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Survival probabilities in the double trapping reaction $A + B \rightarrow B, B + C \rightarrow C$

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Abstract

We consider the double trapping reaction $A + B \rightarrow B, B + C \rightarrow C$ in one dimension. The survival probability of a given A particle is calculated under various conditions on the diffusion constants of the reactants, and on the ratio of initial B and C particle densities. The results are shown to be of more general form than those obtained in previous work on the problem.

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1. Introduction

The simple trapping reaction $A + B \rightarrow B$ has been studied intensely over the last two decades, motivated in part by studies of the related two-species annihilation problem, $A + B \rightarrow 0$, introduced in the classic paper of Toussaint and Wilczek [1]. These models are relevant to problems in chemical kinetics, as well as various processes in physics and biology. For example, the two-species annihilation reaction $A + B \rightarrow 0$ models the reaction $A + B \rightarrow C$, where the product species C is inert, while the trapping reaction $A + B \rightarrow B$ models a catalytic process. In one spatial dimension the survival probability, $Q_A(t)$, of a single diffusing A particle moving in an initially homogeneous background of diffusing B particles has been proved rigorously to decay as $Q_A(t) \sim \exp(-\lambda t^{1/2})$ [2]. Only recently, however, has an exact expression for the coefficient λ been derived [3]: $\lambda = (4/\sqrt{\pi})\rho_B\sqrt{D_B}$, where ρ_B and D_B are the density and diffusion constant, respectively of the B particles. The result has been generalized [4] to all (continuous) dimensions $d \leq 2$. A curious feature of the result is the absence of any dependence on the diffusion constant, D_A , of the A particle (at least in the leading asymptotics— D_A does appear, however, in subdominant terms [5]). For $d > 2$ the rate-equation approach, which predicts a simple exponential decay, is qualitatively correct [2].

In contrast to the simple trapping reaction, more complex trapping sequences have received little attention. This paper is devoted to the double trapping reaction $A + B \rightarrow B, B + C \rightarrow C$. We try to compute the fraction of A particles remaining at time t , or equivalently, the probability, $Q_A(t)$, that a single A particle has survived up to time t , given that it is initially surrounded by a sea of Poisson distributed traps, the B particles. The B particles themselves are initially

surrounded by Poisson distributed traps—the C particles—and thus disappear from the system at each time step with a probability to be determined. By ‘Poisson distributed’ we mean that the probability of finding N traps in an interval of length L is $[(\rho_{B,C}L)^N/N!]\exp(-\rho_{B,C}L)$, where $\rho_{B,C}$ is the density of B or C particles. Since the C particles diffuse independently, and do not disappear from the system, they remain Poisson distributed at all times. The spatial distribution of the B particles may change, however, as B particles are absorbed.

Of particular interest is the limit $t \rightarrow \infty$. Since the B -particle density ultimately decays to zero, the function $Q_A(t)$ will approach a non-zero limit $Q_A(\infty)$ which, on dimensional grounds, can only depend on the density ratio ρ_{B0}/ρ_C , where $\rho_{B0} = \rho_B(0)$ is the initial B -particle density, and on the ratios $D_A/D_B, D_B/D_C$ of diffusion constants. The calculation of $Q_A(\infty)$ is our main goal.

This double trapping problem has been studied using a mean-field (i.e. rate equation) approach, which should again be qualitatively valid for $d > 2$, and by a version of the Galanin model for $d = 1$ [6]. The latter approach predicts the following limiting result:

$$Q_A(\infty) = \left(1 + \frac{\rho_{B0}}{\rho_C} \sqrt{\frac{D_A + D_B}{D_B + D_C}}\right)^{-1}. \quad (1)$$

This paper considers various limiting regimes of the general problem in which exact results or bounds can be obtained for comparison with equation (1). We also obtain some results on the asymptotic form of the time dependence of $Q_A(t)$, i.e. on the manner in which the asymptotic limit is approached.

2. Analysis of the survival probabilities

Each particle i diffuses according to the Langevin equation $\dot{x}_i = \eta_i(t)$, where $\eta_i(t)$ is Gaussian white noise with mean zero and correlator $\langle \eta_i(t)\eta_j(t') \rangle = 2D\delta_{ij}\delta(t-t')$, where $D = D_A, D_B, D_C$ are the diffusion constants for the three reactant species. From this one can derive in standard fashion a backward Fokker–Planck equation governing the time evolution of the particle’s survival probability $Q(x_i, t)$:

$$\frac{\partial Q(x_i, t)}{\partial t} = D \frac{\partial^2 Q(x_i, t)}{\partial x_i^2}, \quad (2)$$

where x_i is the position of the i th particle at time $t = 0$.

We consider three subsets of the general double trapping problem: the cases where $D_A \ll D_B \ll D_C$, where $D_B = 0$ and where $D_A = D_C = 0$. In the first two cases it will be necessary, to obtain exact results or exact bounds, to limit consideration to the regime $\rho_{B0} \ll \rho_C$. For the case $D_A = D_C = 0$, however, an exact result for $Q_A(\infty)$ is possible for all values of the ratio ρ_{B0}/ρ_C .

2.1. The case $D_A \ll D_B \ll D_C$

We first consider a subset of the general $A + B \rightarrow B, B + C \rightarrow C$ problem in which the diffusion constants of the A, B and C particles are subject to the condition $D_A \ll D_B \ll D_C$. This allows us to approximate each process as an independent ‘target annihilation problem’ [7], i.e. in the reaction $B + C \rightarrow C$ we treat the B particles as static and the C particles as mobile traps, and in the $A + B \rightarrow B$ process we consider the B particles as mobile traps for a static A particle. We also subject this problem to the condition $\rho_{B0} \ll \rho_C$ to ensure that the B particles remain Poisson distributed even at large times, i.e. that no clustering of B particles emerges in regions free of C particles. The reason for this condition will become clear shortly.

We begin by considering a single, static B particle at the origin. The survival probability, Q_1 , of the B particle with only one C present, starting at some $x > 0$, is the solution of (2) subject to the boundary conditions $Q_1(0, t) = 0$, $Q_1(\infty, t) = 1$ and $Q_1(x, 0) = 1$. That is [8]

$$Q_1(x, t) = \operatorname{erf}\left(\frac{x}{\sqrt{4D_C t}}\right),$$

where $\operatorname{erf}(y)$ is the error function. With N traps present, where $N = \rho_C L$, starting at positions x_i uniformly distributed in $[0, L]$, the survival probability of the B particle is (following the argument in [7])

$$Q_N(t) = \prod_{i=1}^N \left[\frac{1}{L} \int_0^L dx_i \operatorname{erf}\left(\frac{x_i}{\sqrt{4D_C t}}\right) \right],$$

where we have averaged over the starting positions. Rewriting the error function in terms of the complementary error function, $\operatorname{erf}(y) = 1 - \operatorname{erfc}(y)$, and using the fact that the C particles are independent, we have

$$Q_N(t) = \left[1 - \frac{1}{L} \int_0^L dx \operatorname{erfc}\left(\frac{x}{\sqrt{4D_C t}}\right) \right]^{\rho_C L}. \quad (3)$$

Taking the limits $N \rightarrow \infty$ and $L \rightarrow \infty$, keeping ρ_C fixed, and evaluating the integral in (3), gives

$$Q(t) = \exp\left(-\frac{2}{\sqrt{\pi}} \rho_C \sqrt{D_C t}\right). \quad (4)$$

We can perform the same calculation on the opposite side of the B particle and, since the results are symmetric and independent, get the same result. So the full survival probability of the B particle is simply the square of (4), i.e.

$$Q_B(t) = \exp\left(-\frac{4}{\sqrt{\pi}} \rho_C \sqrt{D_C t}\right), \quad (5)$$

which is the standard result for the one-dimensional target problem.

For the $A + B \rightarrow B$ process we can use the ‘toy model’ introduced in [9]. In this model, the traps B are assumed to disappear randomly in a manner consistent with the required density $\rho_B(t)$. The model will be an exact representation of the double trapping reaction provided $\rho_{B0} \ll \rho_C$, so that no correlations develop in the positions of surviving B particles. The time dependence of the A -particle survival probability, $Q_A(t)$, within this model is calculated using a similar argument to that outlined above, but with the traps disappearing from the system at each time step with a known probability. In our case, we can describe this decay of traps using the survival probability of a B particle, $Q_B(t)$, as given by (5). The model gives for the survival probability of the A particle [9]

$$Q_A(t) = \exp\left(-2\rho_{B0} \sqrt{\frac{D_B}{\pi}} \int_0^t \frac{d\tau}{\tau^{1/2}} Q_B(\tau)\right).$$

Substituting for $Q_B(\tau)$ from equation (5) gives the result

$$Q_A(t) = \exp\left[-\frac{\rho_{B0}}{\rho_C} \sqrt{\frac{D_B}{D_C}} \left(1 - e^{-\frac{4}{\sqrt{\pi}} \rho_C \sqrt{D_C t}}\right)\right]. \quad (6)$$

Note that this result was derived treating the A particles as static, so it will become asymptotically exact in the limit $D_A \ll D_B$ (and we have already assumed $D_B \ll D_C$).

For the case where $\rho_{B0} \ll \rho_C$ and $D_B \ll D_C$ still hold, but D_A is arbitrary, the ‘Pascal principle’ [10], according to which the A particle survives longest if it does not move, shows that equation (6) provides an upper bound on $Q_A(t)$ for any value of D_A .

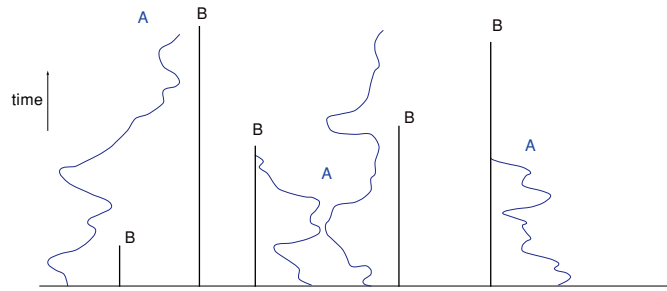


Figure 1. For $D_B = 0$ and $\rho_{B0} \ll \rho_C$, the A particles diffuse among static traps which disappear randomly and independently.

2.2. The case $D_B = 0$

For the $B + C \rightarrow C$ reaction, with the B particles remaining static, we can again use the result in equation (5) for the B -particle survival probability. The $A + B \rightarrow B$ process remains, however, a nontrivial problem, consisting of A particles diffusing among static traps each of which has a survival probability $Q_B(t)$, as shown in figure 1. Taking once again the limit $\rho_{B0} \ll \rho_C$, the survival probabilities of the different B particles can be treated as independent, but the problem is still nontrivial. We can, however, find a lower bound on $Q_A(t)$ by considering an approach based on the span, $R(t)$, of a random walk—the distance from the point of maximum excursion in one direction to maximum excursion in the opposite direction, up to time t . The average value of this quantity is given by (see [11])

$$\langle R(t) \rangle = 4\sqrt{\frac{D_A t}{\pi}}. \quad (7)$$

We formulate the $A + B \rightarrow B$ process as follows. We write the infinitesimal change in the survival probability of a given A particle, dQ_A , in terms of the probability that it is trapped by a B particle in the time interval $t \rightarrow t + dt$ in which the span of the random walk increases by dR :

$$\begin{aligned} dQ_A &= -\rho_{B0} dR Q(A, B; t) \\ &= -\rho_{B0} dR Q_A Q(B|A; t), \end{aligned} \quad (8)$$

where $\rho_{B0} dR$ is the probability of finding a B particle initially in the interval dR (treating, as usual, the initial B particle locations as a Poisson process), $Q(A, B; t)$ is the joint probability that both the A particle and the B particle have survived up to time t , and $Q(B|A; t)$ is the conditional probability that the B particle has survived until time t given that the A particle has survived. To treat the survival probability of the A and the B particles as independent, we must make the assumption that the B particles remain Poisson distributed at all times, i.e. that the positions of the B particles are not spatially correlated. If the B particles survive in clusters and there develop regions totally free of B particles, then the probability that an A particle has survived will depend on whether it is in a B -free region or in a cluster of B particles. In the limit $\rho_{B0} \ll \rho_C$, the assumption of independence is justified, and allows us to write $Q(B|A; t) = Q_B(t)$, with $Q_B(t)$ given by (5). The solution of (8) is then

$$Q_A(t) = \exp\left(-\rho_{B0} \int_0^t Q_B(\tau) \frac{dR}{d\tau} d\tau\right).$$

The span is a stochastic variable so we need to average over all realizations of the function $R(\tau)$, which analytically is not trivial. We can, however, obtain a lower bound by using the

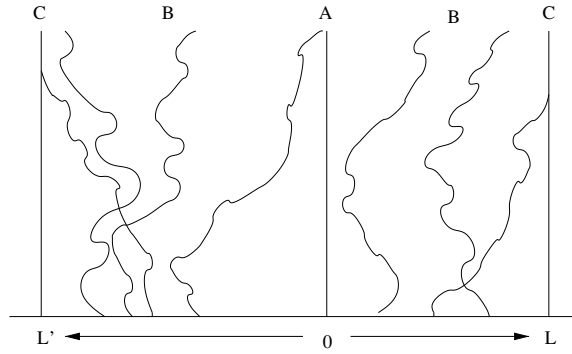


Figure 2. We consider the subset of the problem where $D_A = D_C = 0$. For the A particle to survive, all the B particles between the neighbouring C particles must reach a C particle first, thus being removed from the system before reaching the A particle.

convexity inequality

$$\begin{aligned} \langle Q_A(t) \rangle &= \left\langle \exp \left(-\rho_{B0} \int_0^t Q_B(\tau) \frac{dR}{d\tau} d\tau \right) \right\rangle \\ &\geq \exp \left(-\rho_{B0} \int_0^t Q_B(\tau) \frac{d}{d\tau} \langle R \rangle d\tau \right), \end{aligned}$$

and by substituting for $\langle R(t) \rangle$ using (7) we obtain the result

$$\langle Q_A(t) \rangle \geq \exp \left[-\frac{\rho_{B0}}{\rho_C} \sqrt{\frac{D_A}{D_C}} \left(1 - e^{-\frac{4}{\sqrt{\pi}} \rho_C \sqrt{D_C t}} \right) \right]. \quad (9)$$

2.3. The case $D_A = D_C = 0$

We now consider the case where the A and C particles remain static and the B particles diffuse among them. We can treat this as an extension of the Gambler's Ruin problem [8]. We need only consider a single A particle and the nearest C particle on either side of it, as shown in figure 2. For the probability that the A particle survives, we want the probability that all B particles between the A particle and the nearest C particles on either side reach the C particles before the A particle. The results (after averaging over the distances L and L' in figure 2) will be the same on each side, and independent so we may solve the backward Fokker–Planck equation (2) on one side and simply square the result. We solve equation (2) subject to the boundary conditions $Q(0, t) = 0, Q(L, t) = 1$, where we have an A particle at the origin and a C particle at $x = L$, and the B particle starts at x , uniformly distributed in $[0, L]$. The solution is

$$Q(x, t) = \frac{x}{L} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \sin \left(\frac{n\pi x}{L} \right) \exp \left(-\frac{n^2 \pi^2 D_B t}{L^2} \right). \quad (10)$$

Averaging the result over the starting position x gives

$$\begin{aligned} Q(t; L) &= \frac{1}{L} \int_0^L dx Q(x, t) \\ &= \frac{1}{2} + \frac{4}{\pi^2} \sum_{\text{odd } n} \frac{1}{n^2} \exp \left(-\frac{n^2 \pi^2 D_B t}{L^2} \right). \end{aligned} \quad (11)$$

We now consider an arbitrary number of B particles in this interval $[0, L]$. Since the B particles are Poisson distributed, the probability of having N of them initially in the interval is

$$p_N = \frac{(\rho_{B0}L)^N}{N!} e^{-\rho_{B0}L}.$$

Then the probability that the A survives given $N B$ particles initially in $[0, L]$ is, for large t ,

$$\begin{aligned} \bar{Q}(t; L) &= \sum_{N=0}^{\infty} p_N [Q(t; L)]^N = e^{-\rho_{B0}L[1-Q(t;L)]} \\ &\approx \exp\left(-\frac{\rho_{B0}L}{2} + \frac{4\rho_{B0}L}{\pi^2} e^{-\frac{\pi^2 D_B t}{L^2}}\right), \end{aligned}$$

where we have kept only the lowest mode since we are interested in an asymptotic large- t result.

Finally, we average over all possible lengths L , weighted by the Poisson distribution for the C particle positions:

$$Q_A^{(1)}(t) = \rho_C \int_0^\infty \bar{Q}(t; L) e^{-\rho_C L} dL. \tag{12}$$

We simplify by differentiating with respect to t and evaluate the resulting integral asymptotically for large t using the Laplace method [12]. The result is

$$Q_A^{(1)}(t) \sim \frac{1}{1 + \frac{\rho_{B0}}{2\rho_C}} \left[1 + \frac{8}{(3\pi)^{1/2}} (\rho_{B0}^2 D_B t)^{1/2} \exp\left(-3 \left(\frac{\pi}{2}\right)^{2/3} \left(\frac{\rho_C}{\rho_{B0}} + \frac{1}{2}\right)^{2/3} (\rho_{B0}^2 D_B t)^{1/3}\right) \right]$$

valid for $\rho_{B0}^2 D_B t \gg 1$. To include the contribution from the left side we square this result to obtain, asymptotically,

$$\begin{aligned} Q_A(t) &\sim \frac{1}{\left(1 + \frac{\rho_{B0}}{2\rho_C}\right)^2} \left[1 + \frac{16}{(3\pi)^{1/2}} (\rho_{B0}^2 D_B t)^{1/2} \right. \\ &\quad \left. \times \exp\left(-3 \left(\frac{\pi}{2}\right)^{2/3} \left(\frac{\rho_C}{\rho_{B0}} + \frac{1}{2}\right)^{2/3} (\rho_{B0}^2 D_B t)^{1/3}\right) \right]. \end{aligned} \tag{13}$$

Note that this result does not require any condition on the ratio ρ_{B0}/ρ_C . As a check on the result we evaluate (12) numerically using Gauss–Legendre two-point quadrature. We change variables to $u = 1/(\rho y + 1)$, where $\rho = \rho_C + \rho_{B0}/2$, to map the infinite range of integration onto the finite interval $[0, 1]$. The numerical result along with the asymptotic result (13) is compared in figures 3 and 4 for two values of the ratio ρ_{B0}/ρ_C , 0.5 and 2, respectively. For ease of comparison we first write the result (13) in the form

$$\frac{Q_A(t) - Q_A(\infty)}{Q_A(\infty)\lambda_1(\rho_{B0}^2 D_B t)^{1/2}} = \exp[-\lambda_2(\rho_{B0}^2 D_B t)^{1/3}], \tag{14}$$

where $\lambda_1 = 16/\sqrt{3\pi}$ and $\lambda_2 = 3(\pi/2)^{2/3}(\rho_C/\rho_{B0} + 1/2)^{2/3}$. The result is plotted in log-linear form in figures 3 and 4.

3. Discussion and summary

The asymptotic result (6) for the survival probability of an A particle in the case $D_A \ll D_B \ll D_C$ and the lower bound (9) obtained for $D_B = 0$ are both subject to the condition $\rho_{B0} \ll \rho_C$.

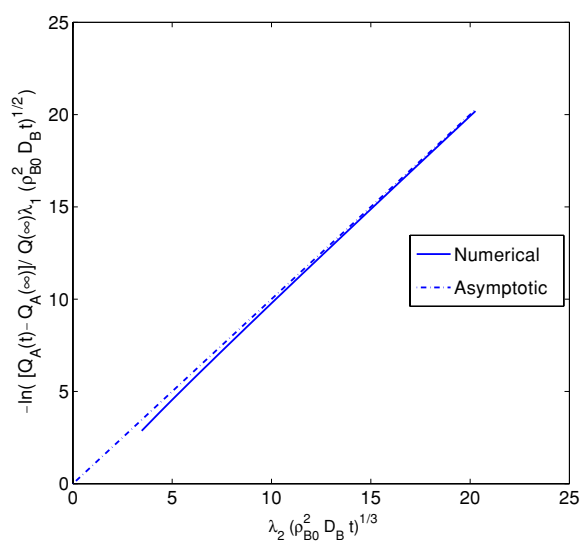


Figure 3. Convergence of the asymptotic solution (13) to the numerical solution of (12) with $\rho_{B0}/\rho_C = 0.5$. The data are presented as a log-linear plot in the form suggested by equation (14). The asymptotic solution has gradient 1.

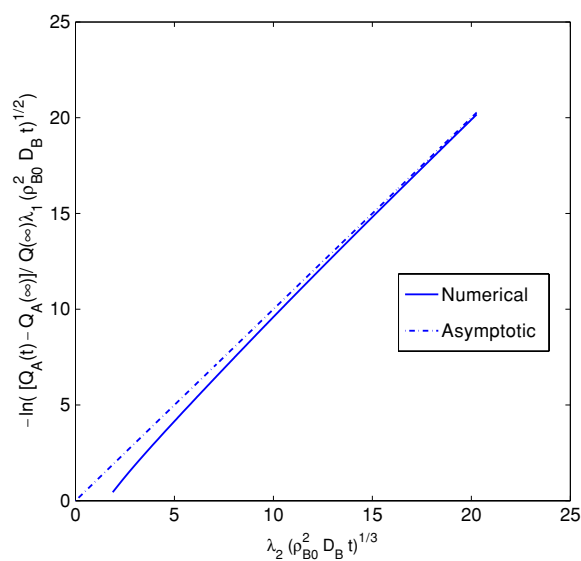


Figure 4. Convergence of the asymptotic solution (13) to the numerical solution of (12) with $\rho_{B0}/\rho_C = 2$. The data are presented as a log-linear plot in the form suggested by equation (14). The asymptotic solution has gradient 1.

Under these conditions both results reduce to the same limiting forms as (1) at late times

$$Q_A(\infty) = 1 - \frac{\rho_{B0}}{\rho_C} \sqrt{\frac{D_{A,B}}{D_C}}, \quad (15)$$

correct to first order in ρ_{B0}/ρ_C . Results (6) and (9) are, however, of a more general form since they indicate the nature of the asymptotic time dependence of $Q_A(t)$. Under the condition $\rho_{B0} \ll \rho_C$ necessary for these results to be valid, the exponentials in (6) and (9) can be expanded to first order in their arguments.

The result (13) for the condition $D_A = D_C = 0$ is still more general since it is valid for any value of the ratio ρ_{B0}/ρ_C . The exact infinite-time result for this case, $Q_A(\infty) = (1 + \rho_{B0}/2\rho_C)^{-2}$, differs from the result $(1 + \rho_{B0}/\rho_C)^{-1}$ obtained from equation (1) under the same conditions, although once more the two results reduce to the same limiting form, $1 - \rho_{B0}/\rho_C$, to leading order in ρ_{B0}/ρ_C . These results suggest the possibility of a systematic expansion in powers of ρ_{B0}/ρ_C .

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