# Survival probability of a subdiffusive particle in a d-dimensional sea of mobile traps

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We investigate the long-time behavior of the survival probability P(t) of a mobile particle in d-dimensional continuous Euclidean media doped with noninteracting mobile traps. The particle is strictly subdiffusive, implying that its mean-square displacement grows as  $t^{\gamma'}$  with  $0 < \gamma' < 1$ . Initially, the traps are scattered randomly and their subsequent mean-square displacement grows as  $t^{\gamma}$  with  $0 < \gamma \le 1$ . Instantaneous annihilation of the particle takes place upon contact with any of the traps. The solution to this problem is obtained by deriving lower and upper asymptotic bounds of the survival probability and showing that they converge to one another for long times, thereby unambiguously determining the long-time decay of P(t). For  $d \ge 2$  we find that at late times the survival probability is that of the pure target problem (the problem where the particle remains immobile) in agreement with previous studies for the d=1 case. These decay laws remain invariant over the whole  $\gamma$  range as opposed to the dynamical crossover observed for the case of a purely diffusive particle ( $\gamma'=1$ ) where, for  $\gamma < 2/(2+d)$ , the survival probability becomes that of the so-called trapping problem (the problem where the particle moves in a sea of static traps). This behavior implies that for sufficiently low values of  $\gamma(\gamma < 2/(2+d))$  the survival probability becomes singular in the limit  $\gamma' \to 1$ : trappinglike for  $\gamma'=1$  and targetlike for any  $\gamma' < 1$ .

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# I. INTRODUCTION

Encounter-controlled processes are widespread in nature. Examples include binary reactions [1-5], quenching of localized excitations [6,7], binding/unbinding kinetics in biological systems [8–12], and search-avoidance strategies in the framework of predator-prey models [13,14] to name but a few. In this context, stochastic transport processes leading to encounter between system constituents are often modeled as ordinary Brownian diffusion obtained from the appropriate limit of a Markovian random walk. However, memory effects arising from geometric constraints or from the complex nature of the constituents (due to internal degrees of freedom, say) may give rise to non-Markovian processes in space and time. A well-known example of the former is the self-avoiding walk [15,16], whose nonintersecting trajectories result in a superlinear growth of the mean-square displacement  $\langle r^2 \rangle$ .

In this paper, we will be concerned with processes where  $\langle r^2 \rangle$  grows sublinearly, i.e.,  $\langle r^2 \rangle \sim t^{\gamma}$  with  $0 < \gamma \le 1$  for long times. This kind of anomalous subdiffusive transport is frequently found in disordered and fractal media. An especially useful model for describing these systems is the continuous time random-walk (CTRW) model [17] with broad-tailed waiting time distributions [5,18–22]. As part of an ongoing research on subdiffusion-limited reactions, in the present work we shall use the mesoscopic fractional diffusion equation (FDE) outgrow of the CTRW [21,22] to discuss how the subdiffusive character of the reactants affects some classical reaction kinetics results for a given class of diffusioncontrolled encounter processes. More specifically, we shall deal with a system consisting of a strictly subdiffusive particle in a sea of subdiffusive or diffusive traps and investigate the long-time behavior of the survival probability P(t) of the particle. In order to place this problem in the appropriate perspective, we next review some previous results for the ordinary diffusion case.

The foundations of the theoretical description of diffusion-influenced kinetics were laid by the seminal work of Smoluchowski on the irreversible reaction  $A+B \rightarrow C$  [23–25]. He showed that under suitable conditions (i.e., negligible A-A and B-B interactions and large excess of one of the species, say B) the kinetics are essentially governed by the diffusive flow of the majority species B toward a *single* molecule of the minority species A. This allows one to obtain approximate expressions for the rate constant and the A-particle concentration decay. At late times, the corresponding survival probability P(t) of the A particle is given by the formula

$$P(t) \sim \begin{cases} \exp[-\rho 4(Dt/\pi)^{1/2}], & d = 1\\ \exp[-4\pi\rho Dt/\ln(Dt/(a+b)^2)], & d = 2\\ \exp[-d(d-2)v_d(a+b)^{d-2}\rho Dt], & d \ge 3, \end{cases}$$
(1)

where  $\rho$  is the mean density of traps, a and b are the radii of the A and B particle, respectively,  $D=D_A+D_B$  is the sum of the diffusion coefficients of the A and B species, and  $v_d=\pi^{d/2}/\Gamma(1+d/2)$  is the volume of a d-dimensional sphere of unit radius [25,26]. P(t) is not only related to the concentration of A particles but also to other relevant quantities such as the mean trapping time [27].

While Smoluchowski originally considered the situation where both A and B diffuse, it was later shown that his method is actually exact for the so-called *target problem*, where the target particle A is assumed to rest immobile [24,25] in a sea of diffusing traps. Conversely, an scenario with a diffusing A particle in a medium with randomly distributed *static* traps B is known as *trapping problem* in the literature. The long-time decay of P(t) in the d=1 trapping problem was first obtained by Balakurov and Vaks [28]. They also conjectured the form of the decay in higher dimensions by exploiting the analogy with the problem of computing the electron density of states in a medium with random

impurities [29,30]. This law was subsequently proved rigorously by Donsker and Varadhan and predicts a stretched-exponential decay [31],

$$P(t) \sim \exp[-k_d \rho^{2/(d+2)} (D_A t)^{d/(d+2)}],$$
 (2)

where  $k_d$  is the *d*-dependent constant [31],

$$k_d = \left(\frac{d+2}{2d}\right) (dv_d)^{2/(d+2)} (2z_1^2)^{d/(d+2)}.$$
 (3)

Here  $z_1$  is the first positive zero of the Bessel function  $J_{d/2-1}(z)$ .

The question now is how the exact asymptotic decay of P(t) looks like when *both* the *A* particle and the traps *B* are allowed to diffuse. For that case, Bramson and Lebowitz proved that the following decay law holds [32]:

$$P(t) \sim \begin{cases} \exp(-\rho c_d t^{1/2}), & d < 2\\ \exp(-\rho c_2 t / \ln t), & d = 2\\ \exp(-\rho c_d t), & d \ge 3 \end{cases}$$
 (4)

in agreement with Smoluchowski's prediction for the time dependence. However, to the general surprise, Bray and Blythe recently found [33,34] that the constants  $c_d$  are not simply functions of the relative diffusion coefficient D [for example,  $c_1$ =4 $(D_B/\pi)^{1/2}$ ]; i.e., these prefactors depend on the diffusion coefficient of the traps only.

The method used by Bray and Blythe consists of finding lower and upper bounds for P(t) and showing that they converge to one another in the long-time limit. The lower bound is obtained by introducing a notional volume centered about the initial A particle location and by requiring that neither traps have entered this volume nor have the particle reached its boundary from the inside up to time t, thereby ensuring that no reaction takes place. In turn, the upper bound is provided by the so-called Pascal principle, stating that the best strategy for the particle to survive is to stand still (a proof for a rather general class of walks can be found in [35]).

Let us now discuss the role played by the subdiffusive character of the two mobile species. The arguments of Bray and Blythe still prove valid in a series of situations where either the particle or both the particle and the traps move subdiffusively, and their stochastic motion is described by a FDE. In [36] this procedure was applied with partial success to the one-dimensional case. For concreteness, let us, respectively, denote by  $\gamma'$  and  $\gamma$  the exponent characterizing the growth of the mean-square displacement  $\langle r_A^2 \rangle$  of the A particle,  $\langle r_A^2(t) \rangle \sim t^{\gamma'}$ , and the corresponding quantity for the traps,  $\langle r_B^2(t) \rangle \sim t^{\gamma}$ . When  $0 < \gamma' < 1$  and  $0 < \gamma \le 1$  the survival probability at late times reads as [36]

$$P(t) \sim \exp[-2\sqrt{\rho^2 K_{\gamma} t^{\gamma}}/\Gamma(1+\gamma/2)], \qquad (5)$$

where  $K_{\gamma}$  is the anomalous diffusion coefficient of the traps (one has  $D_B \equiv \lim_{\gamma \to 1} K_{\gamma}$ ). Note that the time dependence can be straightforwardly obtained by making the simple replacement  $t \to t^{\gamma}$  in Bramson-Lebowitz formula (4) for the d=1 case. When  $\gamma'=1$  (ordinary diffusive particle), Eq. (5) was still found to hold provided that  $2/3 < \gamma \le 1$ . When  $\gamma=2/3$  the bounding procedure yields a behavior akin to the trapping problem scenario,  $P(t) \sim \exp(-\lambda t^{1/3})$ , although the

prefactor  $\lambda$  could only be bounded but not exactly determined in this way. Moreover, when  $\gamma'=1$  and  $0<\gamma<2/3$  the decaying behavior could not be exactly established owing to the fact that lower and upper bounds display a different time dependence and do not converge to each other. Numerical simulations for this case also failed to unequivocally determine the decay law [37].

In Ref. [38], this difficulty for the one-dimensional case with  $\gamma' = 1$  and  $0 < \gamma < 2/3$  was circumvented by introducing a new upper bound based on the so-called anti-Pascal principle. This principle states that the worst possible strategy for the traps to hit the particle is to remain immobile, implying that the trapping problem scenario should provide an upper bound for P(t). For  $\gamma \le 2/3$  this new upper bound turns out to be smaller than the one provided by the Pascal principle and sufficiently tight to converge to the lower bound, thereby allowing one to obtain the full picture for the d=1 case. One of the most remarkable aspects borne out by the calculations is the onset of a dynamical phase transition from targetlike behavior described by the generalized Bramson-Lebowitz formula when  $\gamma_c \le \gamma \le 1$  [cf. Eq. (5)] to trappinglike behavior given by Donsker-Varadhan formula (2) when  $0 < \gamma \le \gamma_c$  (where  $\gamma_c = 2/3$ ). In this latter regime formula (5) valid for  $0 < \gamma' < 1$  no longer holds, implying that the limit  $\gamma' \rightarrow 1$  becomes singular when the traps are sufficiently slow; i.e., for  $\gamma \le 2/3$  the decay kinetics is given by targetlike formula (5) as long as  $\gamma' < 1$ ; however, for  $\gamma' = 1$  the behavior turns out to be completely different, becoming a trappinglike kinetics described by (2). In d=2, a similar crossover from generalized Bramson-Lebowitz or target behavior for  $\gamma > \gamma_c$  to Donsker-Varadhan or trapping behavior for  $\gamma < \gamma_c$  was observed at the smaller value  $\gamma_c = 1/2$ . For  $d \ge 3$ , trappinglike behavior of the survival probability could be ascertained when  $\gamma < 2/(d+2)$ ; however, above this  $\gamma$ value neither the Pascal nor the anti-Pascal upper bound would converge to the lower bound. As a result of this limitation only upper and lower bounds for the characteristic decay exponent could be established.

In the present work, we apply the method employed by Bray and Blythe to extend the results obtained in [36] to d-dimensional media with  $d \ge 2$  or, from another perspective, to extend the results obtained in [38] to include the cases where the particle is subdiffusive. Similarly to the d=1, we shall demonstrate that in higher dimensions P(t) displays a targetlike behavior described by a Bramson-Lebowitz type formula for all dimensions d as long as the motion of the particle is strictly subdiffusive, i.e.,  $\gamma' < 1$ . Thus, the limit  $\gamma' \to 1$  becomes singular when  $\gamma < 2/(d+2)$ . In other words, a minute amount of subdiffusivity in the particle motion is seen to destroy the trappinglike or Donsker-Varadhan behavior observed for sufficiently slow traps when  $\gamma' = 1$ .

Finally, it should be noted that our procedure is not valid for  $\gamma$ =0 or  $\gamma'$ =0 (cf. Secs. III and IV). Therefore, one should not expect our results to hold neither for the subdiffusive target problem ( $\gamma'$ =0,0< $\gamma$ <1) nor for the subdiffusive trapping problem ( $\gamma$ =0,0< $\gamma'$ <1). For results regarding these special cases, see Refs. [19,20,39,40] and references therein.

The remainder of the paper is organized as follows. In Sec. II, we give a brief description of our analytical method

for arbitrary dimension. In Sec. III, we deal with the d=2 case and show that the long-time behavior of P(t) is of Bramson-Lebowitz type, i.e., targetlike when  $0 < \gamma' < 1$ . Subsequently, the analytic result for the decay exponent will be shown to be in good agreement with numerical simulations. Section IV is devoted to the  $d \ge 3$  case for which results along similar lines are obtained. Finally, Sec. V gives a summary of our main findings.

### II. OUTLINE OF THE METHOD

As already mentioned, the method for obtaining the asymptotic behavior of P(t) consists of finding lower and upper bounds for P(t) that converge to one another in the long-time limit. The upper bound is provided by the Pascal principle, which asserts that the best strategy for the particle to survive is to stand still. In other words, the survival probability in the target problem is an upper bound for P(t). This principle is not difficult to prove for the case of a subdiffusive particle and subdiffusive traps. The demonstration essentially follows from the arguments given in Ref. [38], Sec. IV, where it was shown that the anti-Pascal principle corresponding to a configuration with a mobile particle and static traps (trapping problem) provides an upper bound for the survival probability of a *normal* diffusive particle in a sea of subdiffusive traps. The key point is that the arguments given in that proof hold regardless of whether one has normal or subdiffusive motion. In what follows, we reproduce the main arguments slightly modified so that they are applicable to the situation of interest here. In Ref. [38] it was shown that for a system with a random distribution of constituents evolving independently from each other the survival probability of the A particle is

$$P(t) = E^{(a)} \{ e^{-\rho E^{(b)} \{ W[\mathbf{c}_t] \}} \}, \tag{6}$$

where the symbol  $E^{(x)}\{...\}$  denotes an average over all X particle trajectories  $\mathbf{x}_t$  and  $W[\mathbf{c}_t]$  is the volume swept by the "fictitious" particle C of radius a+b following the trajectory  $\mathbf{c}_t = \mathbf{a}_t - \mathbf{b}_t$ . Using Jensen's inequality we find

$$P(t) \le E^{(a)} \{ E^{(b)} \{ e^{-\rho W[\mathbf{c}_t]} \} \} \equiv E^{(c)} \{ e^{-\rho W[\mathbf{c}_t]} \}. \tag{7}$$

Now,  $W[\mathbf{c}_t]$  is a nondecreasing function of the number  $N=N_A+N_B$  of jumps made by the fictitious particle within the time interval (0,t), where  $N_A$  is the number of jumps performed by the A particle and  $N_B$  is the number of jumps made by a randomly chosen trap. Setting  $N_A=0$ , i.e., supposing that the particle is immobile (target problem), clearly diminishes the total number of jumps and hence diminishes  $W[\mathbf{c}_t]$  or at most leaves it unchanged. We therefore conclude that the survival probability in the target problem is an upper bound for P(t). As an aside, we note that a second upper bound for P(t) is obtained by setting  $N_B=0$  (immobile traps), which confirms the validity of the anti-Pascal principle.

Let us now turn on the computation of the lower bound. Consider a strictly subdiffusive  $(0 < \gamma' < 1)$  hyperspherical particle A of radius a in an infinite d-dimensional medium. We assume that at time t=0 an ensemble of subdiffusive hyperspherical traps B of radius b and mean density  $\rho$  are

randomly scattered in space. The A particle disappears upon contact with any of traps B. In order to compute a lower bound for the survival probability P(t) of the A particle, we consider a notional hypersphere  $V_R$  of radius R > a centered about the initial location of the A particle's center. The probability  $Q_1(R)$  that no traps overlap with  $V_R$  at time t=0 is easily obtained from the condition that the trap locations are statistically independent. In the thermodynamic limit (corresponding to infinite system size at constant density  $\rho$ ), one gets

$$Q_1(R) \sim \exp[-v_d \rho (R+b)^d]. \tag{8}$$

The second relevant quantity is the probability  $Q_2(R,t)$  that no traps invade the notional volume up to time t. Because of the spherical symmetry of the traps, this requirement is equivalent to prescribing that the centers of all the traps remain outside a hypersphere of radius R+b. For our purposes, we may regard this hypersphere as a target of radius R+b immersed in a sea of *pointwise* traps which is instantaneously destroyed as soon as any trap attains the surface of the hypersphere. One can then identify  $Q_2(R,t)$  with the survival probability of this target after an elapsed time t. The solution to this problem ("the target problem") reads as [39]

$$\begin{aligned}
Q_{2}(R;t) &= \begin{cases}
\exp\left(-\rho \frac{(4\pi K_{\gamma}t^{\gamma})^{d/2}}{\Gamma(1-d/2)\Gamma(1+\gamma d/2)}\right), & d < 2 \\
\exp\left(-\rho \frac{4\pi K_{\gamma}t^{\gamma}}{\Gamma(1+\gamma)\ln(4K_{\gamma}t^{\gamma}/(R+b)^{2})}\right), & d = 2 \\
\exp\left(-\rho \frac{2(d-2)\pi^{d/2}(R+b)^{d-2}K_{\gamma}t^{\gamma}}{\Gamma(d/2)\Gamma(1+\gamma)}\right), & d > 2.
\end{aligned}$$
(9)

The third quantity required to construct a lower bound is the probability  $Q_3(R,t)$  that the A particle has not attained the surface of  $V_R$  up to time t. Because of the symmetry of the problem, this probability is equal to the probability W(R-a,t) that the particle center does not leave a circle  $V_{R-a}$  of radius R-a. The quantity W(R,t) is calculated in the Appendix.

Once  $Q_3$  is known, one can construct  $Q(R,t) = Q_1(R)Q_2(R,t)Q_3(R,t)$ ; i.e., the joint probability that neither traps are inside  $V_R$  nor have traps reached the surface of  $V_R$  from the exterior and nor has the particle attained it from the interior by time t. If these conditions are met, the particle survives with certainty, and therefore Q(R,t) provides a lower bound for P(t). Subsequent maximization of Q(R,t) with respect to R provides a tight lower bound  $P_L(t) = Q(R_{\max},t)$  whose asymptotic time dependence will be seen to be the same as the upper bound  $P_U(t)$  obtained from the Pascal principle. Since  $P_L(t) \le P(t) \le P_U(t)$ , one eventually concludes that P(t) must satisfy the same asymptotic law as both bounds.

In what follows, we shall deal separately with the d=2 case and the higher dimensional case. In the former case the resulting expression for  $\ln P(t)$  contains a logarithmic term

typical for bidimensional random-walk problems, whereas in the latter case a generic form of  $\ln P(t)$  valid for any  $d \ge 3$  can be found.

## III. SURVIVAL PROBABILITY FOR d=2

In this case, an upper bound is provided by the Pascal principle, which states that the best strategy for the particle to survive is to stand still at the origin [35]. The asymptotic probability  $P_U(t)$  can then be directly obtained from Eq. (9) with d=2 and R=a,

$$P_U(t) = \exp\left[-\omega_2 \rho K_{\gamma} t^{\gamma} / \ln(4K_{\gamma} t^{\gamma} / (a+b)^2)\right], \tag{10}$$

where we have introduced  $\omega_2 = 4\pi/\Gamma(1+\gamma)$ .

Next, let us derive an asymptotic lower bound  $P_L(t)$  for the survival probability. To this end, we need explicit expressions for  $Q_1$ ,  $Q_2$  and  $Q_3$ . For d=2 Eq. (8) gives

$$Q_1(R) = \exp[-\pi\rho(R+b)^2].$$
 (11)

The probability that  $V_R$  remains devoid of traps up to time t is

$$Q_2(R,t) = \exp\left[-\frac{\omega_2 \rho K_{\gamma} t^{\gamma}}{\ln(4K_{\gamma} t^{\gamma}/(R+b)^2)}\right]. \tag{12}$$

Finally,  $Q_3(R,t)$  follows directly from Eq. (A18),

$$Q_3(R,t) = W(R-a,t) = \frac{(R-a)^2}{4\Gamma(1-\gamma')K_{\gamma'}t^{\gamma'}}.$$
 (13)

Our strategy to obtain  $P_L(t)$  will consist of tightening the lower bound by maximizing  $Q(R,t)=Q_1(R)Q_2(R,t)Q_3(R,t)$  with respect to R. The value  $R_{\max}(t)$  that maximizes Q(R,t) can be shown to obey the long-time decay

$$R_{\text{max}} \sim a + \frac{a+b}{\omega_2 \rho K_{\gamma} t^{\gamma}} \ln^2 \left( \frac{4K_{\gamma} t^{\gamma}}{(a+b)^2} \right).$$
 (14)

Therefore

$$P_{L}(t) = Q(R_{\text{max}}, t) \sim e^{-\pi \rho (a+b)^{2}} \exp\left[\frac{-\omega_{2} \rho K_{\gamma} t^{\gamma}}{\ln(4K_{\gamma} t^{\gamma}/(a+b)^{2})}\right] \times \frac{\ln^{4}\left(\frac{4K_{\gamma} t^{\gamma}}{(a+b)^{2}}\right) \left(\frac{a+b}{\omega_{2} \rho K_{\gamma} t^{\gamma}}\right)^{2}}{4\Gamma(1-\gamma')K_{\gamma'} t^{\gamma'}},$$
(15)

or, neglecting subdominant terms,

$$\ln P_L(t) \sim -\frac{\omega_2 \rho K_{\gamma} t^{\gamma}}{\ln[4K_{\gamma} t^{\gamma}/(a+b)^2]}, \quad t \to \infty.$$
 (16)

Note that the long-time behavior of  $\ln P_L(t)$  does not depend on  $\gamma'$ . This results from the fact that the  $\gamma'$  dependence enters Eq. (15) via inverse power law (13) obeyed by  $Q_3(R,t)$  and is thus subdominant with respect to the (up to logarithmic corrections) exponential dependence on  $t^{\gamma}$  displayed by  $Q_2(R,t)$ . This situation is radically different from the case where the A particle performs normal diffusion, where  $Q_2(R,t)$  is the same as previously but  $Q_3(R,t)$  decreases exponentially. Since  $P_L(t) \leq P_U(t)$ , and taking

into account Eq. (10) and the definition of  $\omega_2$ , we see that

$$\ln P(t) \sim -\frac{4\pi\rho K_{\gamma}t^{\gamma}}{\Gamma(1+\gamma)\ln(4K_{\gamma}t^{\gamma}/(a+b)^{2})}$$
(17)

for long times, which is our main result in this section. This law extends Bramson-Lebowitz result (4) to the case with subdiffusive particles and traps. When  $\gamma > 1/2$ , the result coincides with that obtained for  $\gamma' = 1$  in Ref. [38]. However, when  $0 < \gamma \le 1/2$ , the behavior displays a strong departure from the Donsker-Varadhan behavior observed for  $\gamma' = 1$  (cf. Eq. (2) and [38]). In this latter regime, Eq. (2) still predicts a behavior of the form  $\ln P(t) \propto -t^{1/2}$ , implying that the decay exponent is independent of  $\gamma$ , as opposed to Eq. (17). Therefore, we conclude that in this parameter region the limit  $\gamma' \to 1$  is singular. We defer a short discussion on the cause of this behavior to the end of Sec. IV.

In order to check the behavior predicted by Eq. (17), we have performed simulations for a periodic  $\mathcal{L} \times \mathcal{L}$  lattice (torus). In each system realization,  $\mathcal{L}^2\rho$  traps are initially assigned lattice sites at random (since they do not interact with each other, some traps may share the same site) and the A particle is placed at an arbitrarily chosen site. For t > 0 the A and B particles perform nearest-neighbor jumps governed by the Pareto waiting time distribution  $\psi(t) = \alpha/(1+t)^{1+\alpha}$ , with  $\alpha = \gamma'$  for the A particle and  $\alpha = \gamma$  for the B traps, so that on long-time scales this CTRW gives rise to anomalous diffusion with characteristic exponent  $\alpha$  and diffusion constant  $K_{\alpha}=1/[2d\Gamma(1-\alpha)]$ . Any other waiting time distribution with long-time power-law behavior  $\psi(t) \sim t^{-1-\alpha}$  would be suitable for simulation, but the Pareto distribution has the advantage that random waiting times t following this distribution can be easily generated from evaluation of the expression  $r^{1/\alpha}-1$ , where r is a uniformly distributed random number in the interval [0,1]. The chosen density  $\rho$  must be large enough to ensure that finite-size effects already become negligible for relatively small system sizes and that convergence is attained after a comparatively small number of realizations  $N_{real}$ ; however, it must also be small enough to guarantee that in most cases the walkers enter the diffusive regime well before a reactive collision takes place. In order to compute P(t), we record the survival time of the A particle in each individual realization and we then construct the cumulative histogram of realizations  $N(t_i)$  in which the particle has been destroyed before a given time  $t_i$ . From here we compute the mortality function  $F(t_i) = N(t_i)/N_{real}$  and the associated survival probability  $P(t_i) = 1 - F(t_i)$ .

Figure 1 shows a log-log plot of  $-\ln P(t)$  as a function of t obtained from numerical simulations for two different sets of exponents  $\gamma$  and  $\gamma'$ . According to Eq. (17),  $\ln[-\ln P(t)]$  should grow linearly in time up to a logarithmic correction which becomes unimportant for large t. For the case with  $\gamma$ =0.25 and  $\gamma'$ =0.5 (squares) a least-squares fit to the simulation results gives  $\gamma_{\text{sim}}$ =0.27, whereas for  $\gamma$ =0.5,  $\gamma'$ =0.75 (circles) the numerical fit gives  $\gamma_{\text{sim}}$ =0.46, in good agreement with the theoretically expected values. Deviations are most pronounced both for very short times (which is natural, as our results are expected to be valid for long times), and also for the longest simulated times due to the fact that the variance here is very large, as typically only a few successful

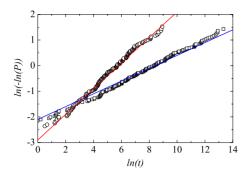


FIG. 1. (Color online) Simulation results for the survival probability of a subdiffusive particle with diffusion exponent  $\gamma'$  in a two-dimensional sea of subdiffusive traps with diffusion exponent  $\gamma$ , with  $\gamma$ =0.25 and  $\gamma'$ =0.5 (squares), and  $\gamma$ =0.5,  $\gamma'$ =0.75 (circles). As a guide to the eyes, we have drawn two lines with the theoretically predicted long-time slope  $\gamma$ . The simulation parameters are  $\mathcal{L}$ =41,  $\rho$ =0.05, and  $N_{real}$ =200.

realizations of long-lived untrapped A particles contribute to the histogram at late times. Even though the theoretical and simulation exponents disagree only by a few per cent, this is enough for impeding any sensible simulation estimate of the prefactor  $\omega_2 \rho K_{\gamma}$  appearing on the rhs of Eq. (17). In contrast, the two cases displayed in Fig. 1 show a remarkable agreement between the simulation results and asymptotic formula (17) even at not very long times (compared to the typical time needed by the A particle to scan the whole system). This is rather fortunate for our purposes since our simulations turn out to be very time consuming because of the need for a detailed bookkeeping and painstaking ordering of the jump times drawn from the Pareto distribution.

## IV. SURVIVAL PROBABILITY FOR $d \ge 3$

Here, we shall apply a similar strategy as in two dimensions for obtaining the asymptotic survival probability P(t) of a particle surrounded by a d-dimensional sea of traps with d > 3

The upper bound provided by the Pascal principle reads as [cf. Eq. (9) and R=a]

$$P(t) \le P_{II}(t) = \exp\left[-\omega_d \rho (a+b)^{d-2} K_{\mathcal{A}} t^{\gamma}\right]$$
 (18)

with  $\omega_d = 2(d-2)\pi^{d/2}/[\Gamma(d/2)\Gamma(1+\gamma)]$ . As discussed in Sec. II, a lower bound of P(t) is given by  $Q(R,t) = Q_1(R)Q_2(R,t)Q_3(R,t)$ . We know [cf. Eq. (8)] that  $Q_1(R) = \exp[-v_d\rho(R+b)^d]$ . The probability  $Q_2$  can be identified as the survival probability of a spherical target of radius R+b and one has [cf. Eq. (9)]

$$Q_2(R,t) = \exp\left[-\omega_d(R+b)^{d-2}\rho K_{\gamma}t^{\gamma}\right]. \tag{19}$$

Finally, by using Eq. (A18) one finds

$$Q_3(R,t) = W(R-a,t) \approx \frac{2^{2-d/2} \alpha_d(1)(R-a)^2}{\Gamma(d/2)\Gamma(1-\gamma')K_{\gamma'}t^{\gamma'}}.$$
 (20)

The coefficient  $\alpha_d(1)$  is expressed in the Appendix in the form of a series. For the three-dimensional case  $\alpha_3(1) = \sqrt{\pi/288}$ .

Let us now obtain the lower bound  $P_L(t)$ . We know that  $Q(R,t) = Q_1(R)Q_2(R,t)Q_3(R,t)$  provides a lower bound for P(t) and, as in the bidimensional case, our strategy to obtain  $P_L(t)$  will consist of tightening the lower bound by maximizing Q(R,t) with respect to R. The value  $R_{\max}(t)$  that maximizes Q(R,t) is given by

$$R_{\text{max}}(t) = a + \frac{1}{\rho} \frac{(a+b)^{3-d}}{2(d-2)\omega_d K_{\mathcal{A}} t^{\gamma}},$$
 (21)

for long times. Therefore

$$P_L(t) = Q(R_{\rm max}, t) \sim \frac{2^{2-d/2} \alpha_d(1) (R_{\rm max} - a)^2}{\Gamma(d/2) \Gamma(1 - \gamma') K_{\gamma'} t^{\gamma'}}$$

$$\times \exp[-v_d\rho(a+b)^d - \omega_d(a+b)^{d-2}\rho K_{\chi}t^{\gamma}],$$
 (22)

or neglecting subdominant terms,  $\ln P_L(t) \sim -\omega_d(a+b)^{d-2}\rho K_\gamma t^\gamma$ . As in the two-dimensional case,  $\ln P_L(t)$  becomes  $\gamma'$ -independent in the long-time regime as a result of the  $t^{-\gamma'}$  behavior displayed by  $Q_3(R,t)$ . Comparing this expression with the upper bound  $P_U(t)$  we see that both converge to

$$\ln P(t) \sim -\omega_d(a+b)^{d-2}\rho K_{\gamma}t^{\gamma}. \tag{23}$$

In particular, for the physically most relevant case of d=3 we get

$$\ln P(t) \sim -\frac{4\pi(a+b)}{\Gamma(1+\gamma)} \rho K_{\gamma} t^{\gamma}$$
 (24)

for long times.

Thus, we find again generalized Bramson-Lebowitz behavior, implying that the replacement  $t \rightarrow t^{\gamma}$  in Eq. (4) provides the correct time dependence. Note that our method also provides an analytic expression for the prefactor appearing in the power law. In contrast, the prefactor could not be computed in the purely diffusive case  $\gamma = \gamma' = 1$ , where the bounding method is only able to provide a pair of bounds for the constant  $c_3$  [34]. Let us now compare the result provided by Eq. (24) with the behavior observed when  $\gamma' = 1$ . As anticipated in the introduction, Donsker-Varadhan law (2) was found to hold below  $\gamma = 2/(2+d)$ , i.e.,  $\ln P(t) \propto t^{d/(2+d)}$  in this regime. In contrast, Eq. (24) predicts  $\ln P(t) \propto -t^z$  with  $z = \gamma$ for any  $\gamma' < 1$ . Therefore, as in the d=2 case, the limit  $\gamma' \rightarrow 1$  is again singular. On the other hand, when  $\gamma'=1$  and  $2/(d+2) \le \gamma < d/(d+2)$ , one has  $d/(d+2) \le z$  $\leq (d-2+2\gamma)/d$  [38]. Thus, in this parameter region z is strictly larger than  $\gamma$ , which is the prediction of Eq. (24). Finally, when  $d/(d+2) \le \gamma \le 1$ , one has  $\gamma \le z \le (d-2+2\gamma)/d$ ; as a result of this, Eq. (24) might still hold in this regime since the predicted exponent coincides with the lower bound determined in [38].

At this stage, a more detailed discussion on the singular character of P(t) in the  $\gamma'=1$  limit is in order. As we have seen, this singularity appears when one switches from the  $t^{-\gamma'}$  long-time behavior of  $Q_3(R,t)$  in the  $0 < \gamma' < 1$  region [Eqs. (13) and (20)] to the exponential regime of  $Q_3(R,t)$  at  $\gamma'=1$ . Had we used  $\ln Q_3(R,t) \sim -t$  in our calculations, then we would have indeed recovered the results in [38]. In the Appendix we show that the singular  $\gamma'$ -dependence of

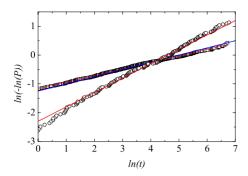


FIG. 2. (Color online) Simulation results for the survival probability of a subdiffusive particle with diffusion exponent  $\gamma'$  in a three-dimensional sea of subdiffusive traps with diffusion exponent  $\gamma$ , with  $\gamma$ =0.25 and  $\gamma'$ =0.5 (squares), and  $\gamma$ =0.5,  $\gamma'$ =0.75 (circles). We have drawn as a guide to the eyes two lines with the theoretically predicted long-time slope  $\gamma$ . The simulation parameters are  $\mathcal{L}$ =41,  $\rho$ =0.1, and  $N_{real}$ =500.

 $Q_3(R,t)$  stems from the fact that for large arguments the Mittag-Leffler function follows the law  $E_{\alpha}(z) \sim 1/z$  for  $\alpha < 1$  and  $E_{\alpha}(z) = \exp(-z)$  for  $\alpha = 1$ . As a result of this, the long-time behavior of W(R,t) as given by (A13) is also singular when  $\gamma' \rightarrow 1$ . The character and implications of this singularity become more transparent in Laplace space. The Laplace transform of the Mittag-Leffler function is  $\mathcal{L}[E_{\alpha}(-t^{\alpha})] = s^{\alpha-1}/(1+s^{\alpha})$ . When  $\alpha=1$  we recover the Laplace transform of the exponential  $\mathcal{L}[\exp(-t)] = 1/(1+s)$ ]. However, for  $\alpha < 1$  the small-s (long-time) behavior of the Laplace transform is quite different,  $\mathcal{L}[E_{\alpha}(-t^{\alpha})] \sim s^{\alpha-1}$ , i.e., one has power-law behavior no matter how close  $\alpha$  gets to 1; in other words, the two limits  $\alpha \rightarrow 1$  and the long-time limit  $t \rightarrow \infty$  are not interchangeable. Note that the closer  $\alpha$  gets to 1, the smaller s [the larger t] must become for the power-law behavior to show up.

Figure 2 shows simulations which have been carried out for a periodic  $\mathcal{L} \times \mathcal{L} \times \mathcal{L}$  lattice along the same lines as the ones for the two-dimensional case. For the case  $\gamma$ =0.25 and  $\gamma$ '=0.5 (squares) we get the numerical fit  $\gamma$ <sub>sim</sub>=0.23, whereas for the case  $\gamma$ =0.5,  $\gamma$ '=0.75 (circles) we find  $\gamma$ <sub>sim</sub>=0.51. We thus see that the difference between the numerical estimates and the theoretical values lies in the same order of magnitude as in the previous section. Once again, we find that these simulation results behave as predicted by asymptotic formula (24) even for not too long times.

#### V. CONCLUSIONS

We have determined the long-time behavior of the survival probability P(t) of a subdiffusive particle in a d-dimensional Euclidean media doped with noninteracting mobile (subdiffusive or normal diffusive) traps. We find that this behavior is targetlike, i.e., the survival probability of the subdiffusive particle is asymptotically equal to the survival probability of a static particle surrounded by the sea of mobile traps. Thus, P(t) is given by Bramson-Lebowitz formula (4) if one performs the replacement  $t \rightarrow t^{\gamma}$  and uses the prefactors  $c_2 = 4\pi K_{\gamma}/(1+\gamma)$  and  $c_d = 2(d-2)\pi^{d/2}(a+b)^{d-2}K_{\gamma}/[\Gamma(d/2)\Gamma(1+\gamma)]$  for  $d \ge 3$ . The

above behavior is at odds with Donsker-Varadhan behavior (2) observed when the particle is normal diffusive  $(\gamma'=1)$  and  $0 < \gamma \le 2/(2+d)$ .

Quite remarkably,  $\ln P(t)$  is found not to depend on  $\gamma'$  or  $K_{\gamma'}$  in the long-time regime. Physically, this conclusion is certainly striking but not completely unexpected in view of previous works by Bray and Blythe [33,34]. For systems with  $d \le 2$  these authors established that when both the particle and the traps perform normal diffusion the long-time survival probability does not depend on the diffusion coefficient of the particle. It would then seem natural to interpret these results using similar arguments to those put forward by Bray  $et\ al.\ [41]$  for the normal diffusion problem, namely, that the dominant contribution to the long-time survival probability arises solely from the subset of trajectories where the A particle remains stationary.

The present work extends the series of results presented in [36,38] to the higher dimensional case where both interacting species are subdiffusive. Thus, results for arbitrary dimension are now available when  $0 < \gamma' < 1$  and  $0 < \gamma \le 1$ .

In contrast, analytic results are more scarce for the case  $\gamma'=1$ . For d=1 and d=2 the behavior has been determined in detail for all  $\gamma$ , including the aforementioned transitions from targetlike to trappinglike behavior (i.e., from Bramson-Lebowitz formulas to Donsker-Varadhan formulas). However, for  $d \ge 3$  and  $\gamma > 2/(2+d)$ , neither the exponent of the time nor the prefactor  $c_d$  in the argument of the exponential are known (although there exist bounds for the exponent). Thus, the determination of these quantities requires an alternative route to the refinement of the upper bound, since it is difficult to conceive upper bounds other than the "natural" ones provided by the Pascal and anti-Pascal principle. In contrast, the lower bound used in [38] and in the present work is based upon rather restrictive assumptions, for this reason there is some hope that a procedure to refine the lower bound can be developed in the future.

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# APPENDIX: PROBABILITY THAT A SUBDIFFUSIVE PARTICLE REMAINS INSIDE A d-DIMENSIONAL HYPERSPHERICAL VOLUME

Let P(r,t)dr be the probability to find a *point* particle at a distance between r and r+dr from the origin after an elapsed time t; this distribution function P(r,t) obeys the subdiffusion equation

$$\frac{\partial P(r,t)}{\partial t} = K_{\gamma'} \,_0 D_t^{1-\gamma'} \left( \frac{\partial^2 P(r,t)}{\partial r^2} + \frac{d-1}{r} \frac{\partial P(r,t)}{\partial r} \right), \text{ (A1)}$$

where  $K_{\gamma'}$  is the anomalous diffusion coefficient of the A particle (the limit  $\lim_{\gamma'\to 1}K_{\gamma'}=D_A$  corresponds to the ordi-

nary diffusion case). The nonlocal integrodifferential operator

$${}_{0}D_{t}^{1-\gamma'}P(r,t) = \frac{1}{\Gamma(\gamma')}\frac{\partial}{\partial t}\int_{0}^{t}dt'\frac{P(r,t')}{(t-t')^{1-\gamma'}},\qquad(A2)$$

is the Riemann-Liouville fractional derivative of P(r,t) with respect to time. This operator reflects memory effects typically arising from a CTRW characterized by a broad waiting time distribution. Such a random walk is indeed known to lead to Eq. (A1) in the diffusion limit [22].

We must find the solution of Eq. (A1) that complies with the initial condition  $P(r,0)=\delta(\mathbf{r})$ , the absorbing boundary condition P(R,t)=0 (which describes the fact that at r=R the point particle is absorbed and disappears), and the (implicit) condition that P(r,t) remains finite everywhere (and in particular at the origin). To this end we will use the method of separation of variables and set P(r,t)=T(t)X(r). This ansatz leads to

$$\frac{T'(t)}{K_{\gamma',0}D_t^{1-\gamma'}T(t)} = \frac{X''(r) + (d-1)X'(r)/r}{X(r)} = \lambda, \quad (A3)$$

where  $\lambda$  is a constant. The solution of the equation

$$T'(t) = \lambda K_{\gamma'} {}_{0}D_{t}^{1-\gamma'}T(t) \tag{A4}$$

for the time dependence of P(r,t) is known as [22]

$$T(t) = E_{\gamma'}(\lambda K_{\gamma'} t^{\gamma'}) \tag{A5}$$

where

$$E_{\gamma'}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(1 + n\gamma')}$$
 (A6)

is the Mittag-Leffler function [42]. The equation and boundary conditions that determine the spatial part X(r) of the solution are exactly the same as for the normal diffusive case; we can thus solve this problem as usual and find that there are only valid solutions when  $\lambda = \lambda_j \equiv -z_j^2/R^2$  (eigenvalues),  $z_j$  being the j-th positive zero of the Bessel function of the first kind and order d/2-1, i.e.,  $J_{d/2-1}(z_j)=0$ . The corresponding solutions (eigenfunctions) are

$$X_{i}(r) = r^{1-d/2} J_{d/2-1}(z_{i}r/R).$$
 (A7)

Therefore, the general solution of this problem is

$$P(r,t) = \sum_{j=1}^{\infty} c_j X_j(r) T_j(t)$$

$$= \sum_{j=1}^{\infty} c_j r^{1-d/2} J_{d/2-1} \left( \frac{z_j r}{R} \right) E_{\gamma'} \left( -z_j \frac{K_{\gamma'} t^{\gamma'}}{R} \right). \quad (A8)$$

The coefficients  $c_j$  can be determined using the orthogonality properties of the Bessel functions. In particular, from

$$\int_{0}^{1} x J_{\alpha}(z_{j}x) J_{\alpha}(z_{m}x) dx = \frac{1}{2} J_{\alpha+1}^{2}(z_{j}) \delta_{m,j}$$

one gets

$$\langle X_m | X_j \rangle = \frac{1}{R^2} \int_0^R r^{d-1} X_m(r) X_j(r) dr = \frac{1}{2} J_{d/2}^2(z_j) \, \delta_{mj} = ||X_j||^2 \, \delta_{mj}$$

so that

$$c_j = \frac{\langle X_j | P(r,0) \rangle}{\|X_j\|^2}.$$
 (A9)

Our Dirac delta initial condition can be expressed as

$$P(r,0) = \delta(\mathbf{r}) = \frac{\delta_{+}(r)}{s_{d}(r)}$$
(A10)

where the  $\delta_+(r)$  is the slightly modified delta function with the property  $\int_0^R \delta_+(r) dr = 1$  for any R > 0, and

$$s_d(r) = \frac{2\pi^{d/2}r^{d-1}}{\Gamma(d/2)}$$

is the surface of a *d*-dimensional hypersphere of radius *r*. Inserting Eq. (A10) into Eq. (A9) and using the property that  $J_{\alpha}(x) \rightarrow (x/2)^{\alpha}/\Gamma(1+\alpha)$  for  $x \rightarrow 0$ , one readily finds

$$c_j = \left(\frac{z_j}{2R}\right)^{d/2 - 1} \frac{1}{\pi^{d/2} R^2 J_{d/2}^2(z_i)}.$$
 (A11)

Therefore Eq. (A8) becomes

$$\begin{split} P(r,t) &= \sum_{j=1}^{\infty} \left(\frac{z_{j}}{2R}\right)^{d/2-1} \frac{r^{1-d/2}}{\pi^{d/2} R^{2} J_{d/2}^{2}(z_{j})} J_{d/2-1} \left(\frac{z_{j} r}{R}\right) E_{\gamma'} \\ &\times \left[ -\left(\frac{z_{j}}{R}\right)^{2} K_{\gamma'} t^{\gamma'} \right]. \end{split} \tag{A12}$$

The probability that a subdiffusive particle has not reached the surface of a hypersphere of radius R by time t is then

$$\begin{split} W(R,t) &= \int_{0}^{R} s_{d}(r) P(r,t) dr \\ &= \frac{2^{2-d/2}}{\Gamma(d/2)} \sum_{j=1}^{\infty} \frac{z_{j}^{d/2-2}}{J_{d/2}(z_{j})} E_{\gamma'} \left[ -\left(\frac{z_{j}}{R}\right)^{2} K_{\gamma'} t^{\gamma'} \right]. \end{split} \tag{A13}$$

For d=3, this formula adopts an especially simple form

$$W(R,t) = 2\sum_{i=1}^{\infty} (-1)^{j} E_{\gamma'}(-j^{2} \pi^{2} K_{\gamma'} t^{\gamma'}/R^{2}).$$
 (A14)

For  $\gamma'=1$  one recovers the corresponding normal diffusive equations for P(r,t) and W(R,t) [43,44],

Since we are interested in the long-time reaction kinetics, we can use the following asymptotic expansion of the Mittag-Leffler function [42]

$$E_{\gamma'}(-z) \sim \sum_{n=1}^{\infty} \frac{(-1)^{m+1}}{\Gamma(1-m\gamma')} z^{-m}, \quad z \to \infty$$
 (A15)

and get

(A18)

$$W(R,t) \sim \frac{2^{2-d/2}}{\Gamma(d/2)} \sum_{m=1}^{\infty} \frac{(-1)^{m+1} \alpha_d(m)}{\Gamma(1-m\gamma')} \left(\frac{R^2}{K_{\gamma'}t^{\gamma'}}\right)^m$$
(A16)

with

$$\alpha_d(m) = \sum_{i=1}^{\infty} \frac{z_j^{d/2 - 2m - 2}}{J_{d/2}(z_i)}.$$
 (A17)

For  $t \rightarrow \infty$  we can approximate Eq. (A16) by its dominant term

- then be easily calculated for m=1:  $\alpha_1(1) = \sqrt{\pi/32}$  and  $\alpha_3(1) = \sqrt{\pi/288}$ . Evaluation for other values of d is much more involved, but eventually it is possible to prove that  $\alpha_d(1) = 2^{d/2-3}\Gamma(d/2)/d$  [45]. In particular, one gets d=2 for  $\alpha_2(1) = 1/8$ . Note, however, that it is not necessary to know the actual value of  $\alpha_d(m)$  in order to get the long-time
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asymptotic behavior of P(t) for all d [see Eqs. (17) and (23)].

 $W(R,t) \sim \frac{2^{2-d/2}\alpha_d(1)R^2}{\Gamma(d/2)\Gamma(1-\gamma')K_{\gamma'}t^{\gamma'}}.$ 

For d=1 and d=3, the Bessel functions can be written in

terms of circular functions and the sum (A17) can

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