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The survival probability of a diffusing particle constrained by two moving, absorbing boundaries

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Abstract
We calculate the exact asymptotic survival probability, Q, of a one-dimensional Brownian particle, initially located at the point $x \in (-L, L)$, in the presence of two moving, absorbing boundaries located at $\pm(L + ct)$. The result is $Q(y, \lambda) = \sum_{n=-\infty}^{\infty}(-1)^n \cosh(ny)\exp(-n^2\lambda)$, where $y = cx/D$, $\lambda = cL/D$ and D is the diffusion constant of the particle. The results may be extended to the case where the absorbing boundaries have different speeds. As an application, we compute the asymptotic survival probability for the trapping reaction $A + B \to B$, for evanescent traps with a long decay time.

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(Some figures in this article are in colour only in the electronic version)

Physical systems described by partial differential equations with moving boundary conditions are ubiquitous in nature [1]. Unfortunately, such equations are notoriously difficult to solve. The case of a single moving boundary is often amenable to analysis, for example by transforming to the moving frame, but the case of more than one moving boundary is, in general, intractable.

First-passage problems are another field of research for which there are relatively few exact results [2, 3]. The simplest such problem, for which some exact results are available, is that of a Brownian particle (i.e. random walker) moving in the presence of one or more absorbing boundaries [2]. The case of a single boundary, moving at constant speed, can be solved exactly [2] but, to our knowledge, the survival probability of a single Brownian walker in the presence of two moving boundaries with different velocities had not been solved up to now.

In the present paper, we apply 'backward Fokker–Planck' methods to solve this problem exactly. As an application, we consider the one-dimensional trapping reaction $A + B \to B$, where the density of traps, ρ, decays exponentially with time, and obtain the exact asymptotic form of the final A-particle density in the limit where the decay time, τ, of the traps is large.

We consider a Brownian walker moving according to the Langevin equation $\dot{X}(t) = \eta(t)$, with initial condition $X(0) = x$, where $\eta(t)$ is Gaussian white noise with mean zero and correlator $\langle\eta(t_1)\eta(t_2)\rangle = 2D\delta(t_1 - t_2)$. The particle is flanked by two receding, absorbing

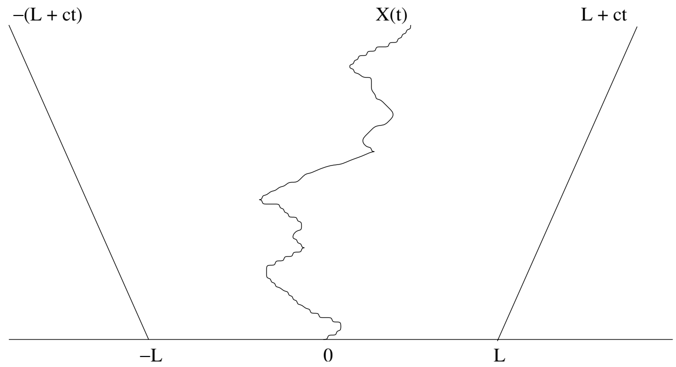

Figure 1. Brownian walker, starting from the origin, in a linearly expanding cage.

walls with coordinates $\pm(L + ct)$, as shown in figure 1. We can derive a backward Fokker–Planck equation for the probability, $Q(x, L, t)$, that the particle has survived up to time t having started at position $x \in (-L, L)$. We note that, after infinitesimal time Δt, the particle will have moved to position $x + \Delta X$, and the walls will have moved to positions $\pm(L + c\Delta t)$. It follows that $Q(x, L, t) = \langle Q(x + \Delta X, L + c\Delta t, t - \Delta t)\rangle$, where the average is over the distribution of the spatial increment ΔX. Expanding to first order in Δt, using $\langle \Delta X\rangle = 0$ and $\langle(\Delta X)^2\rangle = 2D\Delta t$, yields the backward Fokker–Planck equation

$$\frac{\partial Q}{\partial t} = D\frac{\partial^2 Q}{\partial x^2} + c\frac{\partial Q}{\partial L}. \tag{1}$$

The infinite-time result is obtained by setting the time derivative to zero. It is convenient to introduce the variables $y = cx/D$ and $\lambda = cL/D$ to represent the dimensionless initial positions of the particle and the walls. Equation (1) then reads, at infinite time,

$$\frac{\partial^2 Q}{\partial y^2} + \frac{\partial Q}{\partial \lambda} = 0, \tag{2}$$

where $-\lambda \leqslant y \leqslant \lambda$, subject to the absorbing boundary conditions, $Q(\pm\lambda, \lambda) = 0$, and $Q(y, \infty) = 1$, since if the particle starts at one of walls it is immediately absorbed, while if the walls are initially infinitely far away the particle will survive with probability 1. A solution of equation (2) satisfying the boundary conditions may be deduced by inspection, noting the symmetry of the problem under reflection, $y \to -y$:

$$Q(y, \lambda) = \sum_{n=-\infty}^{\infty} (-1)^n \cosh(ny)\, \mathrm{e}^{-n^2\lambda}. \tag{3}$$

Despite the simplicity of its derivation, equation (3) is, to our knowledge, a new result. It should be noted that this result seems difficult to obtain using conventional ('forward') Fokker–Planck methods. The backward Fokker–Planck method has eliminated the time-dependent boundary conditions from the problem at the cost of introducing the initial wall parameter, L, as an additional independent variable.

In figure 2, we present the results of numerically evaluating the sum in equation (3) for various values of the starting coordinate, y.

For a particle starting at the origin, the survival probability $Q(0, \lambda)$, written simply as $Q(\lambda)$, is

$$Q(\lambda) = \sum_{n=-\infty}^{\infty} (-1)^n\, \mathrm{e}^{-n^2\lambda}. \tag{4}$$

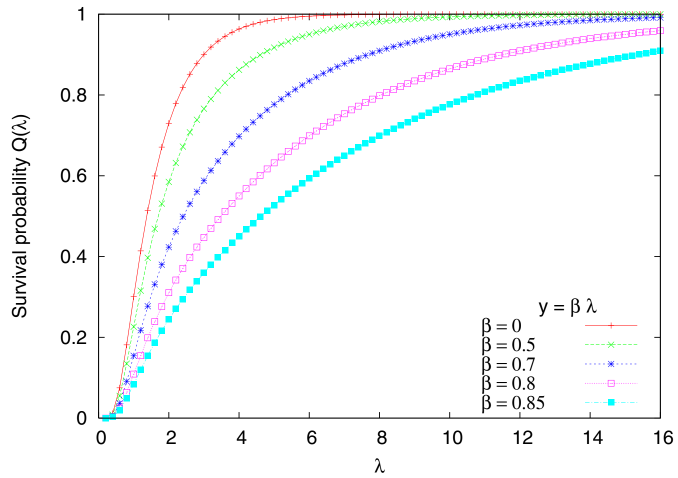

Figure 2. Survival probability $Q(\lambda)$ for various values of the initial coordinate y.

To leading order for large λ we may approximate the sum by the $n = 0$ and $n = \pm 1$ terms:

$$Q(\lambda) \sim 1 - 2\,\mathrm{e}^{-\lambda}. \tag{5}$$

This result agrees, to first order in $\mathrm{e}^{-\lambda}$, with the approximate infinite-time result, $Q(\lambda) \sim \exp(-2\,\mathrm{e}^{-\lambda})$, obtained using the method of Krapivsky and Redner [4] for a rapidly expanding cage. In this approach, one writes the joint probability distribution that the particle survives till time t, and is located at x, in the approximate form [4] $P(x,t) = [Q(t)/\sqrt{4\pi Dt}]\exp(-x^2/4Dt)$, i.e. one multiplies the free diffusion propagator by the probability, $Q(t)$, for the particle to survive till time t, ignoring the boundary conditions at the walls, where the density is anyway small. The rate of change of $Q(t)$ is minus the total probability flux through the walls, $\mathrm{d}Q/\mathrm{d}t = 2D(\partial P/\partial x)_{x=L+ct}$. Integrating the resulting equation from $t = 0$ to $t = \infty$, using the method of steepest descents (valid for $\lambda \gg 1$), gives the quoted result. We see that this method only gives the leading departure from unity correctly.

For small λ, the leading-order behaviour can be obtained by rewriting equation (4) using the Poisson sum formula, $\sum_{n=-\infty}^{\infty} f(n) = \sum_{k=-\infty}^{\infty} \tilde{f}(2\pi k)$, where $\tilde{f}(k)$ is the Fourier transform of the function $f(n)$. This gives

$$Q(\lambda) = \sqrt{\frac{\pi}{\lambda}} \sum_{k=-\infty}^{\infty} \exp(-\pi^2(2k-1)^2/4\lambda) \tag{6}$$

The leading behaviour at small λ is

$$Q(\lambda) \sim 2\sqrt{\pi/\lambda}\,\exp(-\pi^2/4\lambda), \tag{7}$$

which contains an essential singularity at $\lambda = 0$. We are unaware of any approximate methods for which even the leading behaviour, equation (7), can be recovered.

We have performed the sum in equation (4) numerically and plot the result together with the large- and small-λ forms, equations (5) and (7), in figure 3. We see that the asymptotic forms describe the data well over a considerable range of λ. This is readily understood on noting that the leading corrections to the asymptotic forms are of order $\exp(-4\lambda)$ and $\exp(-9\pi^2/4\lambda)$ for large and small λ, respectively.

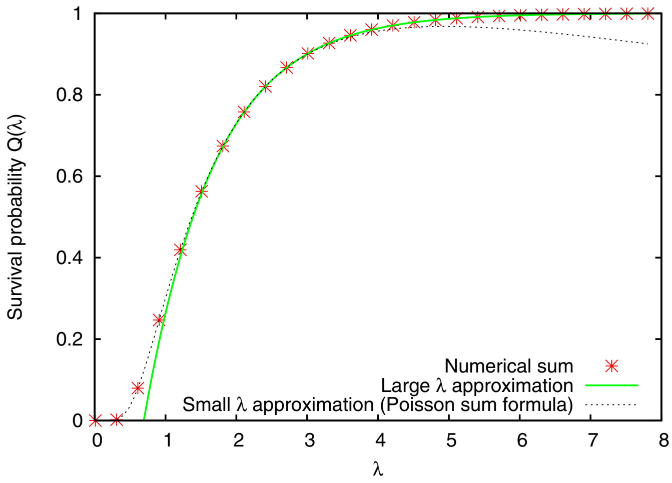

Figure 3. Survival probability for a particle starting at the mid-point of a linearly expanding cage with the asymptotic forms for small and large values of λ, the dimensionless measure of the initial locations of the walls.

To discuss the general case of walls with different speeds, we first consider the problem of a Brownian walker with drift αc following a path $X(t)$, $X(0) = x$, with an absorbing boundary at the origin, and a receding absorbing boundary at position $L + ct$, where $x \in (0, L)$. The path $X(t)$ of the walker satisfies the Langevin equation $\dot{X}(t) = \eta(t) + \alpha c$, where $\eta(t)$ is again Gaussian white noise. We can write a backward Fokker–Planck equation for the survival probability of the particle at infinite time which, making the same changes of variable as those used in equation (2), takes the form

$$\frac{\partial^2 Q}{\partial y^2} + \alpha \frac{\partial Q}{\partial y} + \frac{\partial Q}{\partial \lambda} = 0, \tag{8}$$

subject to the boundary conditions $Q(y = 0, \lambda) = Q(y = \lambda, \lambda) = 0$. In the limit $\lambda \to \infty$, we impose as a boundary condition the solution of equation (8) with $\partial Q/\partial\lambda = 0$, i.e. $Q(y, \lambda \to \infty) = 1 - \exp(-\alpha y)$, which is the survival probability of a diffusing particle that drifts with mean velocity αc away from a fixed absorbing boundary or, equivalently, the survival probability of a particle with no drift in the presence of one wall receding at speed αc (see, for example, [2] and references therein).

A solution to equation (8) satisfying all the boundary conditions is

$$Q(y, \lambda) = \sum_{n=-\infty}^{\infty} (\mathrm{e}^{ny} - \mathrm{e}^{-(n+\alpha)y})\, \mathrm{e}^{-n(n+\alpha)\lambda}. \tag{9}$$

On shifting to the left both the path of the particle and the coordinates of the barriers by a distance $(L/2 + \alpha ct)$, we see that equation (9) solves the expanding cage problem for a particle with no drift and with asymmetrically receding walls—the left wall having coordinates $-(L/2 + \alpha ct)$, and the right $(L/2 + (1 - \alpha)ct)$, and may be shown to be equivalent to equation (3) when $\alpha = 1/2$ (noting that the separation of the walls and drift velocities need to be doubled to show an exact mapping between the two problems).

As an application of these results, we consider the trapping reaction, $A + B \to B$ [5], with evanescent traps. We find the infinite-time survival probability of a particle, A, surrounded by an infinite sea of Poisson-distributed, evanescent traps, B, with initial density ρ, undergoing the trapping reaction in one dimension. By Poisson-distributed we mean that, at $t = 0$, each infinitesimal interval $\mathrm{d}x$ contains a trap with probability $\rho\,\mathrm{d}x$. In particular, the probability of finding no traps in an interval of length L is $\exp(-\rho L)$. The traps are evanescent in the sense that they randomly and independently disappear from the system in such a way that the overall trap density decreases in a prescribed fashion, $\rho(t) = f(t)\rho(0)$. The particle and traps both perform Brownian motion, with diffusion coefficients D_A and D_B, respectively. This problem has recently been studied in detail for various functions $f(t)$ for the case of a fixed target ($D_A = 0$) [6]. It was shown that, in this case, there is a non-zero infinite-time survival probability whenever $f(t)$ falls off more rapidly than $t^{-1/2}$ for large-t. Here, we address the general and more difficult problem of a moving A-particle and specialize to the case of exponentially decaying trap density, $f(t) = \exp(-t/\tau)$, anticipating a non-zero infinite-time survival probability. This survival probability for a single A-particle also gives the *fraction* of A-particles that survive if the initial state contains a macroscopic number of them.

We approach the problem in the spirit of Bray and Blythe [7], who considered the trapping reaction without trap decay, by finding upper and lower bounds on the survival probability and showing that they asymptotically agree. In the calculation of both bounds we use the formalism introduced by Bray, Majumdar and Blythe [8]. They define a quantity $\mu(t)$, the mean number of different traps that would meet the A-particle up to time t, for a given A-particle trajectory $z(t)$, in a fictitious model where the A- and B-particles do not react. It satisfies the integral equation

$$\rho(t) = \int_0^t \mathrm{d}t' \dot{\mu}(t') G(z(t), t|z(t'), t'), \tag{10}$$

where $\rho(t)$ is the trap density and $G(z(t), t|z(t'), t') = \exp[-(z(t) - z(t'))^2/4D_B(t - t')]/\sqrt{4\pi D_B(t - t')}$ is the trap diffusion propagator. Note that $\mu[z]$ is implicitly a functional of the A-particle trajectory and that $\mu\,(t = 0) = 0$. The survival probability of the A-particle is then given by [8, 9]

$$Q(t) = \langle \mathrm{e}^{-\mu[z]} \rangle_z, \tag{11}$$

with the average taken over the A-particle trajectories with the usual Wiener measure. When the fraction of surviving traps is $f(t)$, equation (10) is modified thus [8]

$$\rho = \int_0^t \mathrm{d}t' \frac{\dot{\mu}(t')}{f(t')} G(z(t), t|z(t'), t'), \tag{12}$$

where we now use ρ to refer to the *initial* trap density. This minor modification means that we may simply define a new quantity $\dot{\phi}(t) = \dot{\mu}(t)/f(t)$ in equation (12), solve as in the non-decaying case, and find that

$$\mu(t) = \int_0^t \mathrm{d}t' \dot{\phi}(t') f(t'). \tag{13}$$

We first derive an exact upper bound on the survival probability, as in [7, 8], by arguing that the particle will survive longest if it remains stationary at the origin (the 'target problem' [10]). This is the so-called Pascal principle [11]. We solve equation (12) with $z(t) = 0$,

$$\rho = \int_0^t \mathrm{d}t' \frac{\dot{\phi}(t')}{\sqrt{4\pi D_B(t - t')}}, \tag{14}$$

and get the solution found in [7], that is $\phi = 4(\rho^2 D_B t/\pi)^{1/2}$ which, using equation (13) with $t = \infty$ and $f(t') = \exp(-t'/\tau)$, and equation (11), gives an upper bound on the eventual survival probability as

$$Q \leqslant \exp[-2(\rho^2 D_B \tau)^{1/2}]. \tag{15}$$

We can prove that this is a rigorous upper bound following the procedure outlined in [8]. If we write $\phi = \phi_0 + \phi_1$ in equation (12), where ϕ_0 is the solution to equation (14), we can show that $\phi_1 \geqslant 0$, proving that $\phi \geqslant \phi_0$.

In [7], Bray and Blythe bound the survival probability from below by considering a notional box centred on the origin, from where the A-particle's trajectory is chosen to begin. They then select a subset of surviving trajectories by imposing three independent conditions that together guarantee the A-particle's survival: (i) the A-particle does not leave the box up to time t; (ii) no trap enters the box up to time t and (iii) no traps were inside the box at time $t = 0$. These conditions undercount the number of possible surviving trajectories of the A-particle—for example, a trap may enter the box without trapping the particle—so the probability of fulfilling them underestimates the actual survival probability. We follow a similar line of argument here, but with a modification to adjust for the exponentially decaying traps: we allow the walls of the box to recede linearly. Then we may use the result obtained in equation (4) to determine the probability of satisfying condition (i). We consider, therefore, the survival at infinite time. The probability corresponding to condition (iii) follows simply from the Poisson property of the trap density, and for a box of length $2L$ is simply $\exp(-2\rho L)$.

To obtain the probability that no traps have entered the box, we consider each side independently and square the result. This is then equivalent to the survival probability of a ballistic A-particle in an infinite sea of traps, which was solved in [12]. The problem may be solved using a modified form of equation (12) to allow for traps on only one side of the wall, a modification introduced in [8]. With the linear trajectory $z(t) = ct$ one obtains

$$\frac{\rho}{2}\left[1 + \mathrm{erf}\left(\frac{c\sqrt{t}}{\sqrt{4D_B}}\right)\right] = \int_0^t \mathrm{d}t' \dot{\phi}(t') \frac{\exp\left(-\frac{c^2}{4D_B}(t-t')\right)}{\sqrt{4\pi D_B (t-t')}}. \tag{16}$$

We solve this for $\dot{\phi}(t)$ by Laplace transform and, using equation (13), obtain the probability

$$\exp\left(-2\rho\sqrt{D_B\tau + \frac{c^2\tau^2}{4}} - \rho c\tau\right), \tag{17}$$

that no traps have ever entered the box.

We now combine these three factors to obtain a lower bound on Q:

$$Q \geqslant \exp\left(-2\rho\sqrt{D_B\tau + \frac{c^2\tau^2}{4}} - \rho c\tau - 2\rho L - \frac{\pi^2 D_A}{4cL}\right), \tag{18}$$

where the last term comes from using the small-λ result (7) and we have neglected a logarithmic correction in the exponent coming from the pre-exponential factor in equation (6). The result is valid for $cL/D_A \ll 1$ (corresponding to small λ in the rescaled coordinates of equations (2)–(7)). This bound contains two free parameters, L and c, so we obtain the best lower bound by maximizing equation (18) with respect to both of these quantities, giving

$$Q \geqslant \exp\left(-2(\rho^2 D_B\tau)^{1/2} - \tfrac{3}{2}(4\pi^2\rho^2 D_A\tau)^{1/3}\right). \tag{19}$$

This is valid as long as $\rho^2 D_A\tau \gg 1$, and $\rho^2 D_A\tau \gg (D_A/D_B)^3$, which are satisfied for large enough τ for any values of ρ, D_A and D_B.

Comparing the two bounds, (15) and (19), we see that they agree, for large τ, to leading order in the exponent. They therefore determine the exact large τ asymptotics in the form $Q \sim \exp[-2(\rho^2 D_B\tau)^{1/2} + \cdots]$, where the ellipsis indicates subdominant terms. Note that the leading term is independent of D_A, just as was found for the time-dependent asymptotics of the survival probability for non-decaying traps [7].

The fact that the bounds pinch indicates that the choice of linearly receding walls to obtain the lower bound is optimal for the case of exponentially decaying traps with a long decay time. Other forms for the trap decay function $f(t)$ will require a different choice for the wall motion to optimize the bound. We recall that for non-decaying traps the bound is optimal for static walls [7].

In summary, we have obtained exact results for the infinite-time survival probability of a diffusing particle flanked by two receding, absorbing boundaries, including the case where the boundaries move at different speeds. We have used the results to compute the survival probability of a particle diffusing in a sea of diffusing, evanescent traps in the limit where the trap decay time is large. Extensions to systems with general spatial dimensionality are possible and will be discussed elsewhere.

Acknowledgment

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