gamma}}}{\Gamma(1+\gamma/2)}\right]. \quad (31)$$

2. Traps with $\gamma = 2/3$. Now

$$P_L(t) \leq P_{L^*}(t) = \frac{4}{\pi} \exp\left[-\left(\frac{2\sqrt{\rho^2 K_{\gamma}}}{\Gamma(4/3)} - 3(\pi^2 \rho^2 D'/4)^{1/3}\right) t^{1/3}\right], \quad (32)$$

that is, the second contribution in the exponent in Eq. (29) is of the same order as the first and must thus be retained.

3. Traps with $0 < \gamma < 2/3$. Now the second term in the exponent of Eq. (29) is dominant:

$$P_{L^*}(t) = \frac{4}{\pi} \exp\left[-3(\pi^2 \rho^2 D' t/4)^{1/3}\right]. \quad (33)$$

In the next section we examine our upper and lower bound results to establish the behavior of the survival probability of A whenever possible.

4. SURVIVAL PROBABILITY

We now combine our upper and lower bound results. Recall that the label and exponent γ is associated with the traps and γ' is associated with the particle A . The upper bound on the survival probability is in all cases given in Eq. (14), but the lower bound depends on the anomalous diffusion exponent of the particle. We distinguish the following cases:

1. Subdiffusive particle ($0 < \gamma' < 1$) and diffusive or subdiffusive traps ($0 < \gamma \leq 1$). The lower bound is given in Eq. (25), so that $P_{L^*}(t) \leq P(t) \leq P_U(t)$ leads to

$$\frac{2}{\Gamma(1 + \gamma/2)} \leq -\frac{\ln P(t)}{\sqrt{\rho^2 K_\gamma t^\gamma}} \leq \frac{2}{\Gamma(1 + \gamma/2)} + \frac{2 \ln \left[\sqrt{\rho^2 K_{\gamma'} t^{\gamma'}} \right] + 2 + \ln [2\Gamma(1 - \gamma')]}{\sqrt{\rho^2 K_\gamma t^\gamma}} + O\left(\frac{(\rho^2 K_\gamma t^\gamma)^{-1/2}}{\rho^2 K_{\gamma'} t^{\gamma'}}\right). \quad (34)$$

For $t \rightarrow \infty$, $\ln \left[\sqrt{\rho^2 K_{\gamma'} t^{\gamma'}} \right] \ll \sqrt{\rho^2 K_\gamma t^\gamma}$ and the upper and lower bounds converge asymptotically. We therefore arrive at the explicit asymptotic survival probability

$$P(t) \sim \exp \left[-\frac{2}{\Gamma(1 + \gamma/2)} \sqrt{\rho^2 K_\gamma t^\gamma} \right] \quad (35)$$

for $0 < \gamma \leq 1$ and $0 < \gamma' < 1$. Note that for $\gamma = 1$ we recover the normal diffusive result obtained earlier.¹⁰ A noteworthy result here is that the survival probability depends only on the exponent γ that characterizes the traps and not on γ' that characterizes the particle. This is interesting vis a vis the subordination issue.

2. Diffusive particle ($\gamma' = 1$) and subdiffusive traps with $2/3 < \gamma \leq 1$. The bounds here are exactly as above, and the asymptotic survival probability is again given by Eq. (35).
3. Diffusive particle ($\gamma' = 1$) and subdiffusive traps with $\gamma = 2/3$ (marginal case). Now $P_{L^*}(t) \leq P(t) \leq P_U(t)$ leads to the more ambiguous inequalities

$$\frac{2}{\Gamma(4/3)} \leq -\frac{\ln P(t)}{\sqrt{\rho^2 K_\gamma t^\gamma}} \leq \frac{2}{\Gamma(4/3)} + 3 \left(\frac{\pi}{2\rho} \right)^{2/3} \frac{D^{1/3}}{K_\gamma^{1/2}}. \quad (36)$$

The bounding procedure is therefore not able to predict the value of the prefactor λ in $P(t) = \exp(-\lambda t^{1/3})$, but the asymptotic behavior $-\ln P(t) \propto t^{1/3}$ is evident.

4. Diffusive particle ($\gamma' = 1$) and subdiffusive traps with $0 < \gamma < 2/3$. The inequalities $P_{L^*}(t) \leq P(t) \leq P_U(t)$ now lead to

$$\frac{2}{\Gamma(1 + \gamma/2)} \leq -\frac{\ln P(t)}{\sqrt{\rho^2 K_\gamma t^\gamma}} \leq \frac{2}{\Gamma(1 + \gamma/2)} + 3 \left(\frac{\pi}{2\rho} \right)^{2/3} \frac{D^{1/3}}{K_\gamma^{1/2}} t^{1/3 - \gamma/2}, \quad (37)$$

so that the bounding procedure is not able to determine the asymptotic behavior of $P(t)$ at all for this case. We are not even able to assert the asymptotic form $P(t) \sim \exp(-\lambda t^\beta)$.

5. PANORAMA AND DISCUSSION

Bray and Blythe^{10,11} have calculated the asymptotic survival probability of a diffusive particle A in a randomly distributed sea of diffusive traps B in one dimension, and have determined the precise value of the coefficient λ in the classic result $P(t) \sim \exp(-\lambda t^{1/2})$ first obtained by Bramson and Lebowitz.^{8,9} We have attempted to generalize this result to the case where one or both of the species move subdiffusively. Our particle A is characterized by the anomalous diffusion exponent γ' and generalized diffusion coefficient $K_{\gamma'}$, and the traps

by γ and K_γ . These may be the first results in the literature involving two subdiffusive species with different anomalous diffusion exponents.

When both species are subdiffusive (γ and γ' both smaller than unity), the survival probability is independent of γ' and determined entirely by the subdiffusive properties of the traps, cf. Eq. (35). When the particle moves diffusively ($\gamma' = 1$), on the other hand, we are unable to unequivocally determine the coefficient λ for all cases using this procedure. If the traps move sufficiently rapidly ($2/3 < \gamma \leq 1$) then the result Eq. (35) is still valid. Note that this reduces to the Bray and Blythe result when $\gamma = 1$. The case $\gamma = 2/3$ is marginal in the sense that we can establish the behavior $P(t) \sim \exp(-\lambda t^{1/3})$, but are not able to determine the constant λ . Note that this particular time dependence of the survival probability is the same as the classic result for the survival probability of a diffusive particle in a sea of immobile traps.^{45–48} If the traps are too slow (“extremely subdiffusive”), $0 < \gamma < 2/3$, it is no longer possible to determine even the time dependence of the survival probability on the basis of this approach.

We thus find that in so far as one can even think of some sort of subordination principle (and whether such thinking is appropriate is debatable), it is determined by the behavior of the traps, i.e., by the replacement of t by t^γ . Even in the range of exponents where this is possible, it is only possible for the main asymptotic contribution to $P(t)$ but not for the correction terms to the leading asymptotic term.

It is interesting to note that the value $L^* = 2/\rho$ that maximizes the lower bound of the survival probability for a subdiffusive particle A does not grow with time. This implies that finite particle size effects could become relevant with increasing density ρ . This is completely different from the case of a Brownian particle A , since the growth $L^* \propto t^{1/3}$ now suppresses such finite size contributions for any given density.

A number of questions and opportunities for further work arise from our analysis. In our analysis (as in that of Bray and Blythe^{10,11}) we have simply applied the Pascal principle that the best survival strategy of a particle in a sea of moving traps is to remain stationary. While it seems intuitively obvious that this principle would hold whether the motions are diffusive or subdiffusive, the proof has only been presented for the diffusive case.^{40,41} As an interesting aside, we note that while the proof of the Pascal principle has assumed an equal concentration of traps on either side of the particle, we conjecture that this is not a necessary condition, and that the Pascal principle also holds with an asymmetric distribution and even if the traps are all located on one side of the particle. This, too, remains to be proved.

At this point we inject a digression that is relevant not only to our analysis but also to the original work of Bray and Blythe.^{10,11} They assumed that the particle A is initially surrounded by a random (Poisson) distribution of mobile traps, an assumption also made in our analysis, cf. Eq. (17). On the other hand, if at the start of the observations ($t = 0$) the process has already been taking place for some time $-\tau$ (i.e., if the process started at some time τ in the past), then it is known that the distribution around the surviving particles at time $t = 0$ is not of Poisson form. Those particles that initially had close-by traps are more likely to have been trapped already than those that did not, so that those particles that have survived are surrounded by a region of fewer than average traps (sometimes referred to as a “gap”). Bramson and Lebowitz arrive at the conclusion that the configuration of B particles is nevertheless dominated by a Poisson random measure.⁹ In Appendix A we confirm that for any finite τ the gap does not affect the asymptotic survival probability results of Bray and Blythe. The detailed nature of the gap is different in the diffusive and subdiffusive cases, and unknown in the latter. However, we conjecture that it is no more pronounced in the subdiffusive than in the diffusive system, and that it does not affect our results either.

Our own results of course leave a number of questions unanswered. One obvious question concerns the marginal role of the trap exponent $\gamma = 2/3$ when the particle is diffusive. Why is this a marginal exponent? A connection between this critical value and the fact that for a Brownian particle the length that maximizes the lower bound of the survival probability grows as $L^* \sim t^{1/3}$ seems plausible, but the conceptual basis for such a relation is not clear.

The most pressing and intriguing puzzle to resolve is that of calculating the survival probability when the particle A is diffusive ($\gamma' = 1$) and the traps are extremely subdiffusive ($0 < \gamma < 2/3$). Because the upper and lower bounds in this case do not have the same asymptotic time dependence, we are not able to say anything about this case on the basis of the procedures used in this paper.

APPENDIX A. MODIFIED INITIAL CONDITION

Suppose that the process $A + B \rightarrow B$ with a diffusive particle and diffusive traps began at time $-\tau$, but our observation of the system starts at time $t = 0$. Even if at time $-\tau$ the distribution of B 's around A was random (Poisson), it will not be so at time $t = 0$. Let $p(r)$ be the probability density of finding an empty region of length r to the right of A at time $t = 0$, so that the first trap is found to be located between r and $r + dr$. This function is unknown for our system, but one can conjecture a behavior on the basis of known (analytic and numerical) approximate results for the bimolecular reactions $A + A \rightarrow \emptyset$ and $A + B \rightarrow \emptyset$,^{49,50}

$$p(r) \sim r/\langle r \rangle \quad \text{for } r/\langle r \rangle \ll 1 \quad (38a)$$

$$p(r) \sim \exp(-r/\langle r \rangle) \quad \text{for } r/\langle r \rangle \gg 1 \quad (38b)$$

where $\langle r \rangle$ is the mean size of the gap next to particle A at the initial time of observation. Next we need to define the function $q(r)$, the probability density that a particle B is located at a distance r from A at $t = 0$. This function can be related to $p(r)$, most easily by considering a discrete lattice and then going to the continuum limit. Let p_n be the probability of a gap of size n and a particle B at position $n + 1$ to the right of A . Thus $p_n = \prod_i^n (1 - q_i)q_i$, where q_i is the probability that there is a trap B at distance i from A . It then follows that $\ln p_n = \ln(q_i) + \sum_i^n \ln(1 - q_i) \approx \ln(q_i) - \sum_i^n q_i$ and thus in the continuum limit

$$p(r) = q(r) \exp \left[- \int_0^r q(x) dx \right]. \quad (39)$$

To find $q(r)$ one thus needs to solve a nonlinear integral equation, a difficult task not worth the attempt given our imperfect knowledge of $p(r)$. It is nevertheless straightforward to conclude that the solution $q(r) = p(r)$ for $r \ll \langle r \rangle$ is compatible with (38a), and that $q(r) = \text{const.}$ for $r \gg \langle r \rangle$ is compatible with (38b). For our purposes it is thus sufficient to approximate $q(r)$ by

$$q(r) = \begin{cases} \frac{1}{R} \frac{r}{\langle r \rangle}, & 0 \leq r \leq \langle r \rangle, \\ \frac{1}{R}, & r \geq \langle r \rangle, \end{cases} \quad \text{for } R \rightarrow \infty. \quad (40)$$

The coefficient $1/R$ has been set by requiring that the integral of $q(r)$ from zero to R be normalized to unity. Thus, the presence of A affects the distribution of B 's within a distance $\langle r \rangle$ from A but not beyond, where the distribution remains random.

How does this deviation from a random distribution affect the survival probability? For this calculation we also introduce $q(r; R) = q(r) / \int_0^R q(r) dr$, the probability density for a B particle to be found at a distance r from A given that there is a B particle somewhere in an interval of length R that begins at A . An upper bound is obtained, as before, by invoking the Pascal principle. Generalizing the derivation for a Poisson distribution one straightforwardly arrives at the expression

$$\begin{aligned} Q_\infty(t) &= \lim_{R \rightarrow \infty} \left[\int_0^R q(r; R) Q_1(t|r) dr \right]^{\rho R} \\ &= \lim_{R \rightarrow \infty} \left[\int_0^R q(r; R) - \int_0^R q(r; R) \widehat{Q}_1(t|r) dr \right]^{\rho R}, \end{aligned} \quad (41)$$

where Q_1 is given in Eq. (5) and $\widehat{Q}_1 \equiv 1 - Q_1$. Since $\lim_{R \rightarrow \infty} \int_0^R q(r; R) dr = 1$, it follows that

$$\begin{aligned} Q_\infty(t) &= \lim_{R \rightarrow \infty} \exp \left[-\rho R \int_0^R q(r; R) \widehat{Q}_1(t|r) dr \right] = \lim_{R \rightarrow \infty} \exp \left[-\frac{\rho R}{\int_0^R q(r) dr} \int_0^R q(r) \widehat{Q}_1(t|r) dr \right] \\ &= \lim_{R \rightarrow \infty} \exp \left[-\rho R \int_0^R q(r) \widehat{Q}_1(t|r) dr \right] \\ &= \exp \left[-\rho \left(\int_0^{\langle r \rangle} \frac{r}{\langle r \rangle} \widehat{Q}_1(t|r) dr + \int_{\langle r \rangle}^\infty \widehat{Q}_1(t|r) dr \right) \right], \end{aligned} \quad (42)$$

where we have introduced the explicit form (40) in the last line. The integrals can be carried out in the long time limit, to yield

$$Q_\infty(t) = \exp \left[-\rho \left(\frac{\langle r \rangle}{2} + \sqrt{\frac{4Dt}{\pi}} \right) \right] \quad \text{for } t \rightarrow \infty. \quad (43)$$

Since $\langle r \rangle$ is a constant (no matter how large), eventually the second term in the exponent dominates, and the upper bound on the survival probability in the diffusive case is exactly the same as obtained for an initially Poisson distribution of B 's around A .

Consider now the lower bound on the survival probability. The probabilities Q_2 and Q_3 are not changed by a modification of the initial distribution of traps around the particle. The probability Q_1 that at $t = 0$ a box of size L around A contains no traps is changed. It is again easiest to start with a discrete lattice and define $\bar{\omega}_n$ as the probability that there is a gap of n sites to the right of A given that there is a single trap to the right of A as determined by the distribution q_i . Thus

$$\bar{\omega}_n = \prod_{i=0}^n (1 - q_i) \Rightarrow \ln \bar{\omega}_n = \sum_{i=0}^n \ln(1 - q_i) \approx - \sum_{i=0}^n q_i. \quad (44)$$

The continuum limit gives

$$\bar{\omega}(x) = \exp \left(- \int_0^x q(r) dr \right). \quad (45)$$

If there are $N = \rho R$ to the right of A , with $R \rightarrow \infty$, the probability of a gap of size x to the right of A is $\omega(x) = \bar{\omega}^N(x) = \bar{\omega}^{\rho R}(x)$. Inserting the expression for $q(r)$ and carrying out the integrals for $R \rightarrow \infty$ gives

$$\omega(x) = \begin{cases} \exp \left[-\rho x^2 / (2\langle r \rangle) \right], & x \leq \langle r \rangle \\ \exp \left[-\rho(x - \langle r \rangle / 2) \right], & x \geq \langle r \rangle \end{cases} \quad (46)$$

The same result is valid for a gap to the left of A , so that the probability Q_1 for there to be a gap of length L centered at A then is

$$Q_1 = \exp \left[-\rho L^2 / (4\langle r \rangle) \right], \quad \text{for } L/2 \leq \langle r \rangle \quad (47)$$

$$Q_1 = \exp \left[-\rho(L - \langle r \rangle) \right], \quad \text{for } L/2 \geq \langle r \rangle \quad (48)$$

The lower bound on the survival probability then is

$$P_L(t) = Q_1 \frac{4}{\pi} \exp \left(-\frac{\pi^2 D' t}{L^2} - 2\rho \sqrt{\frac{4Dt}{\pi}} \right), \quad (49)$$

where we have inserted the explicit expressions for Q_2 and Q_3 found earlier. As before, one can choose the box size L to maximize this lower bound. There are now two possibilities. One is to assume that $L \leq 2\langle r \rangle$, whence

$$P_L(t) = \frac{4}{\pi} \exp \left(-\frac{\pi^2 D' t}{L^2} - \rho \frac{4L^2}{\langle r \rangle} - 2\rho \sqrt{\frac{4Dt}{\pi}} \right). \quad (50)$$

Maximizing with respect to L gives $L^* = (4\pi^2 D' \langle r \rangle t / \rho)^{1/4}$, which grows with time and is therefore in contradiction with the assumption $L \leq 2\langle r \rangle$. Thus we have to take the other possibility, $L \geq 2\langle r \rangle$, whence Eq. (48) leads to

$$P_L(t) = \frac{4}{\pi} \exp \left(-\frac{\pi^2 D' t}{L^2} - \rho L + \rho \langle r \rangle - 2\rho \sqrt{\frac{4Dt}{\pi}} \right), \quad (51)$$

and maximizing with respect to L gives $L^* = (2\pi^2 D't/\rho)^{1/3}$. For $t \rightarrow \infty$, the new term $\rho(r)$ in the exponent is negligible compared to the terms that grow with time. The asymptotic lower bound is therefore identical to that obtained by Bray and Blythe for the Poisson distribution of traps around A .

Although the distribution $q(r)$ is not known in the subdiffusive case, it will surely be the case that at large distances from A it is independent of r even if the trapping process has been going on for a long time τ before the start of the observations at $t = 0$. Therefore in this case as well the asymptotic survival probability results obtained in this paper are applicable.

ACKNOWLEDGMENTS

This work was partially supported by the Ministerio de Ciencia y Tecnología (Spain) through Grant No. FIS2004-01399, and by the National Science Foundation under grant No. PHY-0354937.

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