Trapping reactions with subdiffusive traps and particles characterized by different anomalous diffusion exponents

S. B. Yuste¹ and Katja Lindenberg²

¹Departamento de Física, Universidad de Extremadura, E-06071 Badajoz, Spain

²Department of Chemistry and Biochemistry 0340, and Institute for Nonlinear Science, University of California San Diego,

9500 Gilman Drive, La Jolla, California 92093-0340, USA

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A number of results for reactions involving subdiffusive species, all with the same anomalous exponent γ , have recently appeared in the literature and can often be understood in terms of a subordination principle whereby time *t* in ordinary diffusion is replaced by t^{γ} . However, very few results are known for reactions involving different species 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. We find rigorous results for the asymptotic survival probability of the particle in most cases, with the exception of the case of a particle that diffuses normally while the anomalous diffusion exponent of the traps is smaller than 2/3.

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I. 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, $A+B\rightarrow B$. 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 nonequilibrium statistical mechanics [1–4]. 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 [5].

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 [6,7] proved rigorously that the long-time survival probability 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, recently Bray and Blythe [8] proved in a simple and elegant way, assuming the so-called "Pascal principle" (see below), that the survival probability of a diffusing particle with a 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. They furthermore proved that the survival probability coincides with that of an immobile target (D'=0) in the presence of diffusive traps. In particular, in a one-dimensional medium, $P(t) \sim \exp[-4\rho(Dt/\pi)^{1/2}]$, where ρ is the density of traps. 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.* [9] 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 Pascal principle states that the best strategy for survival is for the *A* particle not to move. This assumption was adopted in one dimension "without proof" by Bray and Blythe [8] to calculate an upper bound for the survival probability for $d \le 2$, although it was already proved in [10] in the context of incoherent exciton quenching. More recently, the principle was proved by Bray, Majumdar, and Blythe [11]. Almost simultaneously but slightly earlier, Moreau *et al.* [12] proved the Pascal principle for a rather general class of random walks on *d*-dimensional lattices. These latter authors are responsible for the name now bestowed on the principle.

The purpose of this paper is to extend the procedure and results of Bray and Blythe [8], which are valid for a Brownian diffusive particle and Brownian diffusive traps, to situations in which the particle and traps move subdiffusively. Anomalous diffusion of a particle is usually characterized by its mean squared displacement x(t) for large t:

$$\langle x^2(t) \rangle \sim \frac{2K_{\gamma}}{\Gamma(1+\gamma)} t^{\gamma}.$$
 (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 sudiffusive when $0 < \gamma < 1$. Subiffusive processes are ubiquitous in nature [13–18], and are particularly useful for understanding transport in complex systems [3,19].

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) with waiting-time distributions between steps that have broad long-time tails and consequently infinite moments, $\psi(t) \sim t^{-1-\gamma}$ for $t \to \infty$ with $0 < \gamma < 1$. Using the CTRW formalism, Blumen *et al.* [20,21] considered a variety of reactions, including the trapping problem $A+B(\text{static}) \to B(\text{static})$, the target problem $A(\text{static})+B \to B$, and the bimolecular reactions $A+A \to \emptyset$ and $A+B \to \emptyset$. The moving particles were modeled as continuous-time random walkers with long-tailed waitingtime densities. Recently, Sung and Silbey [22] 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.* [23] to study the kinetics of the recombination reaction in subdiffusive media.

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) [13,24]

$$\frac{\partial}{\partial t}P(x,t) = K_{\gamma 0} D_t^{1-\gamma} \frac{\partial^2}{\partial x^2} P(x,t), \qquad (2)$$

where K_{γ} is the generalized diffusion coefficient that appears in Eq. (1), and ${}_{0}D_{t}^{1-\gamma}$ is the Riemann-Liouville operator,

$${}_{0}D_{t}^{1-\gamma}P(x,t) = \frac{1}{\Gamma(\gamma)}\frac{\partial}{\partial t}\int_{0}^{t}d\tau \frac{P(x,\tau)}{(t-\tau)^{1-\gamma}}.$$
(3)

Sung et al. [25] directly addressed this problem with a fractional diffusion equation approach. Seki et al. [23] went beyond the CTRW model and derived a fractional reactiondiffusion equation for the geminate recombination problem, and one finds some disagreement between the assumptions and results in this work and that in [25]. 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) [26]. The fractional-diffusion approach has also been employed to study other bimolecular reactions between subdiffusive particles. In particular, the annihilation $A + A \rightarrow \emptyset$ and coagulation $A + A \rightarrow A$ of subdiffusive particles was studied [27] by means of a fractional generalization of the interparticle distribution function method [4]. The evolution of reactionsubdiffusion 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 [28]. Other recent work on fractional diffusion and CTRW models of subdiffusive reacting particles can be found in a number of references [29].

In this paper we implement the fractional diffusion equation approach to study the one-dimensional trapping problem in the long-time regime for subdiffusive (or diffusive) particles that move among a distribution of *nonstatic* traps. The traps can be either subdiffusive or diffusive. For this purpose, we generalize the ideas of Bray and Blythe [8]. Recent contributions to the A+B problem based on the fractional diffusion equation approach [22,26] share the simplifying characteristic that the reaction takes place between a static particle (or fixed boundary) and a subdiffusive particle. The present work differs from those 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. Some of this work has been presented in [30].

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} . 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 [21]). 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 [21]). 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" but not static.

Our paper is organized as follows. In Sec. II we extend the proof of the Pascal principle in one dimension to the case in which both the particle and the traps move subdiffusively and calculate the upper bound for the survival probability. In Sec. III we present an alternative calculation of the upper bound, which is particularly helpful for the calculation of the lower bound in Sec. IV. The survival probability is established, when possible, in Sec. V. Section VI presents a compendiary of results and some comments on open problems.

II. THE PASCAL PRINCIPLE

The Pascal principle of random walks says that the best survival strategy for a random walker A surrounded by a random sea of trapping random walkers B is to stand still. Here we extend the proof of the Pascal principle in one dimension to the case in which both the particle and the traps perform subdiffusive random walks.

As did Bray *et al.* [11], we consider a finite volume V containing $N = \rho V$ traps B initially distributed at random, and a single A particle initially at the origin. The trajectory of the A particle is z(t). Bray *et al.* write the survival probability of A as $P(t) = \exp\{-\mu[z(t)]\}$, where the trajectory-dependent functional μ is to be determined. To find this functional they derive an equation for it by calculating, in two ways, the

probability density to find a *B* particle at the point z(t) at time *t*:

$$\rho = \int_0^t dt' \dot{\mu}(t') G[z(t), t|z(t'), t'] + \rho P[\mu(t)].$$
(4)

That the left side is this probability density is obvious. On the right side $\dot{\mu}(t')dt' = (-\dot{P}/P)dt'$ is the probability that a *B* particle intersected *A* in the time interval (t', t' + dt') for the first time, and the propagator *G* is the probability density for this particular *B* to be at z(t) at time *t*. We have slightly augmented Bray *et al.*'s fundamental starting point by including the second term on the right hand side, which is the probability that the first intersection of a *B* with *A* occurs at time *t* and not before. This term is ultimately unimportant because it decays much more quickly than the first term and so we omit it henceforth, but it is satisfying that the fundamental equation now holds at all times.

Proof of the Pascal principle requires us to show that the trajectory z(t)=0 for all t gives the smallest possible value of $\mu[z]$. For this trajectory the fundamental equation is

$$\rho = \int_0^t dt' \,\dot{\mu}_0(t') G[z(t) = 0, t|z(t') = 0, t'], \tag{5}$$

where $\mu_0(t) = \mu[z(t=0)]$. The propagator G[z(t)=0,t|z(t')=0] is a function only of t-t', which we abbreviate as G(t-t'), so Eq. (5) is a convolution. Denoting the Laplace transform of f(t) as $\hat{f}(s)$ yields for the transform of (5)

$$\hat{\rho}(s) = s\hat{\mu}_0(s)\hat{G}(s), \tag{6}$$

where we have noted that $\mu_0(t'=0)=0$ because the initial survival probability is unity. It follows that

$$\hat{\mu}_0(s) = \frac{\hat{\rho}(s)}{s\hat{G}(s)}.$$
(7)

Inversion for the subdiffusive case in one dimension gives

$$G(t) = \frac{t^{-\gamma/2}}{\sqrt{4\pi K_{\gamma}}} H_{1,2}^{2,0} \left[0 \left| \begin{pmatrix} (1 - \gamma/2, \gamma/2) \\ (0,1), (1/2,1) \end{pmatrix} \right| = \frac{t^{-\gamma/2}}{\sqrt{4K_{\gamma}} \Gamma\left(1 - \frac{\gamma}{2}\right)},$$
(8)

where γ is the anomalous diffusion exponent for the traps, K_{γ} is the associated generalized diffusion constant, and $H_{1,2}^{2,0}$ is Fox's *H* function [31,32], whose value at the given arguments we have used to write the last equality. The Laplace transform of G(t) is

$$\hat{G}(s) = \frac{s^{\gamma/2-1}}{\sqrt{4K\gamma}}.$$
(9)

The inverse of Eq. (7) then immediately follows,

$$\mu_0(t) = \frac{\rho \sqrt{4K_\gamma t^\gamma}}{\Gamma\left(1 + \frac{\gamma}{2}\right)}.$$
(10)

To prove that z(t)=0 gives the global minimum of $\mu[z(t)]$ we again follow Bray *et al.* and write $\mu = \mu_0 + \mu_1$ in Eq. (4) (without the last term),

$$\rho = \int_0^t dt' [\dot{\mu}_0(t') + \dot{\mu}_1(t')] G[z(t), t|z(t'), t'].$$
(11)

Adding and subtracting $(t-t')^{-\gamma/2}/\sqrt{4K_{\gamma}}\Gamma(1-\gamma/2)$ to *G* in the integrand allows cancellation of the left side of Eq. (11) against one of the terms on the right, leaving

$$0 = -\int_{0}^{t} dt' \frac{\dot{\mu}(t')}{\sqrt{4K_{\gamma}}\Gamma\left(1 - \frac{\gamma}{2}\right)} \frac{R}{(t - t')^{\gamma/2}} + \int_{0}^{t} dt' \frac{1}{\sqrt{4K_{\gamma}}\Gamma\left(1 - \frac{\gamma}{2}\right)} \frac{\dot{\mu}_{1}(t')}{(t - t')^{\gamma/2}},$$
 (12)

where

$$R = 1 - \frac{\Gamma\left(1 - \frac{\gamma}{2}\right)}{\sqrt{\pi}} H_{1,2}^{2,0} \left[0 \left| \begin{array}{c} (1 - \gamma/2, \gamma/2) \\ (0,1), (1/2,1) \end{array} \right] \right].$$
(13)

An explicit expression for μ_1 is obtained by Laplace transforming this result, solving for $\hat{\mu}(s)$, and inverting,

$$\mu_{1}(t) = \frac{1}{\Gamma\left(\frac{\gamma}{2}\right)\Gamma\left(1-\frac{\gamma}{2}\right)} \int_{0}^{t} \frac{dt_{1}}{(t-t_{1})^{1-\gamma/2}} \int_{0}^{t_{1}} dt_{2} \frac{R\dot{\mu}(t_{2})}{(t_{1}-t_{2})^{\gamma/2}}.$$
(14)

The rest of the argument follows exactly as in Bray *et al.* [11,30]. Since $R \ge 0$ and $\dot{\mu} \ge 0$ [because P(t) is a nonincreasing function of time], it follows that $\mu_1(t) \ge 0$ for all paths z(t), with equality when z(t)=0 for all t. The survival probability of our A particle averaged over all possible trajectories z is $P(t) = \langle e^{-\mu(t)} \rangle_z = \langle e^{-\mu_0(t)-\mu_1(t)} \rangle_z$, and the above proof shows that $\langle e^{-\mu_0(t)-\mu_1(t)} \rangle_z \le e^{-\mu_0(t)}$. Therefore

$$P_U(t) = \exp[-\mu_0(t)] = \exp\left[-\frac{\sqrt{4\rho^2 K_{\gamma} t^{\gamma}}}{\Gamma\left(1 + \frac{\gamma}{2}\right)}\right]$$
(15)

is a strict upper bound for the survival probability P(t), thus extending the proof of the Pascal principle to subdiffusive particles in one dimension.

III. ALTERNATIVE CALCULATION OF UPPER BOUND FOR THE SURVIVAL PROBABILITY

The survival probability $P_U(t)$ of a static particle A surrounded by a distribution of mobile traps (the "target problem") was considered as early as 1986 using a CTRW model [21], and more recently for the three-dimensional case by means of a fractional diffusion approach [25]. In the previous section we obtained the result (15) following the approach of Bray *et al.* [11]. Here we recalculate $P_U(t)$ by generalizing

the original approach of Bray and Blythe [8] to the subdiffusive case because it provides results useful for the calculation of the lower bound in the next section.

Consider a target A of size $2\mathcal{L}$ centered at the origin, and let $Q_1(t|y)$ be the probability that the trap initially placed at $y > \mathcal{L}$ has not reached the end of the target at $y = \mathcal{L}$ by time t. Then, in terms of the Fox's H function [33]

$$\mathcal{Q}_1(t|y) = 1 - H_{11}^{10} \left[\left. \frac{y - \mathcal{L}}{\sqrt{K_{\gamma} t^{\gamma}}} \right|^{(1, \gamma/2)}_{(0, 1)} \right] \equiv 1 - H \left[\frac{y - \mathcal{L}}{\sqrt{K_{\gamma} t^{\gamma}}} \right].$$
(16)

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

$$Q_1(t|y) = 1 - \operatorname{erfc}\left(\frac{y - \mathcal{L}}{\sqrt{4Dt}}\right), \quad \gamma = 1.$$
 (17)

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

$$\mathcal{Q}_{N}(t) = \prod_{i=1}^{N} \frac{1}{R} \int_{\mathcal{L}}^{\mathcal{L}+R} dy_{i} \Biggl\{ 1 - H\Biggl[\frac{y_{i} - \mathcal{L}}{\sqrt{K_{\gamma} t^{\gamma}}} \Biggr] \Biggr\}$$
$$= \Biggl\{ 1 - \frac{1}{R} \int_{\mathcal{L}}^{\mathcal{L}+R} dy H\Biggl[\frac{y - \mathcal{L}}{\sqrt{K_{\gamma} t^{\gamma}}} \Biggr] \Biggr\}^{N}, \qquad (18)$$

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

$$Q_{\infty}(t) = \lim_{R \to \infty} \left\{ 1 - \frac{1}{R} \int_{0}^{R} dy H\left[\frac{y}{\sqrt{K_{\gamma}t^{\gamma}}}\right] \right\}^{\rho R}$$
$$= \exp\left\{ -\rho \sqrt{K_{\gamma}t^{\gamma}} \int_{0}^{\infty} dz H[z] \right\}.$$
(19)

Note that the result is independent of the size of the target. We need to evaluate the integral

$$I_{\gamma} = \int_{0}^{\infty} dz H_{11}^{10} \left[z \left| \begin{pmatrix} 1, \gamma/2 \\ 0, 1 \end{pmatrix} \right],$$
(20)

which can be done from the properties of the Fox's H function [31]. One finds that

$$H_{11}^{10} \left[z \left| \begin{pmatrix} 1, \gamma/2 \\ 0, 1 \end{pmatrix} \right] = \frac{d}{dz} H_{11}^{10} \left[z \left| \begin{pmatrix} 1+\gamma/2, \gamma/2 \\ 0, 1 \end{pmatrix} \right].$$
(21)

But

$$H_{11}^{10} \left[\infty \left| \begin{array}{c} (1 + \gamma/2, \gamma/2) \\ (0,1) \end{array} \right] = 0$$
 (22)

and

$$H_{11}^{10} \left[0 \left| \begin{pmatrix} (1+\gamma/2,\gamma/2) \\ (0,1) \end{pmatrix} \right] = \frac{1}{\Gamma(1+\gamma/2)},$$
(23)

so that $I_{\gamma} = 1/\Gamma(1 + \gamma/2)$. Therefore,

$$Q_{\infty}(t) = \exp\left[-\frac{\sqrt{\rho^2 K_{\gamma} t^{\gamma}}}{\Gamma(1+\gamma/2)}\right].$$
 (24)

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. (24),

$$P_U(t) = \mathcal{Q}_{\infty}^2(t) = \exp\left[-\frac{\sqrt{4\rho^2 K_{\gamma} t^{\gamma}}}{\Gamma(1+\gamma/2)}\right].$$
 (25)

This result, which is of course identical to Eq. (15), 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 [21,34],

$$P_U(t) = e^{-\rho \langle S(t) \rangle + \cdots}, \qquad (26)$$

where the dots represent higher moments that decay more rapidly with time. Comparing this expression with Eq. (25), one finds that the asymptotic 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

$$\langle S(t) \rangle \sim \frac{2\sqrt{K_{\gamma}t^{\gamma}}}{\Gamma(1+\gamma/2)}.$$
 (27)

This result agrees with that found by Yuste and Acedo [26] using a different approach.

IV. LOWER BOUND FOR THE SURVIVAL PROBABILITY

Let $P_L(t)$ be the probability that the mobile particle A remains inside a box of size \mathcal{L} and that all the traps remain outside this box until time t (we distinguish between \mathcal{L} , the size of the box, and L, which denotes lower bound). 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 because there exist many other trajectories involving the simultaneous presence of the particle and traps within the box \mathcal{L} that allow the particle A to survive. This lower bound was first calculated for diffusive particles and traps by Redner and Kang [35] and further considered (and in some cases corrected) in [6,36].

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 \mathcal{L} contains no traps

$$Q_1 = e^{-\rho \mathcal{L}}.$$
 (28)

(2) The probability Q_2 that no traps enter the box of size \mathcal{L} up to time t

$$Q_2 = \exp\left[-\frac{2}{\Gamma(1+\gamma/2)}\sqrt{\rho^2 K_{\gamma} t^{\gamma}}\right] = P_U(t).$$
 (29)

Note that it is the derivation of the previous section, which explicitly shows this probability to be independent of the size of the box, that allows us to write this result.

(3) The probability Q_3 that the particle has not left the box of size \mathcal{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 $x=\pm \mathcal{L}/2$. Solving the fractional diffusion equation by means of separation of variables [13] one finds

$$W(x,t) = \frac{2}{\mathcal{L}} \sum_{n=0}^{\infty} (-1)^n \sin\left[\frac{(2n+1)\pi(x+\mathcal{L}/2)}{\mathcal{L}}\right] \\ \times E_{\gamma'} [-K'_{\gamma'}(2n+1)^2 \pi^2 t^{\gamma'} / \mathcal{L}^2],$$
(30)

where $K'_{\gamma'}$ and γ' are the generalized diffusion constant and the anomalous diffusion exponent of the particle *A*. Therefore,

$$Q_{3} = \int_{-\mathcal{L}/2}^{\mathcal{L}/2} W(x,t) dx$$

= $\frac{4}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^{n}}{2n+1} E_{\gamma'} [-K'_{\gamma'}(2n+1)^{2} \pi^{2} t^{\gamma'} / \mathcal{L}^{2}].$ (31)

Next we distinguish two cases in the handling of the sum in Eq. (31): first we deal with a subdiffusive particle, and subsequently with an ordinary diffusive particle. In the subdiffusive case, we note that for large arguments $(z \ge 1)$ the Mittag-Leffler function has the expansion

$$E_{\gamma'}(-z) = \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{\Gamma(1-\gamma'm)} z^{-m}$$
(32)

so that

$$Q_3 = \frac{4}{\pi} \sum_{m=1}^{\infty} \frac{(-1)^{m+1} \mathcal{L}^{2m}}{\Gamma(1-\gamma'm) [\pi^2 K'_{\gamma'} t^{\gamma'}]^m} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^{2m+1}}.$$
(33)

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

$$Q_{3} = \frac{1}{8\Gamma(1-\gamma')} \frac{\mathcal{L}^{2}}{K_{\gamma'}^{\prime} t^{\gamma'}} + O\left(\frac{\mathcal{L}^{2}}{K_{\gamma'}^{\prime} t^{\gamma'}}\right)^{2}.$$
 (34)

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

$$P_{L}(t) = Q_{1}Q_{2}Q_{3}$$

$$= e^{-\rho\mathcal{L}} \exp\left[-\frac{2}{\Gamma(1+\gamma/2)}\sqrt{\rho^{2}K_{\gamma}t^{\gamma}}\right]$$

$$\times \frac{1}{8\Gamma(1-\gamma')} \frac{\mathcal{L}^{2}}{K_{\gamma'}t^{\gamma'}} \left[1 + O\left(\frac{\mathcal{L}^{2}}{K_{\gamma'}t^{\gamma'}}\right)\right]. \quad (35)$$

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

$$P_{L^{*}}(t) = \frac{e^{-2}}{8\Gamma(1-\gamma')} \left(\frac{2}{\rho}\right)^{2} \frac{1}{K_{\gamma'}t^{\gamma'}}$$
$$\times \exp\left[-\frac{2}{\Gamma(1+\gamma/2)}\sqrt{\rho^{2}K_{\gamma}t^{\gamma}}\right]$$
$$\times \left[1 + O\left(\frac{1}{\rho^{2}K_{\gamma'}t^{\gamma'}}\right)\right]. \tag{36}$$

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

When the particle A diffuses normally, Eq. (31) becomes

$$Q_3 = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} \exp[-D'(2n+1)^2 \pi^2 t/\mathcal{L}^2]$$
(37)

with $D' \equiv K'_1$. For long times [8]

$$Q_3 \sim \frac{4}{\pi} \exp[-D' \pi^2 t / \mathcal{L}^2], \quad t \ge 1$$
 (38)

so that

$$P_{L}(t) = Q_{1}Q_{2}Q_{3} \sim \frac{4}{\pi}e^{-\rho\mathcal{L}}\exp\left[-\frac{2}{\Gamma(1+\gamma/2)}\sqrt{\rho^{2}K_{\gamma}t^{\gamma}}\right]$$
$$\times \exp\left[-D' \pi^{2}t/\mathcal{L}^{2}\right]$$
(39)

for $t \ge 1$. This lower bound can again be maximized by optimizing the value of \mathcal{L} . The optimal value is [8] $\mathcal{L}^* = (2\pi^2 D' t/\rho)^{1/3}$ (time dependent), so that

$$P_{L}(t) \leq P_{L^{*}}(t) = \frac{4}{\pi} \exp\left[-\frac{2\sqrt{\rho^{2}K_{\gamma}t^{\gamma}}}{\Gamma(1+\gamma/2)} - 3(\pi^{2}\rho^{2}D't/4)^{1/3}\right].$$
(40)

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 $2/3 < \gamma \le 1$. In this case, for $t \ge 1$

$$\frac{2\sqrt{\rho^2 K_{\gamma} t^{\gamma}}}{\Gamma(1+\gamma/2)} \gg 3(\pi^2 \rho^2 D' t/4)^{1/3}$$
(41)

so that

$$P_{L^*}(t) = \frac{4}{\pi} \exp\left[-\frac{2\sqrt{\rho^2 K_{\gamma} t^{\gamma}}}{\Gamma(1+\gamma/2)}\right].$$
 (42)

(2) Traps with
$$\gamma = 2/3$$
. Now
 $P_L(t) \leq P_{L^*}(t) = \frac{4}{\pi} \exp\left[-\left(\frac{2\sqrt{\rho^2 K_\gamma}}{\Gamma(4/3)} - 3(\pi^2 \rho^2 D'/4)^{1/3}\right)t^{1/3}\right],$
(43)

that is, the second contribution in the exponent in Eq. (40) 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. (40) is dominant,

$$P_{L^{*}}(t) = \frac{4}{\pi} \exp[-3(\pi^{2}\rho^{2}D't/4)^{1/3}].$$
 (44)

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

V. 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. (25), 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 $(0 < \gamma \le 1)$. The lower bound is given in Eq. (36), so that $P_{L^*}(t) \le P(t) \le P_U(t)$ leads to

$$\frac{2}{\Gamma(1+\gamma/2)} \leq -\frac{\ln P(t)}{\sqrt{\rho^2 K_{\gamma} t^{\gamma}}}$$

$$\leq \frac{2}{\Gamma(1+\gamma/2)}$$

$$+\frac{2 \ln[\sqrt{\rho^2 K_{\gamma'} t^{\gamma'}}] + 2 + \ln[2\Gamma(1-\gamma')]}{\sqrt{\rho^2 K_{\gamma} t^{\gamma}}}$$

$$+ O\left(\frac{(\rho^2 K_{\gamma'} t^{\gamma'})^{-1/2}}{\rho^2 K_{\gamma'} t^{\gamma'}}\right).$$
(45)

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

$$P(t) \sim \exp\left[-\frac{2}{\Gamma(1+\gamma/2)}\sqrt{\rho^2 K_{\gamma} t^{\gamma}}\right]$$
(46)

for $0 < \gamma \le 1$ and $0 < \gamma' < 1$. Note that for $\gamma = 1$ we recover the normal diffusive result obtained earlier [8]. 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 $2/3 < \gamma \le 1$. The bounds here are

$$\frac{2}{\Gamma(1+\gamma/2)} \leq -\frac{\ln P(t)}{\sqrt{\rho^2 K_{\gamma} t^{\gamma}}} \leq \frac{2}{\Gamma(1+\gamma/2)} + 3\left(\frac{\pi^2}{4\rho}\right)^{1/3} \frac{D'^{1/3}}{K_{\gamma}^{1/2}} t^{1/3-\gamma/2}, \quad (47)$$

and the asymptotic survival probability is again given by Eq. (46).

(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

$$\frac{2}{\Gamma(4/3)} \le -\frac{\ln P(t)}{\sqrt{\rho^2 K_{\gamma} t^{\gamma}}} \le \frac{2}{\Gamma(4/3)} + 3\left(\frac{\pi^2}{4\rho}\right)^{1/3} \frac{D'^{1/3}}{K_{\gamma}^{1/2}}.$$
 (48)

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 bounds here are also given by (47) 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 stretched exponential form $P(t) \sim \exp(-\lambda t^{\beta})$.

VI. PANORAMA AND DISCUSSION

Bray and Blythe [8] 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 [6,7]. Within some constraints, we have generalized 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 the generalized diffusion coefficient $K_{\gamma'}$, and the traps by γ and $K_{\gamma'}$. In the process of this generalization, we have extended the proof of the Pascal principle, that the best survival strategy of a particle in a sea of moving traps is to remain stationary, to the case of particles and/or traps that move subdiffusively. These results may be the first 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. (46). 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 $(2/3 < \gamma \le 1)$, then the result Eq. (46) 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 [37]. If the traps are too slow ("strongly subdiffusive"), $0 < \gamma < 2/3$, we are not able to determine even the time dependence of the survival probability on the basis of this approach. However, since we find the same stretched exponential behavior when $\gamma = 2/3$ and when $\gamma = 0$, a conjecture as to the behavior throughout this slow trap regime might be appropriate. The conjecture is that the survival probability decays as $P(t) \sim \exp(-\lambda t^{1/3})$ in the entire regime $0 \le \gamma \le 2/3$.

We thus find that in so far as one can think of some sort of subordination principle (and whether such thinking is appropriate here 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 asymptoic contribution to P(t) but not for the correction terms to the leading asymptotic term.

It is interesting to note that the value $\mathcal{L}^*=2/\rho$ 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 $\mathcal{L}^* \propto t^{1/3}$ now suppresses such finite size contributions for any given density.

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 [8]. They assumed that the particle A is initially surrounded by a random (Poisson) distribution of mobile traps, an assumption also made in our explicit analysis, cf. Eq. (28). 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 nearby 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 [7]. In Ref. [30] 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 $\mathcal{L}^* \sim t^{1/3}$ 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 strongly subdiffusive ($0 < \gamma < 2/3$). While we conjecture that the survival probability in this regime decays as $P(t) \sim \exp(-\lambda t^{1/3})$, the upper and lower bounds in this case do not have the same asymptotic time dependence so we are not able to test these conjectures on the basis of the procedures used in this paper.

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