Survival probability of a diffusing particle in the presence of Poisson-distributed mobile traps

R. A. Blythe[1] and A. J. Bray[1,2]

[1]*Department of Physics and Astronomy, University of Manchester, Manchester M13 9PL, United Kingdom*
[2]*Laboratoire de Physique Quantique (UMR C5626 du CNRS), Université Paul Sabatier, 31062 Toulouse Cedex, France*

The problem of a diffusing particle moving among diffusing traps is analyzed in general space dimension d. We consider the case where the traps are initially randomly distributed in space, with uniform density ρ, and derive upper and lower bounds for the probability $Q(t)$ (averaged over all particle and trap trajectories) that the particle survives up to time t. We show that, for $1 \leq d \leq 2$, the bounds converge asymptotically to give $Q(t) \sim \exp(-\lambda_d t^{d/2})$ for $1 \leq d < 2$, where $\lambda_d = (2/\pi d)\sin(\pi d/2)(4\pi D)^{d/2}\rho$ and D is the diffusion constant of the traps, and that $Q(t) \sim \exp(-4\pi\rho Dt/\ln t)$ for $d=2$. For $d>2$ bounds can still be derived, but they no longer converge for large t. For $1 \leq d \leq 2$, these asymptotic forms are independent of the diffusion constant of the particle. The results are compared with simulation results obtained using a new algorithm [V. Mehra and P. Grassberger, Phys. Rev. E **65**, 050101 (2002)] which is described in detail. Deviations from the predicted asymptotic forms are found to be large even for very small values of $Q(t)$, indicating slowly decaying corrections whose form is consistent with the bounds. We also present results in $d=1$ for the case where the trap densities on either side of the particle are different. For this case we can still obtain exact bounds but they no longer converge.

I. INTRODUCTION

Reaction-diffusion processes represent a large and important class of systems with nonequilibrium dynamics. From a fundamental physical viewpoint, the interest in these systems lies in the fact that the concentration of reactants is governed, in general, by irreversible reaction events that depend on the spatial distribution of particles rather than through equilibrium fluctuations controlled by a chemical potential. Such model systems have a range of applications, most notably to chemical kinetics [1,2] but also to interfacial growth [3], domain coarsening [4,5], and aggregation [6].

The most intensively studied reactions are single-species annihilation ($A+A \rightarrow \varnothing$) and coalescence ($A+A \rightarrow A$) as well as two-species annihilation ($A+B \rightarrow \varnothing$)—see, e.g., Refs. [7–9] for reviews. In this paper we focus on the two-species problem. It is known to exhibit two different classes of long-time behavior depending on whether the initial concentrations of A and B particles are equal or not. (As an aside, we note that a similar dependence on the initial condition also holds for the $A+A \rightarrow \varnothing$ reaction when the reactant motion is deterministic rather than diffusive [10,11]). The reason for this is that when the initial densities of A and B particles are the same, they remain so for all times, whereas if, say, the initial density of A particles $\rho_A(0)$ is less than that of the B particles $\rho_B(0)$, the ratio $\rho_A(0)/\rho_B(0) \rightarrow 0$ as $t \rightarrow \infty$ and at late times one has a few, isolated A particles diffusing in a background of B particles.

The case of equal initial densities is well understood, and results similar to those for the $A+A \rightarrow \varnothing$ with diffusive particle motion have been obtained [12,13]. In low dimensions, here $d<4$, fluctuation effects are important and one finds a density decay $\rho_A(t) = \rho_B(t) \sim t^{-d/4}$ in this *diffusion-limited* regime. Above the critical dimension $d>d_c=4$ one finds that the mean-field result $\rho_{A,B}(t) \sim 1/t$ applies. This result

also holds for the $A+A \rightarrow \varnothing$ process above its critical dimension $d_c=2$.

By contrast, the density decay forms for the $A+B \rightarrow \varnothing$ process when the initial densities $\rho_A(t)$ and $\rho_B(t)$ are not equal are less well understood. In fact, since the exposition of the process as a model of monopole-antimonopole annihilation in the early universe nearly twenty years ago [12], only a few results are known exactly. Most notably, Bramson and Lebowitz [14] proved rigorously that, at large times, the density of the minority species (which we will take to be the A particles) behaves as

$$\rho_A(t) \sim \begin{cases} \exp(-\lambda_d t^{d/2}), & d<2 \\ \exp(-\lambda_2 \ln t/t), & d=2 \\ \exp(-\lambda_d t), & d>2 \end{cases} \tag{1}$$

revealing $d=2$ to be critical in this case. To the best of our knowledge, no predictions for the constants λ_d were given until recently [15]. Furthermore, there has been no convincing numerical verification of the predicted decay even in one dimension, despite the development of sophisticated simulation techniques [16] that allow the probing of extremely small densities that emerge at large times. In this paper, we expand on the bounding arguments reported in Ref. [15] that give rise to precise values of λ_d for $d \leq 2$. We also present a detailed description of the simulation algorithm introduced in Ref. [16] and extend it to test our bounding arguments and understand the approach to the asymptopia described by Eq. (1).

As noted above, the late-time regime is characterized by a few isolated A particles diffusing in a sea of B particles. Thus it is appropriate to consider the extreme case of a single A particle in a sea of B particles that has a uniform (Poisson) density. In this case, the quantity $\rho_A(t)$ is just the *survival probability* of the A particle. Furthermore, if the diffusion

constants of the A and B particles are the same, one can also view $\rho_A(t)$ as the fraction of particles that have not met any other particles. Thus the reaction $A+B\rightarrow\varnothing$ in the limit of a low density of A particles has been discussed under the guises of *uninfected walkers* [17] in which random walkers infect each other on contact, *diffusion in the presence of traps* [16,18] in which the B particles are considered as traps for the A particles, and *predator-prey models* [19] in which one asks for the survival of a prey (the A particle) being chased by diffusing predators (the B particles). To avoid confusion, we shall adopt only the trapping terminology in our discussion.

In this work, we show how the survival probability of a diffusing particle in the presence of mobile traps can be understood in terms of the *target annihilation problem* [20–22] (or first passage problem [23]) where one asks for the probability that none of the traps has entered a particular region (target) in the d-dimensional space. In turn, the asymptotics of the target annihilation problem are intimately related to the *recurrence* or *transience* of diffusion in various dimensions. A process is said to be recurrent if the probability of returning to the initial configuration is unity. In the context of diffusion, this implies that with probability one, a walker will visit a particular point in space infinitely often. It is well known (see, e.g, Refs. [23,24]) that diffusion is recurrent in dimensions $d\le 2$, whereas in more than two dimensions it is transient (i.e., the return probability is less than one). It is precisely this property of diffusion that gives rise to the critical dimension of two for the trapping reaction and hence the asymptotic results (1) for the $A+B\rightarrow\varnothing$ process.

The principal result of the paper is the determination of the constants λ_d in Eq. (1) for $d\le 2$, and the derivation of upper and lower bounds for $d=3$. A striking feature of the results is that, for $d\le 2$, the value of λ_d is independent of the diffusion constant of the A particle.

We begin in the following section of this paper by defining the trapping reaction model. Then, in Sec. III we present in detail our analysis of the one-dimensional case, testing our predictions in Sec. IV where we discuss how the model may be simulated efficiently. In Sec. V, we show how the method used to treat the one-dimensional case can be extended to general dimensions $d>1$. Only when the underlying diffusion process is recurrent (i.e., for $d\le 2$) do our upper and lower bounds converge asymptotically to give exact predictions for λ_d. Finally, in Sec. VI, we present a discussion and summary of the results.

II. DEFINITION OF THE MODEL

The trapping reaction model we consider is defined as follows. At time $t=0$ a particle is placed at the origin of a d-dimensional coordinate system. Surrounding this particle is a uniform sea of traps whose initial positions $\vec{x}_i$ are chosen independently. This initial condition ensures that the distribution of traps is Poisson, i.e., the probability that a volume V contains N traps is $[(\rho V)^N/N!]\exp(-\rho V)$ in which ρ is the mean number of traps per unit volume.

The dynamics of the particle and traps can be expressed using the Langevin equation

$$\dot{x}_i^\alpha = \eta_i^\alpha(t) \tag{2}$$

in which the subscript $i=0$ denotes the particle, $i\ge 1$ one of the traps and the superscript α indicates a component of the position vector $\vec{x}_i$. The noise $\eta_i^\alpha(t)$ is a Gaussian white noise with zero mean and correlator

$$\langle \eta_i^\alpha(t)\eta_j^\beta(t')\rangle = 2D_i\delta_{ij}\delta_{\alpha\beta}\delta(t-t'). \tag{3}$$

We take all the traps to have a diffusion constant D and the particle to have a diffusion constant D'. Hence $D_0=D'$ and $D_i=D$ for $i>0$. The quantity of interest in this model is the probability $Q(t)$, averaged over all initial conditions and realizations of the random walks, that the particle has not yet met any of the diffusing traps.

III. ANALYTICAL RESULTS IN ONE DIMENSION

For clarity, we restrict ourselves initially to the case $d=1$. Later, in Sec. V we will explain how the arguments presented in detail here can be generalized to higher dimensions. We begin with a description of the target annihilation problem before moving on to discuss how it applies to the more general problem of a particle's survival in a sea of diffusing traps. The target annihilation problem can be solved exactly for any d [20–22]. The asymptotic form of the solution, and the leading corrections to it (for $d>1$), play a central role in our bounding arguments. To establish the notation and to make our presentation self-contained, we present in this paper a brief derivation of the main results as a prelude to deriving the bounds.

A. The target annihilation problem

Consider a one-dimensional line containing a target of length $2l$ centered on the origin (i.e., lying between $x=-l$ and $x=l$). We wish to calculate the probability $Q_T(t)$ that none of the diffusing traps initially placed outside this region has hit the target by a time t. This quantity can be calculated if one knows the probability $Q_1(t|y)$ that a trap initially at position y has not yet entered the target region. Since the target is static and each trap executes independent diffusion, we can simply multiply the probabilities for each individual trap together and average over all possible initial positions to find $Q_T(t)$.

Let us consider then a trap that has its initial position to the right of the target, i.e., $y>l$. The probability $Q_1(t|y)$ that the trap has not reached the target satisfies the backward Fokker-Planck equation

$$\frac{\partial Q_1(t|y)}{\partial t} = D\frac{\partial^2 Q_1(t|y)}{\partial y^2} \tag{4}$$

with the boundary conditions $Q_1(t|l)=0$, $Q_1(0|y)=1$ if $y>l$ and $Q_1(t|\infty)=1$. These express the facts that the probability that the target has been reached if the trap started at $y=l$ is one, that it is reached in zero time from $y>l$ is zero

and that it is reached from infinity *in a finite time* is zero respectively. The solution to Eq. (4) that satisfies these boundary conditions is

$$Q_1(t|y) = \text{erf}\left(\frac{y-l}{\sqrt{4Dt}}\right) \tag{5}$$

in which erf(x) is the error function.

Instead of a single trap to the right of the target, consider N independently diffusing traps, each initially placed at random in the interval $y_i \in [l, l+L]$. Then, the probability that none of the traps has reached the target by time t is

$$Q_N(t) = \prod_{i=1}^{N} \frac{1}{L} \int_l^{l+L} dy_i \, \text{erf}\left(\frac{y_i-l}{\sqrt{4Dt}}\right). \tag{6}$$

It is convenient now to rewrite the error function in terms of the complementary error function, erf(x) = 1 − erfc(x). Then one has

$$Q_N(t) = \left[1 - \frac{1}{L} \int_l^{l+L} dy \, \text{erfc}\left(\frac{y-l}{\sqrt{4Dt}}\right)\right]^N. \tag{7}$$

Since we wish to consider an infinite sea of traps, we take $N = \rho L$ and then the limit $L \to \infty$ holding ρ, the density of traps, fixed. This yields

$$Q_\infty(t) = \lim_{L\to\infty} \left[1 - \frac{1}{L} \int_l^{l+L} dy \, \text{erfc}\left(\frac{y-l}{\sqrt{4Dt}}\right)\right]^{\rho L}$$

$$= \exp\left(-\frac{2\rho\sqrt{Dt}}{\sqrt{\pi}}\right). \tag{8}$$

This gives the probability that no traps initially positioned on one side of the target have reached the target by time t. Since we have in mind a target surrounded on both sides by traps, and that the motion on each side is independent, we obtain the probability that the target has not been annihilated by a trap by squaring Eq. (8). That is,

$$Q_T(t) = \exp\left(-\frac{4\rho\sqrt{Dt}}{\sqrt{\pi}}\right). \tag{9}$$

Note that the size of the one-dimensional target l does not appear in this exact expression for its survival probability. Later, in Sec. V, we will find that at suitably large times, the size of the target is unimportant for all $d < 2$ (where diffusion is recurrent).

B. Bounding argument for a diffusing particle in the presence of mobile traps

We now discuss how to construct upper and lower bounds on the particle's survival probability $Q(t)$ using the result for the target annihilation problem (9) in one dimension. We claim that, on average, a particle surrounded by a uniform, isotropic distribution of traps survives longer if it is stationary than if it is allowed to diffuse. We are currently unable to
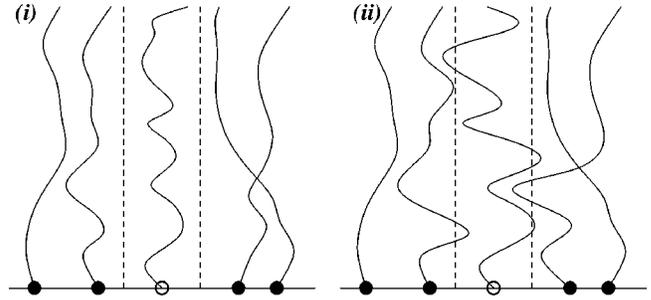
FIG. 1. Two walker trajectories (space-time plots, with $t = 0$ at the bottom) for which the particle (unfilled) survives contact with a trap. Trajectories of type (i) have the property that the particle remains inside a notional box, and the traps outside. This forms a subset of the entire class of surviving trajectories, which includes paths of type (ii) in which the particle leaves the box and the traps enter but nevertheless no particle-trap contact occurs.

prove this statement rigorously, although it is supported by intuition and numerical data (see Sec. IV below). We also note that when we say "on average" we mean "after averaging over all possible initial trap positions and trajectories of both particle and traps."

If this claim is accepted, we obtain an upper bound $Q_U(t)$ on the particle's survival probability from Eq. (9) by noting that requiring the particle to remain stationary is equivalent to having a target region of size $l = 0$. Then we immediately have that

$$Q(t) \leq Q_U(t) = \exp\left(-\frac{4\rho\sqrt{Dt}}{\sqrt{\pi}}\right). \tag{10}$$

To derive a lower bound on the survival probability $Q(t)$ we introduce a notional box of size l centered on the origin. If we ask for the particle to remain inside this box until a time t, and for all the traps to remain outside it, the traps and particle may never meet and hence the particle survives until time t. There are, of course, other trajectories for which the particle survives, and so those just described form a subset of all possible surviving trajectories—see Fig. 1. Hence the probability that the particle remains within the box and traps outside is a lower bound $Q_L(t)$ on $Q(t)$.

There are three independent contributions to this bound: (i) the probability that there are initially no traps in the box of size l; (ii) the probability that no traps enter the box up to time t; and (iii) the probability that the particle has not left the box up to time t. The first two contributions are easily obtained. From the definition of the Poisson distribution, we have that the probability the box initially contains no traps is exp($-\rho l$). Second, the probability that no traps enter the box is independent of the box size and is given by Eq. (9). The third contribution, the probability that the particle remains inside the box, is obtained as follows.

Since the system is translationally invariant, we can just as easily consider a particle initially sandwiched between absorbing boundaries at $x = 0$ and $x = l$. The probability $Q_P(t|y)$ that the particle starting at $y = l/2$ has not crossed the absorbing boundaries satisfies a backward Fokker-Planck equation

$$\frac{\partial Q_P(t|y)}{\partial t} = D' \frac{\partial^2 Q_P(t|y)}{\partial y^2} \tag{11}$$

subject to the absorbing boundary conditions $Q_P(t|0) = Q_P(t|l) = 0$ and the initial condition $Q_P(t|y) = 1$ for $0 < y < l$. The general solution to this equation that satisfies the absorbing boundary conditions is obtained by separating the time and space variables in the usual way. One obtains the Fourier sine series

$$Q_P(t|y) = \sum_{k=1}^{\infty} a_k \exp\left(-\frac{k^2 \pi^2 D' t}{l^2}\right) \sin\left(\frac{k\pi y}{l}\right). \tag{12}$$

The expansion coefficients a_k are fixed through the initial condition. Using the orthogonality of the sine functions one finds

$$a_k = \begin{cases} \dfrac{4}{\pi k}, & k \text{ odd} \\[2mm] 0, & k \text{ even.} \end{cases} \tag{13}$$

For the purposes of the present calculation, we need consider only the long-time form of $Q_P(t|y)$ for a particle that starts at $y = l/2$. Thus we keep only the longest-lived ($k = 1$) mode in expansion (12) to find

$$Q_P(t|l/2) \sim \frac{4}{\pi} \exp\left(-\frac{\pi^2 D' t}{l^2}\right). \tag{14}$$

Including this along with the contributions to the lower bound $Q_L(t)$ on the diffusing particle's survival probability $Q(t)$ discussed above, we have

$$Q(t) \geq Q_L(t) = \frac{4}{\pi} \exp\left(-\frac{\pi^2 D' t}{l^2} - \rho l - \frac{4\rho\sqrt{Dt}}{\sqrt{\pi}}\right), \tag{15}$$

once the time t is sufficiently large. Note that this provides a bound for a particular box size l. Since the box is an artificial construct, we can choose its size so that the lower bound is maximized at a particular (predetermined) time t^*. One finds that the corresponding box size is $l^* = (2\pi^2 D' t^*/\rho)^{1/3}$. Using this box size in Eq. (15) we find the largest lower bound is given by

$$Q_L(t) = \frac{4}{\pi} \exp\left(-\frac{4\rho\sqrt{Dt}}{\sqrt{\pi}} - 3\left[\frac{\pi^2 \rho^2 D' t}{4}\right]^{1/3}\right). \tag{16}$$

Combining this lower bound with the upper bound $Q_U(t)$ of Eq. (10) we find

$$\frac{4}{\sqrt{\pi}} \leq -\frac{\ln Q(t)}{(\rho^2 D t)^{1/2}} \leq \frac{4}{\sqrt{\pi}} + 3\left(\frac{\pi}{2}\right)^{2/3} \frac{(D'/D)^{1/3}}{(\rho^2 D t)^{1/6}}. \tag{17}$$

This implies that the constant λ_1 in the expressions of Bramson and Lebowitz (1) is precisely determined as

$$\lambda_1 = -\lim_{t \to \infty} \frac{\ln Q(t)}{\sqrt{t}} = 4\rho\sqrt{\frac{D}{\pi}}. \tag{18}$$

Note that this constant depends only on the density and diffusion constant of the traps, and is independent of the diffusion constant of the particle.

C. Extensions to the basic trapping reaction model

It is straightforward to incorporate two generalizations of the one-dimensional trapping model defined in Sec. II into the bounding arguments discussed above. The first of these is to allow the traps to the left and right of the origin at time 0 to have different densities. We denote the larger (respectively, smaller) of these densities as ρ_+ (ρ_-) and their average as $\bar{\rho} = \frac{1}{2}(\rho_+ + \rho_-)$. Additionally we shall place n particles at the origin at time 0 and study the probability that *all* survive until a time t.

To obtain an upper bound on the survival probability, we note that the survival probability of the particles can only increase (or remain constant) as either ρ_+ or ρ_- is decreased. Hence the survival probability for the case of unequal densities is bounded from above by the case where the density of traps is on both sides equal to ρ_-. For the case of a single diffusing particle, we argued above that an upper bound on its survival probability is found by setting its diffusion constant D' to 0. Clearly, if $D' = 0$ the number of particles at the origin is irrelevant, and so an upper bound on $Q(t)$ is given by Eq. (10) with $\rho = \rho_-$, i.e.,

$$Q(t) \leq Q_U(t) = \exp\left(-\frac{4\rho_- \sqrt{Dt}}{\sqrt{\pi}}\right). \tag{19}$$

To obtain a lower bound on the particles' survival probability we once again introduce a notional box, inside which all the particles must remain and no traps may enter until time t. This time, however, we respect the asymmetry of the problem by allowing the box to extend a distance l_- into the low-density region of traps and l_+ into the high-density region. We will again seek to maximize the lower bound by varying l_- and l_+.

A lower bound $Q_L(t)$ is obtained using an argument analogous to that leading to Eq. (16). Considering once again late times, we find

$$Q_L(t) \propto \exp\left(-\frac{n\pi^2 D' t}{(l_- + l_+)^2} - (\rho_- l_- + \rho_+ l_+)\right.$$
$$\left. - \frac{2\rho_- \sqrt{Dt}}{\sqrt{\pi}} - \frac{2\rho_+ \sqrt{Dt}}{\sqrt{\pi}}\right). \tag{20}$$

The number of particles n enters into this expression through the fact that the probability for *all* of the n particles to remain inside the box of size $l = l_- + l_+$ is simply the nth power of the corresponding probability for a single particle.

The maximal lower bound for a prescribed time t^* is obtained from Eq. (20) by setting l_+^* to zero (thus discount-

ing particle trajectories that enter the high-density region) and putting $l^*_- = (2n\pi^2 D' t^*/\rho_-)^{1/3}$. Then

$$Q(t) \geqslant Q_L(t) \propto \exp\left(-\frac{4\bar{\rho}\sqrt{Dt}}{\sqrt{\pi}} - 3\left[\frac{n\pi^2\rho_-^2 D' t}{4}\right]^{1/3} \right). \tag{21}$$

Along with the upper bound Eq. (19) we find that

$$\frac{4}{\sqrt{\pi}} \leqslant -\frac{\ln Q}{(\rho_-^2 Dt)^{1/2}} \leqslant \frac{4}{\sqrt{\pi}}\frac{\bar{\rho}}{\rho_-} + 3\left(\frac{n\pi^2 D'}{4D}\right)^{1/3}\frac{1}{(\rho_-^2 Dt)^{1/6}}. \tag{22}$$

Note that, except for the case where $\bar{\rho} = \rho_-$ (which implies $\rho_- = \rho_+$) these two bounds do not converge and so we cannot make a precise prediction for λ when the trap densities are unequal. For the case $\rho_- = \rho_+$, however, the bounds converge to $4/\sqrt{\pi}$, independent of the number of particles n.

IV. SIMULATION ALGORITHM AND RESULTS

A sophisticated algorithm for simulating the trapping reaction in discrete space and time and with a Poisson distribution of traps was recently introduced [16]. The beauty of the algorithm is that it admits (numerically) exact calculation of the survival probability for an arbitrarily long, but fixed, trajectory of the particle. As will be discussed below, the algorithm takes into account all possible paths of the traps, as long as their initial distribution is Poisson. In order to obtain an estimate of the particle survival probability, it is necessary to iterate the algorithm over a sequence of particle paths. We now discuss this algorithm in detail.

A. An efficient simulation algorithm

In order to simulate the trapping reaction model in one dimension, we construct a discretized version in which each walker follows a path $x(t)$ that has $x(t+1) - x(t) = \pm 1$. Since all hops to the left or right occur in parallel, we must ensure that the initial coordinates of all the walkers are even integers so that no two walkers are able to hop over each other.

As a starting point in understanding the simulation algorithm, consider a system comprising the particle, whose trajectory $x_0(t)$ is predetermined, and a single trap, whose trajectory $x_1(t)$ is stochastic given some initial condition $x_1(0) = y_1$. The probability $P_1(x,t)$ of finding the trap at site x after time t, given that it has not absorbed the particle, satisfies the equation

$$P_1(x,t+1) = \frac{1}{2}[P_1(x-1,t) + P_1(x+1,t)] \tag{23}$$

subject to the initial condition $P(x,0) = \delta_{x,y_1}$ and the moving absorbing boundary condition $P(x_0(t),t) = 0$. Note that Eq. (23) is the discrete analog of the diffusion (Fokker-Planck) equation

$$\frac{\partial P_1(x,t)}{\partial t} = D\frac{\partial^2 P_1(x,t)}{\partial x^2}. \tag{24}$$

By Taylor expanding Eq. (23) we find the diffusion constant of both particle and trap to be $D = D' = \frac{1}{2}$.

The solution of the diffusion equation with an arbitrary moving absorbing boundary at $x_0(t)$ is not known analytically. One can obtain it numerically, however, by iterating the following two steps over $t' = 1,2,\ldots,t$.

(1) Construct the probability distribution of the trap's position using the equation $P_1(x,t') = \frac{1}{2}[P_1(x-1,t'-1) + P_1(x+1,t'-1)]$.

(2) Enforce the absorbing boundary condition by subsequently setting $P_1[x_0(t'),t'] = 0$.

In the simulation, we wish to consider not just a single trap, but a Poisson distribution of traps. This can be achieved as follows. Let $P_n(x,t)$ be the probability that there are n traps on lattice site x at time t. We shall assume that this distribution is Poisson, i.e.,

$$P_n(x,t) = \frac{[c(x,t)]^n}{n!}\exp[-c(x,t)] \tag{25}$$

in which $c(x,t)$ is the mean number of traps at site x and time t.

Now, if each trap can hop with equal probability to the left or right in one time step, we have

$$P_n(x,t+1) = \sum_{m=0}^{n} W_m^+(x-1,t) W_{n-m}^-(x+1,t) \tag{26}$$

in which $W_m^{\pm}(x,t)$ is the probability that m particles hop from site x at time t to $x\pm 1$ at time $t+1$. This quantity is given by

$$W_m^{\pm}(x,t) = \sum_{s=m}^{\infty} \frac{[c(x,t)]^s}{s!}\exp[-c(x,t)]\binom{s}{m}\frac{1}{2^s}. \tag{27}$$

Insertion of this expression into Eq. (26) and a little algebra reveals that

$$P_n(x,t+1) = \frac{[\bar{c}(x,t)]^n}{n!}\exp[-\bar{c}(x,t)] \tag{28}$$

in which

$$\bar{c}(x,t) = \frac{c(x-1,t) + c(x+1,t)}{2}. \tag{29}$$

That is, if the distribution of traps at time t is Poisson the distribution of traps at time $t+1$ is also Poisson, with the mean occupation number at each site obeying the discrete diffusion equation

$$c(x,t+1) = \frac{1}{2}[c(x-1,t) + c(x+1,t)]. \tag{30}$$

As with the case of the single-trap described above, we wish to determine the probability distribution of traps given that the particle following the predetermined path $x_0(t)$ has not been absorbed until a time t. We must therefore have at each time step $P_n(x_0(t),t) = \delta_{n,0}$, which can be achieved by enforcing the boundary condition $c(x_0(t),t) = 0$. Thus we can evolve the mean occupation numbers for the Poisson distributed sea of traps in exactly the same way as for the single-trap distribution function described above (albeit with a different initial condition, to be described shortly).

In the simulations, we wish to calculate the probability that the particle has survived until time t. To obtain an expression for this, consider a particular distribution of traps described by the function $c(x,t)$. The probability that site x_0 contains no traps is just $\exp(-c[x_0,t])$ and so $Q(t+1) = Q(t)\exp(-c[x_0,t])$ where the value of $c(x_0,t)$ used is that obtained after the diffusion step, but before enforcing the boundary condition $c(x_0,t) = 0$.

We now give a step-by-step explanation of the algorithm for calculating the particle survival probability for a predetermined particle path $x_0(t)$. One begins by setting up the trap concentration as follows:

$$c(x,t_0) = \begin{cases} 2\rho_L, & x < x_0(0) \\ 0, & x = x_0(0) \\ 2\rho_R, & x > x_0(0), \end{cases} \tag{31}$$

in which ρ_L and ρ_R are the equivalent continuum densities to the left and right of the particle, as used in Sec. III C. The factor of 2 emerges because that is the effective lattice spacing in the discrete model. We also set $Q(0) = 1$ (i.e., we assume there are no traps at the origin to begin with). Then, for each time $t' = 1,2,\ldots,t$ we perform the following steps.

(1) The trap concentration variables are evolved using $c(x,t') = \frac{1}{2}[c(x-1,t'-1) + c(x+1,t'-1)]$.

(2) The cumulative particle survival probability is calculated using $Q(t') = Q(t'-1)\exp[-c(x_0(t'),t')]$.

(3) The boundary condition is enforced by setting $c(x_0(t'),t') = 0$.

Note that this algorithm can be run for paths of arbitrary length and that, at a particular time t', the trap density at positions $x < x_0(0) - t'$ and $x > x_0(0) + t'$ is uniform. Hence at each time step, one need deal only with $t' + 1$ concentration variables to simulate the infinite system.

Using the above algorithm, one obtains the survival probability for a particle following a particular path $x_0(t)$. To reach an estimate of the particle survival probability averaged over all paths, it is most efficient to perform Monte Carlo sampling. That is, one generates a binomial random walk by choosing the particle displacement $x_0(t') - x_0(t'-1) = \{-1,1\}$ with equal probability. Then, one estimates the mean particle survival probability as

$$Q(t) \approx \frac{1}{N}\sum_{k=1}^{N} Q^{(k)}(t) \tag{32}$$

in which $Q^{(k)}$ is the value of the survival probability for the kth random walk. One can, of course, estimate other quanti-
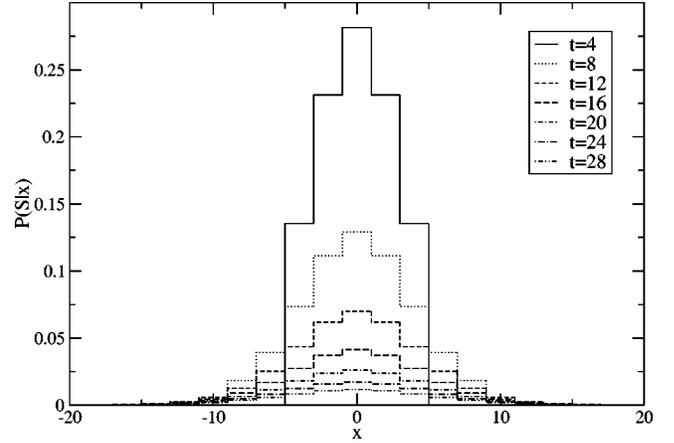
FIG. 2. Survival probability $P(S,t|x)$ given that the particle is at site x at early times and with $\rho_L = \rho_R = 0.5$.

ties, such as the mean and variance of the particle's displacement. Also, if one is interested only in the short-time behavior, one can obtain the particle survival probability for each possible path. We should also note that the one-dimensional algorithm described here generalizes straightforwardly to higher (integer) dimensions.

B. Numerical results

We first investigate the entire set of short particle paths in order to get a feel for those that give rise to the greatest probability of survival. For each time $t \leq 28$ we found that the paths which have the greatest survival probability are those with the smallest width (defined as the distance between the extrema of the path), i.e., the sequences $x(t) = (0,1,0,1,0,\ldots)$ and $x(t) = (0,-1,0,-1,0,\ldots)$. This result gives support to the supposition in Sec. III that staying still (i.e., a diffusion constant $D' = 0$) gives rise to the greatest chance of survival. We also established this to be case for two-dimensional walks up to a time $t = 12$.

It is a simple matter to use the algorithm presented above to find the probability $P(x,t|S)$ for the particle to be at coordinate x after time t given that it has survived. Then, an application of Bayes' theorem yields the more telling quantity $P(S,t|x)$, i.e., the probability that the particle has survived to time t given that it ends at coordinate x. The resulting data are plotted in Fig. 2 and one sees quite clearly that the particle is most likely to survive if it is at the origin, at least for times $t \leq 28$. This figure provides further weight to our assertion that staying still is the best particle survival strategy.

As stated in the preceding section, one can obtain estimates of various quantities at later times if one performs Monte Carlo sampling over particle paths. In fact, we produced histograms of $P(S,t|x)$ this way and obtained data very similar to those shown in Fig. 2 (except with poorer statistics). Hence we do not present them here. Instead we concentrate on the survival probabilities for a range of trap densities to compare with the bounds given by Eq. (22).

First we consider the case of equal trap densities either side of the origin and the case of $n = 1$ and 2 particles start-
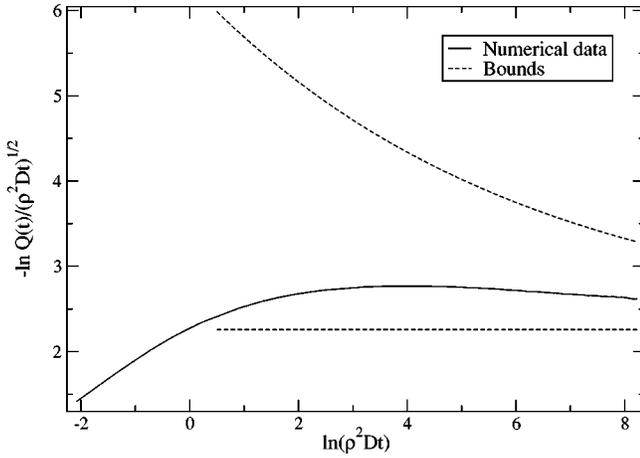
FIG. 3. Single particle survival probability and bounds with $\rho_L = \rho_R = 0.5$.

FIG. 5. Single particle survival probability and bounds with $\rho_+ / \rho_- = 2$, 4, and 8. The symbols on the solid lines (representing the numerical data) are included purely for the purpose of identifying each curve with the corresponding density ratio.

ing at the origin. We generated the data for the case $n=1$ using the algorithm described above, and densities $\rho_L = \rho_R = 0.5$ until a time $t = 30\,000$. Bearing in mind the form of the bounds Eq. (22) it is appropriate to plot the quantity $\lambda(t) = -\ln Q(t)/\sqrt{\rho_-^2 Dt}$ against log time. In all the simulations, $D = D' = \frac{1}{2}$ and in this case, $\rho_- = 0.5$. Hence the upper and lower bounds in Eq. (22) converge to the constant $\lambda(\infty) = 4/\sqrt{\pi}$. Figure 3 shows that, after an initial transient, $\lambda(t)$ does fall within the bounds. However, even at the late times probed in the simulation, $\lambda(t)$ still seems to be far away from its asymptote. This highlights the fact that the predicted asymptotic form for the particle's survival probability Eq. (1) has not yet been observed in simulation, even with sophisticated methods at our disposal.

The data for the case $n=2$ have been taken from Ref. [16] and are plotted with our bounds in Fig. 4. As with the case $n=1$ we have from Eq. (22) that $\lambda(\infty) = 4/\sqrt{\pi}$ and again the convergence to asymptopia is very slow.

In Fig. 5 we plot the single particle survival probability for the case, where the densities of traps either side of the origin are unequal. Specifically we have the cases ρ_+ / ρ_-

FIG. 4. Two particle survival probability taken from Ref. [16] and bounds with $\rho_L = \rho_R = 0.25$.

$= 2, 4, 8$ with $\rho_R = 0.5$ in each case. Note that the density used to scale the plots is always the smaller of the two, ρ_- . Again we see that the numerical data lie within the bounds predicted by Eq. (22). In these cases, however, the bounds we have presented do not converge so we have no predictions for the limiting value of $\lambda(t)$.

V. ANALYTICAL RESULTS IN DIMENSIONS GREATER THAN ONE

The upper and lower bounds on $Q(t)$ derived in $d=1$ will now be generalized to all d in the range $1 < d < 2$ and to $d = 2$, the latter case requiring a slightly different treatment. The case $d > 2$ will also be discussed.

A. Upper bound

Let the particle, with diffusion constant D', start at the origin, and the traps, with diffusion constant D, be randomly distributed in space with density ρ. As before, we assert, on intuitive grounds, that the "best strategy" for the particle is to stay at rest at the origin. With this assumption (which was verified numerically for $d=2$, for all times up to $t=12$, in the preceding section) the survival probability for $D'=0$ provides an upper bound on the survival probability for any $D' > 0$. Let $Q_1(t|r)$ be the probability that a given trap, starting a distance r from the origin, has not yet visited the origin at time t. It obeys the backward Fokker-Planck equation

$$\frac{\partial Q_1}{\partial t} = D\nabla^2 Q_1 = D\left(\frac{\partial^2 Q_1}{\partial r^2} + \frac{d-1}{r} \frac{\partial Q_1}{\partial r} \right), \qquad (33)$$

where we have exploited the spherical symmetry of the problem. The boundary conditions are $Q_1(t|0)=0$ for all t and $Q_1(t|\infty)=1$ for all t, while the initial condition is $Q_1(0|r)=1$ for all $r>0$. Since there is no length scale in the problem, $Q_1(t|r)$ must have the scaling form

$$Q_1(t|r) = f(r/\sqrt{Dt}). \qquad (34)$$

Substituting this form into Eq. (33) gives an ordinary differential equation for $f(x)$:

$$\frac{d^2 f}{dx^2} + \frac{d-1}{x}\frac{df}{dx} + \frac{x}{2}\frac{df}{dx} = 0, \qquad (35)$$

with boundary conditions $f(0) = 0$, $f(\infty) = 1$. The solution is

$$f(x) = \left[\Gamma\left(\frac{2-d}{2}\right)\right]^{-1}\int_0^{x^2/4} ds\, s^{-d/2}e^{-s}. \qquad (36)$$

For $d=1$ our previous result, $f(x) = \mathrm{erf}(x/2)$, is recovered. Note that Eq. (36) is only valid for $d<2$, since the integral diverges for $d \geq 2$. This regime will therefore require a different treatment.

Equation (36) gives the survival probability of a stationary particle in the presence of a single diffusing trap. Consider N traps in a large sphere of volume V centered on the origin. Each trap starts anywhere in the volume with equal probability. The average, over the initial positions of the traps, of the probability that none of the traps has yet reached the origin at time t is

$$Q(t) = \left[\frac{1}{V}\int_V d^d r\, f\left(\frac{r}{\sqrt{Dt}}\right)\right]^N$$

$$= \left[1 - \frac{1}{V}\int_V d^d r\left\{1 - f\left(\frac{r}{\sqrt{Dt}}\right)\right\}\right]^N. \qquad (37)$$

Taking the limit $N \to \infty$, $V \to \infty$, with $\rho = N/V$ held fixed, gives

$$Q(t) = \exp\left[-\rho\int d^d r\left\{1 - f\left(\frac{r}{\sqrt{Dt}}\right)\right\}\right], \qquad (38)$$

where the integral is now over all space. Inserting the function $f(x)$ from Eq. (36) and evaluating the integral gives the final result, which serves as an upper bound, $Q_U(t)$, for the problem with general $D' > 0$:

$$Q_U(t) = \exp[-a_d \rho (Dt)^{d/2}], \qquad (39)$$

where

$$a_d = \frac{2}{\pi d}(4\pi)^{d/2}\sin\left(\frac{\pi d}{2}\right). \qquad (40)$$

B. Lower bound

Our strategy for constructing a rigorous lower bound follows that employed in one dimension. We construct an imaginary (d-dimensional) sphere of radius l centered on the origin, and calculate the probability that (i) there are no traps inside the sphere at $t=0$, (ii) the particle stays inside the sphere up to time t, and (iii) no traps enter the sphere up to time t. As before, the set of trajectories (of particle and traps) selected by these constraints are a subset of all trajectories in

which no traps meet the particle, so the probability weight of this subset provides a lower bound on $Q(t)$. We compute these probabilities in turn.

(i) The probability that the sphere initially contains no traps is simply $\exp(-\rho V_d l^d)$, where $V_d = 2\pi^{d/2}/d\Gamma(d/2)$ is the volume of a d-dimensional unit sphere.

(ii) The probability, $Q_P(t|r,l)$ that the particle stays inside the sphere up to time t is obtained by solving the backward Fokker-Planck equation (33), with D replaced by D', subject to the boundary conditions $Q_P(t|l,l) = 0$ and $Q_P(t|r,l)$ is analytic at $r=0$, and the initial condition $Q_P(0|r,l) = 1$ for $r<l$. The solution has the form

$$Q_P(t|r,l) = r^\nu \sum_{n=1}^{\infty} c_n \exp(-D'k_n^2 t)J_{-\nu}(k_n r), \qquad (41)$$

where $J_{-\nu}(z)$ is a Bessel function of the first kind,

$$\nu = (2-d)/2, \qquad (42)$$

and $k_n l = z_n$ is the nth zero of $J_{-\nu}(z)$. The coefficients c_n are obtained from the initial condition, but their precise values are of no interest here. Since the particle starts at $r=0$, we need $Q_P(t|0,l)$. Its asymptotic form is

$$Q_P(t|0,l) \sim \exp(-z_1^2 D't/l^2). \qquad (43)$$

(iii) To compute the probability, $Q_T(t)$, that no trap enters the sphere up to time t (the target annihilation problem) we begin by calculating this probability, $Q_1(t|r,l)$, for a single trap. Then the probability that none of the traps enter the sphere is given by a natural generalization of Eq. (38),

$$Q_T(t) = \exp\left[-\rho\int_{r>l} d^d r\{1 - Q_1(t|r,l)\}\right]. \qquad (44)$$

In contrast to the case $l=0$ used for the upper bound, there is no simple scaling form analogous to Eq. (34) for $Q_1(t|r,l)$ because l provides an additional length scale.

The function $Q_1(t|r,l)$ obeys the backward Fokker-Planck equation (33), with boundary conditions $Q_1(t|l,l) = 0$ for all t, $Q_1(t|\infty,l) = 1$ for all t, and initial condition $Q_1(0|r,l) = 1$ for $r>l$. The solution can be found by Laplace transform techniques. The result is [25]

$$Q_1(t|r,l) = \frac{2}{\pi}\left(\frac{r}{l}\right)^\nu\int_0^\infty \frac{dk}{k}\exp(-Dk^2 t)G_\nu(kr,kl), \qquad (45)$$

where

$$G_\nu(x,y) = \frac{Y_\nu(x)J_\nu(y) - J_\nu(x)Y_\nu(y)}{J_\nu^2(y) + Y_\nu^2(y)}, \qquad (46)$$

and $Y_\nu(z)$ is a Bessel functions of the second kind.

Before continuing, we can first simplify Eq. (44) as follows. First define

$$F(t) = \int_{r>l} d^d r \{1 - Q_1(t|r,l)\}, \tag{47}$$

where $F(0)=0$ follows from the initial condition $Q_1(0|r,l)=1$ for all $r>l$. Then we use the backward Fokker-Planck equation (33) to write

$$\partial_t F = -D \int_{r>l} d^d r \, \nabla^2 Q_1(t|r,l) = -D \int_A d\mathbf{A} \cdot \boldsymbol{\nabla} Q_1(t|l,l)$$

$$= DS_d l^{d-1} \partial_r Q_1(t|r,l)|_{r=l}, \tag{48}$$

where A is the surface of the sphere, $d\mathbf{A}$ is a surface element directed along the inward normal to the sphere, and

$$S_d = \frac{2\pi^{d/2}}{\Gamma(d/2)} \tag{49}$$

is the surface area of the unit sphere in d dimensions. Integrating result (48) with respect to time, with initial condition $F(0)=0$, Eq. (44) takes the form [22]

$$Q_T(t) = \exp\left[-\rho DS_d l^{d-1} \int_0^t dt' \, \partial_r Q_1(t'|r,l)|_{r=l}\right]. \tag{50}$$

We are interested in the behavior of $Q_T(t)$ for large t. At this point it is convenient to discuss separately the cases $1<d<2$, $d=2$, and $d>2$.

1. The case $1<d<2$

For $1<d<2$, the function $Q_1(t|r,l)$, given by Eq. (45), has the large-t expansion [25]

$$Q_1(t|r,l) = \left[\left(\frac{r}{l}\right)^{2\nu} - 1\right]\left\{\frac{\tau^{-\nu}}{\Gamma(1+\nu)} + \frac{\tau^{-2\nu}}{\Gamma^2(1+\nu)}\right.$$

$$\left. \times \frac{\Gamma^2(1-\nu)}{\Gamma(1-2\nu)} + \cdots\right\}, \tag{51}$$

where $\tau = 4Dt/l^2$ and we recall that $\nu = (2-d)/2$. Taking the derivative with respect to r, setting $r=l$, inserting the result into Eq. (50), and evaluating the integrals over t', gives the probability, that the target has not been annihilated by a trap,

$$Q_T(t) = \exp[-a_d\rho(Dt)^{d/2} - b_d\rho(Dt)^{d-1}l^{2-d} + \cdots], \tag{52}$$

where a_d is given by Eq. (40) and

$$b_d = \frac{2^{2d-1}\pi^{d/2}\Gamma(d/2)}{(2-d)\Gamma^2(1-d/2)\Gamma(d)}. \tag{53}$$

Note that, as with the case $d=1$, the leading term is independent of l. This phenomenon can be attributed to the recurrence of diffusion in dimensions $d<2$.

Finally we assemble the contributions (i)–(iii) above to obtain a rigorous lower bound on the asymptotic behavior for $1<d<2$,

$$Q_L(t) \sim \exp[-a_d\rho(Dt)^{d/2}]$$

$$\times \exp[-\rho V_d l^d - z_1^2 D't/l^2 - b_d\rho(Dt)^{d-1}l^{2-d}]. \tag{54}$$

As usual, for a given time t^* we choose a sphere radius l^* to optimize the lower bound. The dominant l-dependent terms for $t\to\infty$ are the final two terms in the second exponential. Ignoring constants of order unity, we find that the value of l^* that gives the greatest lower bound is

$$l^* \sim \left(\frac{D'}{\rho D^{d-1}}\right)^{1/(4-d)} (t^*)^{(2-d)/(4-d)}. \tag{55}$$

Inserting this into Eq. (54) the second exponential takes the form

$$\exp[-\text{const}(D')^{(2-d)/(4-d)}(\rho D^{d-1})^{2/(4-d)}t^{d/(4-d)}]. \tag{56}$$

The neglected first term in the second exponential in Eq. (54) behaves as $l^d \sim t^{d(2-d)/(4-d)}$, which is indeed negligible compared to $t^{d/(4-d)}$ for large t (recalling that $d>1$ here).

In summary, the best lower bound behaves as

$$Q_L(t) \sim \exp[-a_d\rho(Dt)^{d/2} + O(t^{d/(4-d)})]. \tag{57}$$

Since $d/(4-d)<d/2$ for $d<2$, the two bounds pinch asymptotically, to give the exact result

$$\lim_{t\to\infty} -\frac{\ln Q(t)}{\rho(Dt)^{d/2}} = a_d, \quad 1\le d<2, \tag{58}$$

where we recall that a_d is given by Eq. (40). The constant λ_d in Eq. (1) is therefore given by

$$\lambda_d = \frac{2\rho}{\pi d} \sin\left(\frac{\pi d}{2}\right)(4\pi D)^{d/2}, \quad 1\le d<2. \tag{59}$$

Note that the subdominant term in Eq. (57) decays more slowly relative to the leading term as $d\to2$, signaling a change of behavior at $d=2$. Note also that the coefficient a_d vanishes at $d=2$, suggesting a *slower* decay than a simple exponential in two dimensions. We now show that this expectation is correct, and determine the constant λ_2 in Eq. (1).

2. The case $d=2$

For $d=2$ the asymptotic form of $Q_1(t|r,l)$ is [25]

$$Q_1(t|r,l) = 2\ln\left(\frac{r}{l}\right)\left[\frac{1}{\ln\tau} + O\left(\frac{1}{\ln^2\tau}\right)\right], \tag{60}$$

where $\tau = 4Dt/l^2$ as before. Inserting this into Eq. (50), with $d=2$, gives the probability that no trap has entered the circle of radius l up to time t:

$$Q_T(t) = \exp\left[-\frac{4\pi\rho Dt}{\ln(4Dt/l^2)} + O\left(\frac{t}{\ln^2 t}\right)\right]. \tag{61}$$

Following our previous procedure, the asymptotic lower bound is given by

$$Q_L(t) \sim \exp\left[-\frac{4\pi\rho Dt}{\ln(4Dt/l^2)} + O\left(\frac{t}{\ln^2 t}\right) - \rho\pi l^2 - z_1^2 \frac{D't}{l^2} \right],$$

$$(62)$$

where z_1 is now the smallest zero of $J_0(z)$. The dominant terms in the exponential for large t are the first and last terms. Extremizing this bound with respect to l at some fixed t^* gives

$$l^* \sim z_1 \left(\frac{D'}{4\pi\rho D} \right)^{1/2} \ln\left(\frac{\rho D^2 t^*}{D'} \right) \qquad (63)$$

to leading order, and

$$Q_L(t) \sim \exp\left[-\frac{4\pi\rho Dt}{\ln(\rho D^2 t/D')} + O\left(\frac{t\ln(\ln t)}{\ln^2 t}\right) \right]. \quad (64)$$

As far as the upper bound is concerned, Eq. (39) is not useful in $d=2$, since $a_2=0$. This tells us that the probability that a trap will reach a specified region of zero volume (i.e., a specified point) is zero in two dimensions. The A particle has to be given a nonzero size (or the system put on a lattice) for a nonzero trapping probability. We therefore assign the particle a nonzero radius a, but still treat it as stationary for the upper bound. The traps will, for the moment, continue to be treated as point particles. With the definition that trapping occurs if a trap enters within the particle's radius (so that a is an interaction range), our upper bound is just given by the probability $Q_T(t)$, Eq. (61), but with l replaced by a, to give

$$Q_U(t) \sim \exp\left[-\frac{4\pi\rho Dt}{\ln(4Dt/a^2)} + O\left(\frac{t}{\ln^2 t}\right) \right]. \qquad (65)$$

In the limit $t\to\infty$, the bounds converge to give the asymptotic result $Q(t) \sim \exp(-4\pi\rho Dt/\ln t)$ or, equivalently

$$\lim_{t\to\infty} -\frac{\ln t \ln Q(t)}{\rho Dt} = 4\pi. \qquad (66)$$

This gives the constant λ_2 in Eq. (1) as

$$\lambda_2 = 4\pi\rho D. \qquad (67)$$

As noted previously, the algorithm described in Sec. IV can be used to simulate the trapping reaction in any integer dimension. Numerical results for the two-dimensional system were presented in Ref. [16] and we compare these data with the asymptotic result (66) in Fig. 6. We find that the deviation of the numerical results from the asymptote is even more marked in two dimensions than in one (see Fig. 3). Part of the reason for this is, presumably, that the increased number of sites in two dimensions means that one cannot probe such late times. A second, and perhaps more important, reason is the very large corrections to scaling evident from our bounding arguments. The *relative* size of the subleading term
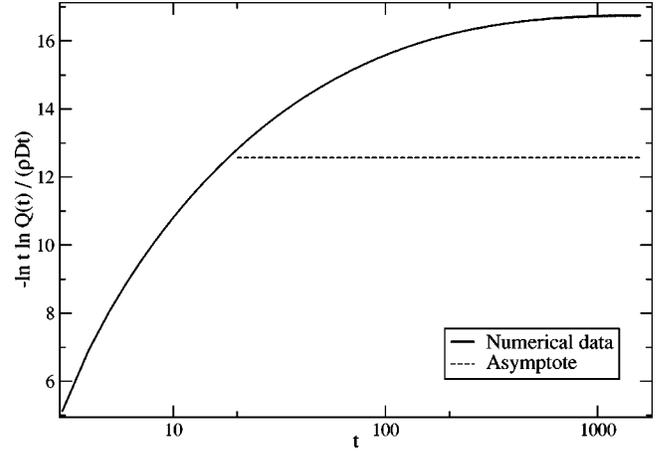
FIG. 6. Numerical data for the two-dimensional trapping reaction taken from Ref. [16]. In the simulation, the trap density $\rho = 1/4$ and the diffusion constants $D=D'=1/4$. The asymptote given by Eq. (66) is plotted for comparison.

in Eq. (65) is $O(1/\ln t)$, while the subleading term for the lower bound, Eq. (64), is even larger, of relative size $O(\ln[\ln t]/\ln t)$. This suggests that convergence to asymptopia will be *extremely* slow in two dimensions. Note also that the particle's survival probability was found to decay to $\sim 10^{-99}$ after $t=1600$ time steps. This emphasizes the importance of determining the corrections to asymptopia in order to determine the form of the survival probability in numerically (and, indeed, experimentally) accessible regimes.

3. The case d>2

The same bounding arguments can be applied equally well in $d>2$. The main difference from $d\leq 2$ is that the bounds no longer converge, so it is not possible to determine λ_d exactly (except for d very close to 2—see below). The basic idea is the same as for $d\leq 2$, except that the particles must be given nonzero sizes (or, equivalently, a nonzero range of interaction). We let the particle have radius a, and the traps radius b. A reaction is deemed to have occurred if there is an overlap between the particle and any trap, i.e., if the centers approach more closely than a distance $R=a+b$, which is the range of interaction. (Note, however, that we continue to assume that the traps do not interact with each other. In particular, there is no excluded volume interaction between traps.)

The upper bound is obtained from the target annihilation problem with target radius R. For $d>2$, the single-trap survival probability, $Q_1(t|r,R)$, has a nonvanishing large-t limit given by the well-known result

$$Q_1(\infty|r,R) = 1 - (R/r)^{d-2}, \qquad (68)$$

which is easily obtained from Eq. (33) on setting the left side to zero, and imposing the boundary conditions $Q_1(\infty|R,R) = 0$, $Q_1(\infty|\infty,R) = 1$ on the resulting ordinary differential equation. Inserting this form in Eq. (50), with $l=R$, and evaluating the time integral, gives an upper bound with the leading large-t behavior

$$Q_U(t) \sim \exp[-(d-2)S_d\rho R^{d-2}Dt]. \qquad (69)$$

The lower bound is obtained in a similar fashion, following the pattern established for $d \leq 2$. One constructs a notional sphere of radius l, centered on the initial position of the particle. The bound is given by the subset of trajectories in which (i) there are no traps initially within the sphere, (ii) the center of the particle remains within a sphere of radius $l - a$, so that the particle remains entirely inside the sphere of radius l, and (iii) the center of every trap remains outside a sphere of radius $l + b$, so that every trap remains entirely outside the sphere of radius l.

The probability of (i) is $\exp[-\rho V_d (l+b)^d]$. The probability of (ii) has the asymptotic form $\exp[-z_1^2 D' t/(l-a)^2]$, where z_1 is the first zero of $J_{-\nu}(z) = J_{(d-2)/2}(z)$. The probability of (iii) is given, for large t, by Eq. (69) with R replaced by $l + b$. Assembling these three contributions gives the asymptotic lower bound

$$Q_L(t) \sim \exp[-(d-2)S_d \rho (l+b)^{d-2} Dt - z_1^2 D' t/(l-a)^2$$
$$- \rho V_d (l+b)^d]. \tag{70}$$

This has to be maximized with respect to l. For $t \to \infty$, the first two terms in the exponent dominate, and the final term is negligible. Setting $l = a + x$, and maximizing with respect to x, gives the equation

$$(d-2)^2 S_d \rho D (x+R)^{d-3} = 2 z_1^2 D'/x^3, \tag{71}$$

where $R = a + b$ as before. This equation cannot be solved analytically for general d, so we concentrate on two soluble cases—the physically interesting case $d = 3$, and the limit $d \to 2+$.

For $d = 3$, we have $S_d = 4\pi$ and $z_1 = \pi$, giving $x = (\pi D'/2\rho D)^{1/3}$ and

$$Q_L(t) \sim \exp[-4\pi \rho DRt - 3(2\pi^2 \rho D \sqrt{D'})^{2/3} t]. \tag{72}$$

Combining the two bounds, we obtain the asymptotic form $Q(t) \sim \exp(-\lambda_3 t)$, as in Eq. (1), with the bounds

$$4\pi \rho DR \leq \lambda_3 \leq 4\pi \rho DR + 3(2\pi^2 \rho D \sqrt{D'})^{2/3}, \quad d = 3. \tag{73}$$

It is worth noting that the second term on the right is negligible compared to the first if $D'/D \ll \rho R^3$, i.e., when D'/D is small compared to the number of traps per interaction volume.

For $d = 2 + \epsilon$, Eq. (71) has the solution

$$x = \frac{1}{\epsilon} \left(\frac{z_1^2 D'}{\pi \rho D} \right)^{1/2}, \tag{74}$$

to leading order for $\epsilon \to 0$, giving the lower bound $Q_L(t) \sim \exp[-2\pi \epsilon \rho D t]$ to leading order in ϵ. In the same limit, the upper bound Eq. (69) has exactly the same form, giving the result $Q(t) \sim \exp(-\lambda_d t)$ with

$$\lambda_d = 2\pi \rho D \epsilon + \cdots. \tag{75}$$

Hence the bounds pinch to leading order in ϵ, but not for general d.

To conclude this section, we consider again the case where n particles start from the origin, and we want the probability that *all* survive until time t. As noted in the discussion of the one-dimensional case, n only enters in the calculation of the lower bound, in the term giving the probability for the particle to stay inside the notional box ($d = 1$), or sphere ($d > 1$), of size l. This probability behaves as $\exp(-\text{const } D' t/l^2)$, so having n particles simply requires raising this factor to the power n, which is equivalent to replacing D' by nD'. Since the asymptotic forms we derive do not depend on D' for $d \leq 2$, it follows that our results are independent of n in this regime. For $d > 2$, however, our results do depend on D' [see Eq. (73)]. In this regime, therefore, the generalization to arbitrary n is achieved through the replacement $D' \to nD'$.

VI. DISCUSSION AND SUMMARY

In this paper we have derived a number of results for the asymptotic survival probability of a particle diffusing among randomly distributed diffusing traps with density ρ. We allow the particle and traps to have different diffusion constants, D' and D respectively. Our results take the forms originally derived by Bramson and Lebowitz [14], as expressed in Eq. (1). With one assumption, supported by numerical evidence, we have obtained exact results for the coefficients λ_d in Eq. (1) for dimensions $d \leq 2$, and an exact inequality for dimensions $d > 2$. These results are given by Eqs. (18), (59), and (73). For $d \leq 2$ the results for λ_d are independent of the diffusion constant D' of the particle.

The results are obtained by deriving upper and lower bounds for λ_d, and showing these coincide for $d \leq 2$. Whilst our lower bound is rigorous, we had to assume that the particle's survival probability for $D' = 0$ provides an upper bound on its survival probability when $D' > 0$ when the trap distribution is symmetric. Indeed, for the $d = 1$ system with different densities of traps to the left and right of the particle, it was found that staying still is *not* the particle's best strategy. Instead, trajectories that survive for long times tend to be those in which the particle drifts to the side with the lower trap density. This emphasizes the crucial role of the symmetry of the trap distribution, an observation supported by perturbative studies for a system with a finite number of traps [15,26].

In all cases the particle and traps are assumed to move in a continuous space, and to have zero size for $d < 2$. For $d \geq 2$ is necessary for the particle and/or the traps to have nonzero size (otherwise the survival probability, for motion on a continuous space, is one for all time). We also take the traps to be randomly distributed in space at time $t = 0$, with uniform density ρ. This raises the question of the extent to which the results are "universal," i.e., independent of the microscopic details of the model, a question which we now address.

We argue that, for $d \leq 2$, the results do indeed have a degree of universality. In $d = 1$, the optimal box size used to obtain the lower bound on $Q(t)$ is *large*, $l \sim t^{1/3}$, as $t \to \infty$, so the effect of the particle having a finite size when confined to this box is negligible. With a little thought one sees that the

same is true for all $d \leq 2$. The optimal length scale for the lower bound *grows with time* as $l \sim t^{(2-d)/(4-d)}$ ($d<2$) or $l \sim \ln t$ ($d=2$), and the results are independent of the particle and trap sizes, as far as the leading-order results are concerned. The same is true of the upper bound—the finite-size corrections come in at subleading order.

The dominance of large length scales at late times, for $d \leq 2$, also suggests that the asymptotic results are independent of whether the model is defined on the continuum (as here) or on a lattice, an assumption implicitly made earlier when we compared our theoretical predictions to numerical results obtained from lattice simulations. For $d>2$, however the dominant value of l that determines the lower bound is time independent. Therefore we expect a lack of universality in this case. The explicit dependence on the interaction range R in Eq. (73) is a signature of this effect. Note, however, that to leading order in $\epsilon = d-2$, λ_d is independent of R [see Eq. (75)] and we expect the result to be universal to this order. Physically, this is because the length scale $l=a+x$ diverges as $\epsilon \to 0$ [see Eq. (74)].

A further universality question concerns universality with respect to the initial conditions. We have taken Poissonian initial conditions, where the probability $P_N(V)$ of having N traps in a volume V is given by $P_N(V) = [(\rho V)^N/N!]\exp(-\rho V)$ for any V. The lattice simulations, where the number of traps on each site has a Poisson distribution (with mean ρ, say) has this property, namely, the number of traps on m sites has a Poisson distribution with mean $m\rho$. Whether there is a larger class of initial conditions sharing the same asymptotic behavior is a question deserving further study.

We conclude by discussing some recent papers related to the present work, and directions for future work. The coefficient λ_d in Eq. (1) has recently been calculated using a diagrammatic method [27] to first order in $(2-d)$. The quoted result, however, exceeds our rigorous upper bound for λ_d [corresponding to the lower bound for $Q(t)$] by a factor of two. This is because in Ref. [27] λ_d depends on D and D' only through their sum $D+D'$ [28], whereas our rigorous upper bound on λ_d depends solely on D. It is interesting to note that in the related process $A+B \to A$, where the single A particle acts as a trap for the B particles, certain properties of the B-particle distribution *can* be expressed as functions of $D+D'$ [29]. However, we stress that for the $A+B \to B$ reaction studied here, the asymptotics are entirely governed by the B-particle diffusion constant for $d \leq 2$.

In a very recent work [30] our approach, as outlined in Ref. [15], has been generalized to diffusion on fractals for the case where the fractal dimension of the traps' trajectories is greater that the physical dimension (this condition is the analog of the condition $d<2$ in the present work). It should be noted, however, that in Ref. [30] the optimal lower bound on $Q(t)$ is not obtained. For $d<2$, only the subdominant corrections to the leading terms are affected, and the upper and lower bounds still pinch asymptotically. For $d=2$, however, the approach used in Ref. [30] yields bounds that no longer converge at large t, so the exact result Eq. (67) for λ_2 is missed.

In this paper and our earlier work [15] we noted that the extant simulation data [16] fail to reach the asymptotic regime even though survival probabilities are so small that they can only be measured using sophisticated methods. Perhaps the most important challenge, therefore, is to obtain a better understanding of the corrections to asymptopia in order to make testable, quantitative predictions. Other directions for future work include exploring further the extent to which our results are universal, and establishing rigorously the validity of our upper bound.

[1] S.W. Benson, *The Foundations of Chemical Kinetics* (McGraw-Hill, New York, 1960).

[2] S.A. Rice, *Diffusion-limited Reactions* (Elsevier, Amsterdam, 1985).

[3] J. Krug and H. Spohn, in *Solids Far From Equilibrium,* edited by C. Godrèche (Cambridge University Press, Cambridge, 1991).

[4] A.J. Bray, Adv. Phys. **43**, 357 (1994).

[5] B. Derrida and R. Zeitak, Phys. Rev. E **54**, 2513 (1996).

[6] J.L. Spouge, Phys. Rev. Lett. **60**, 871 (1988).

[7] S. Redner, in *Nonequilibrium Statistical Mechanics in One Dimension,* edited by V. Privman (Cambridge University Press, Cambridge, 1997), Chap. 1.

[8] D. ben Avraham, in *Nonequilibrium Statistical Mechanics in One Dimension* (Ref. [7]).

[9] D. ben Avraham and S. Havlin, *Diffusion and Reactions in Fractals and Disordered Systems* (Cambridge University Press, Cambridge, 2000).

[10] Y. Elskens and H.L. Frisch, Phys. Rev. A **31**, 3812 (1985).

[11] R.A. Blythe, M.R. Evans, and Y. Kafri, Phys. Rev. Lett. **85**, 3750 (2000).

[12] D. Toussaint and F. Wilczek, J. Chem. Phys. **78**, 2642 (1983).

[13] B.P. Lee and J.L. Cardy, J. Stat. Phys. **80**, 971 (1995).

[14] M. Bramson and J.L. Lebowitz, Phys. Rev. Lett. **61**, 2397 (1988).

[15] A.J. Bray and R.A. Blythe, Phys. Rev. Lett. **89**, 150601 (2002).

[16] V. Mehra and P. Grassberger, Phys. Rev. E **65**, 050101 (2002).

[17] S.J. O'Donoghue and A.J. Bray, Phys. Rev. E **65**, 051114 (2002).

[18] M. Donsker and S.R.S. Varadhan, Commun. Pure Appl. Math. **28**, 525 (1975).

[19] S. Redner and P.L. Krapivsky, Am. J. Phys. **67**, 1277 (1999).

[20] A. Blumen, G. Zumofen, and J. Klafter, Phys. Rev. B **30**, 5379 (1984).

[21] M. Tachiya, Radiat. Phys. Chem. **21**, 167 (1983).

[22] S.F. Burlatsky, and A.A. Ovchinnikov, Zh. Éksp. Teor. Fiz. **92**, 1618 (1987) [Sov. Phys. JETP **65**, 908 (1987)].

[23] S. Redner, *A Guide to First-passage Processes* (Cambridge University Press, Cambridge, 2001).

[24] G.H. Weiss, *Aspects and Applications of the Random Walk* (North-Holland, Amsterdam, 1994).

[25] A.V. Barzykin and M. Tachiya, J. Chem. Phys. **99**, 9591 (1993).

[26] R.A. Blythe and A.J. Bray, J. Phys. A **35**, 10 503 (2002).

[27] F. van Wijland, J. Phys. A **35**, 5391 (2002).

[28] F. van Wijland (private communication).

[29] A.D. Sánchez, M.A. Rodriguez, and H.S. Wio, Phys. Rev. E **57**, 6390 (1998).

[30] G. Oshanin, O. Bénichou, M. Coppey, and M. Moreau, Phys. Rev. E **66**, 060101 (2002).