Exact Asymptotics for One-Dimensional Diffusion with Mobile Traps

Alan J. Bray and Richard A. Blythe

Department of Physics and Astronomy, University of Manchester, Manchester, M13 9PL, United Kingdom

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We consider a diffusing particle, with diffusion constant D', moving in one dimension in an infinite sea of noninteracting mobile traps with diffusion constant D and density ρ. We show that the asymptotic behavior of the survival probability, $P(t)$, satisfies $\lim_{t\to\infty}[-\ln P(t)]/\sqrt{\rho^2 Dt} = 4/\sqrt{\pi}$, independent of D'. The result comes from obtaining upper and lower bounds on $P(t)$, and showing that they coincide asymptotically. We also obtain exact results for $P(t)$ to first order in D'/D for an arbitrary finite number of traps.

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The asymptotics of the survival probability, $P(t)$, for a particle diffusing among mobile traps is a long-standing challenge. Over ten years ago Bramson and Lebowitz [1] showed by rigorous arguments that in one dimension $P(t)$ has a stretched-exponential decay for large t,

$$P(t) \sim \exp(-\lambda t^{1/2}). \tag{1}$$

The computation of the constant λ, however, has thus far proved intractable, both analytically and numerically. This long-standing problem is resolved in this Letter.

The problem addressed by Bramson and Lebowitz was first posed almost 20 years ago in the seminal paper of Toussaint and Wilczek (TW) [2]. These authors introduced the two-species annihilation process, $A + B \to 0$, as a model of monopole-antimonopole annihilation in the early Universe, though applications to chemical kinetics and condensed matter physics are more numerous [3]. TW showed that if the initial densities, $\rho_A(0)$ and $\rho_B(0)$, of the A and B particles are equal (and the particles are randomly distributed in space), the densities decay asymptotically as $t^{-d/4}$ in space dimensions $d < 4$. If the initial densities are *different*, however, the density of the minority species (A, say) decays much more rapidly.

The connection with the trapping problem is as follows. At late times $\rho_A(t) \ll \rho_B(t)$ and the A particles can be regarded as independently diffusing in a background of the majority B particles, which act as traps for the A particles by virtue of the annihilation reaction. An equivalent problem, therefore, is to consider a single A particle moving among B particles (which do not interact with each other) and ask for the probability, $P(t)$, that the A particle survives to time t. In the context of the original $A + B \to 0$ process (or $A + B \to B$ [4], which has the same asymptotics [1]) the "particle" A and "traps" B are taken to have the same diffusion constants, but for generality we will take them to be different, D' and D, respectively.

To our knowledge, no analytical result has been obtained up to now for the constant λ in Eq. (1). Furthermore, attempts to determine λ by numerical simulations (or even to confirm the predicted stretched-exponential decay with exponent 1/2) are severely hampered by large, slowly decaying transients [5–8]. In Ref. [7], a sophisticated numerical approach enabled data to be obtained down to $P(t) \sim 10^{-35}$, but still the asymptotic time dependence could not be unambiguously established.

For this trapping problem, the traps are infinite in number, and distributed randomly on the interval $(-\infty, \infty)$ with density ρ. By contrast, if the number of traps is *finite,* the problem is equivalent to the much studied predator-prey problem [9,10], where the traps are predators and the particle is the prey. In this case the prey survival probability decays as a power law,

$$P(t) \sim t^{-\theta(N_L, N_R, D'/D)}, \tag{2}$$

where N_L (N_R) is the number of predators initially to the left (right) of the prey. To our knowledge the only exactly solved examples are for $N_L + N_R \leq 2$. Obtaining analytical results for more than two predators is another long-standing challenge.

In this Letter we obtain two exact analytical results. First, we finally resolve the question of the asymptotics of $P(t)$ for the trapping problem. We verify the asymptotic form (1), and determine exactly the value of the constant λ, namely, $\lambda = 4\rho(D/\pi)^{1/2}$, i.e.,

$$P(t) \sim \exp[-4\rho(Dt/\pi)^{1/2}]. \tag{3}$$

Note that this asymptotic result depends only on the density, ρ, and diffusion constant, D, of the traps and is *independent of the diffusion constant D' of the particle.* The value of D', however, does affect the rate of approach to asymptopia. Equation (3) is derived by obtaining upper and lower bounds for $P(t)$, and showing that they converge for large t. Furthermore, the form of the lower bound suggests why large corrections to the asymptotic behavior might be expected.

Second, we outline [11] a perturbation theory in D'/D, based on a path-integral formulation, for the computation of the exponent θ in Eq. (2). For small D'/D and arbitrary values N_L and N_R, we find

$$\theta = \frac{N}{2} + \frac{1}{\pi}(N - \Delta^2)\frac{D'}{D} + O\left(\frac{D'^2}{D^2}\right), \tag{4}$$

where $N = N_L + N_R$ is the total number of predators and $\Delta = N_L - N_R$ measures their left-right asymmetry with respect to the prey.

We will first describe the treatment of the trapping problem with infinitely many traps. The bounds that lead to Eq. (3) are obtained as follows.

Upper Bound.—An obvious upper bound, $P_U(t)$, on $P(t)$, for any D', is provided by the problem with $D' = 0$, in which the particle stays at its initial position, which we call $x = 0$. Although we have as yet been unable to make this bound rigorous [12], it is intuitively clear that when, as here, the traps are (statistically) symmetrically placed with respect to the particle, the particle will on average survive longer if it stays still than if it diffuses. This assertion has been checked, using the algorithm outlined in Ref. [7], for all (lattice) walks up to time $t = 28$. It is also supported by Eq. (4), which shows that for any symmetric case ($\Delta = 0$), the decay of $P(t)$ is faster for small D' than for $D' = 0$, for any *finite N*.

For $D' = 0$ (sometimes called the "scavenger model" [13] in predator-prey terminology), $P(t)$ is just the probability that none of the moving traps has reached the origin up to time t. This problem is exactly soluble [14]. Since similar techniques will be needed to derive the lower bound, we outline the solution here.

The N traps move independently according to the Langevin equations

$$\dot{x}_i = \eta_i(t), \qquad i = 1, \ldots, N, \tag{5}$$

where $\eta_i(t)$ is Gaussian white noise with mean zero and correlator

$$\langle \eta_i(t)\eta_j(t')\rangle = 2D\,\delta_{ij}\delta(t - t'). \tag{6}$$

The quantity $P(t)$ is just the product of the individual trap probabilities. For a given trap starting at x_i, the required probability is [10] $P_1(x_i, t) = \mathrm{erf}(|x_i|/\sqrt{4Dt})$. So our upper bound is

$$P_U(t) = \left\langle \prod_{i=1}^{N} \mathrm{erf}(|x_i|/\sqrt{4Dt}) \right\rangle, \tag{7}$$

where $\langle\cdots\rangle$ means an average over the initial positions of the traps. Since the x_i are also independent, the latter average also factors. Using $N = \rho L$, where L is the length of the system, and each x_i is uniformly distributed in $(-L/2, L/2)$, gives

$$P_U(t) = \left[1 - 1/L \int_{-L/2}^{L/2} dx\, \mathrm{erfc}(|x|/\sqrt{4Dt})\right]^{\rho L} \to \exp[-4\rho(Dt/\pi)^{1/2}], \tag{8}$$

where the final result follows on taking the limit $L \to \infty$.

Lower Bound.—Consider the same system as before but with a pair of absorbing boundaries at $x = \pm l/2$. We consider the subset of initial conditions in which all the traps lie outside the interval $(-l/2, l/2)$ (and the particle is at $x = 0$), and trajectories in which neither the particle nor any of the traps has crossed a boundary up to time t. We calculate the probability, $P_L(t)$, of such an occurrence over the ensemble of all initial conditions and trajectories. These restricted initial conditions and trajectories are a subset of all the possible initial conditions and trajectories in which the particle never meets a trap. It follows that $P(t) \geq P_L(t)$, i.e., $P_L(t)$ is a lower bound.

The probability that there are no traps in the interval $(-l/2, l/2)$ at $t = 0$ is $\exp(-\rho l)$. Given that there are no traps in this interval at $t = 0$, the probability that no traps enter the interval up to time t is given by the same result as in the derivation of the lower bound, namely, $\exp[-4\rho(Dt/\pi)^{1/2}]$. Finally, the probability that the particle, starting at $x = 0$, has not left the interval $(-l/2, l/2)$ up to time t is given, for times $t \gg l^2/D'$, by [10] $(4/\pi)\exp(-\pi^2 D't/l^2)$. Assembling these contributions gives

$$P(t) \geq (4/\pi)\exp[-4\rho(Dt/\pi)^{1/2} - (\rho l + \pi^2 D't/l^2)]. \tag{9}$$

Since this inequality holds for all l, the best lower bound is obtained by maximizing with respect to l. The optimum value is $l = (2\pi^2 D't/\rho)^{1/3}$, and the best lower bound is

$$P_L(t) = \frac{4}{\pi}\exp[-4\rho(Dt/\pi)^{1/2} - 3(\pi^2\rho^2 D't/4)^{1/3}]. \tag{10}$$

Since the second term in the exponent is negligible compared to the first as $t \to \infty$, the two bounds converge to yield the asymptotic form, Eq. (3), for $P(t)$. More precisely, we can take the logarithm of $P(t)$ and divide out the leading $\sqrt{t}$ dependence to get

$$\frac{4}{\sqrt{\pi}} \leq -\frac{\ln P(t)}{(\rho^2 Dt)^{1/2}} \leq \frac{4}{\sqrt{\pi}} + 3\left(\frac{\pi}{2}\right)^{2/3}\frac{(D'/D)^{1/3}}{(\rho^2 Dt)^{1/6}}, \tag{11}$$

giving $\lim_{t\to\infty} -[\ln P(t)]/(\rho^2 Dt)^{1/2} = 4/\sqrt{\pi}$.

As an aside we note that, while the left-hand inequality in (11) holds for *all t*, since Eq. (8) does, the right-hand inequality is strictly a large t result. This is because the factor $(4/\pi)\exp(-\pi^2 D't/l^2)$ in Eq. (9) comes from the lowest mode in the Fourier decomposition of the survival probability of the particle in the interval $(-l/2, l/2)$. This mode dominates for $D't \gg l^2$, which requires $\rho^2 D't \gg 1$. A lower bound on $P(t)$ valid for all t can easily be written down by including all Fourier modes, but the large-t form (10) is sufficient for present purposes.

In Fig. 1, the left and right-hand sides of Eq. (12), representing the two asymptotic bounds, are plotted and compared to the numerical data of Ref. [7]. The data are

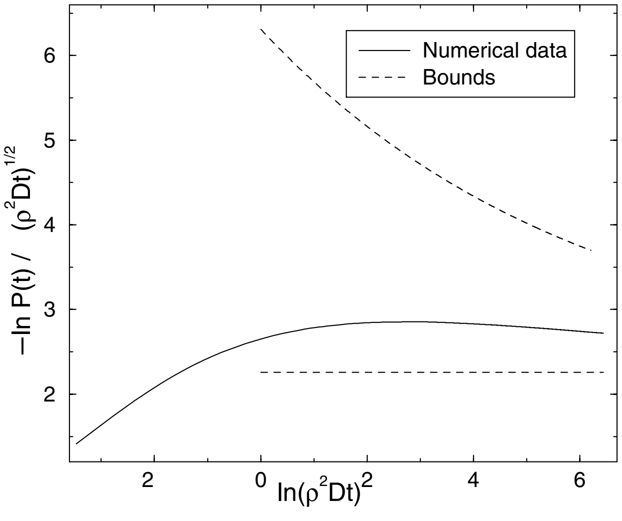

FIG. 1. Numerical data from Ref. [7] and the upper and lower bounds, Eq. (12), for $D' = D$. The numerical data were generated with $D = D' = 1/2$ and $\rho = 1/4$.

plotted using the dimensionless time $\rho^2 Dt$, and the axes are chosen to test the asymptotic form (3). The data lie between the bounds (except at early times where lattice effects are important [8]). The bounds displayed are for the case $D' = D$. The very slow convergence of the bounds is consistent with the observed trend in the data.

Some comments on Eq. (11) are in order. First, the right-hand inequality already suggests the possibility that the approach to asymptopia could be *very* slow, as observed in simulations, since the second term vanishes only as $t^{-1/6}$. For the case $D' = D$ that is usually simulated, the asymptotic result (3) gives, for a dimensionless time $\rho^2 Dt = 10^4$, say, a survival probability of order 10^{-98}. This is far smaller than can be reached in simulations (or experiments) even with sophisticated methods [7]. Yet even at this large time, the second term on the right-hand side of (11) is still 39% as big as the first. This term would give a further factor of 10^{-38} in the survival probability, i.e., a total probability of order 10^{-136}. Of course, this second term is only a bound, and the true correction to the asymptotic form could be smaller. The form of the bound is nonetheless suggestive and illustrates how large subdominant terms could arise. A clearer understanding of these subdominant terms is necessary before a detailed comparison with numerical or experimental data can be made.

A second interesting point is that the mean-square displacement of the particle, averaged over the surviving trajectories used to derive the lower bound, grows as $l^2 \sim (D't/\rho)^\nu$ with $\nu = 2/3$. This can be compared with the estimate $\nu = 0.5$ to 0.6 obtained from recent simulations [7]. Note, however, that these simulations were not in the asymptotic regime, so the numerical estimates should be treated with caution. Furthermore, the value $\nu = 2/3$ obtained from the lower bound for $P(t)$ does not necessarily represent any kind of bound for ν. Nevertheless, the rough agreement between the measured value and that obtained from our very simple arguments is again suggestive.

Our approach is also readily generalized to dimensions $d > 1$ [11]. For $d < 2$ we find $P(t) \sim \exp[-a_d \rho (Dt)^{d/2}]$, where $a_d = (2/\pi d)(4\pi)^{d/2} \sin(\pi d/2)$ while, for $d = 2$, $P(t) \sim \exp[-4\pi\rho Dt/\ln t]$. The latter agrees with the functional form obtained in [1], but with a precise value for the constant. For $d > 2$, simple exponential decay is obtained, in agreement with [1], but the bounds no longer converge and the decay constant cannot be determined.

In the remainder of this Letter we sketch [11] the derivation of the perturbation theory, for a finite number of traps, that leads to Eq. (4). We recall that the N traps move independently according to Langevin equations (5) with noise correlator (6). We call the particle coordinate $x_0(t)$. It obeys the Langevin equation $\dot{x}_0 = \eta_0(t)$, where $\eta_0(t)$ is independent of the other noise terms, with correlator $\langle \eta_0(t)\eta_0(t')\rangle = 2D'\delta(t - t)$, corresponding to a particle diffusion constant D'. It is convenient to introduce the relative coordinates $y_i = x_i - x_0$, $i = 1, \ldots, N$. The corresponding Langevin equations are $\dot{y}_i = \xi_i(t)$ where the noise terms, $\xi_i(t) = \eta_i(t) - \eta_0(t)$, have correlators

$$\langle \xi_i(t)\xi_j(t')\rangle = 2D_{ij}\delta(t - t'), \tag{12}$$

where $D_{ij} = D\delta_{ij} + D'$. The equivalent Fokker-Planck equation, $\partial P/\partial t = \sum_{i,j=1}^{N} D_{ij}\, \partial^2 P/\partial y_i \partial y_j$, has to be solved subject to absorbing boundary conditions at $y_i = 0$ for any i (i.e., when any trap meets the particle). In principle, this equation can be solved by a coordinate transformation that diagonalizes the matrix D to give isotropic diffusion. This transformation, however, also rotates the edges of the absorbing region so that they are no longer mutually orthogonal but form the edges of an N-dimensional wedge. For $N = 2$, the problem can be solved exactly [9,10], but to our knowledge there are no exact solutions for $N \geq 3$.

An alternative starting point is the path-integral representation for the survival probability of the particle,

$$P(t) = \frac{\int_R D\vec{y}(t)\, \exp(-S[\vec{y}])}{\int D\vec{y}(t)\, \exp(-S[\vec{y}])}, \tag{13}$$

where $\vec{y}$ is a shorthand for $(y_1, \ldots, y_n)$, $S[\vec{y}] = (1/4)\sum_{i,j=1}^{N} (D^{-1})_{ij} \int_0^t dt'\, \dot{y}_i(t')\dot{y}_j(t')$, and the subscript R indicates that the path integral is restricted to "surviving" paths, in which none of the y_i has changed sign up to time t. The matrix D is easily inverted to give $(D^{-1})_{ij} = (1/D)(\delta_{ij} - \lambda)$, where $\lambda = D'/(D + ND')$ will be our expansion parameter. Thus

$$S[\vec{y}] = S_0[\vec{y}] - S_1[\vec{y}], \tag{14}$$

$$S_0[\vec{y}] = \frac{1 - \lambda}{4D} \sum_i \int_0^t dt'\, [\dot{y}_i(t')]^2, \tag{15}$$

$$S_1[\vec{y}] = \frac{\lambda}{2D}\sum_{i<j}\int_0^t dt'\,\dot{y}_i(t')\,\dot{y}_j(t'), \tag{16}$$

where the diagonal terms, $i = j$, have been absorbed into S_0.

A convenient normalization of the path integral is provided by the path integral for the survival probability, $P_0(t) \sim t^{-N/2}$, of the same problem with $D' = 0$ and $D \to D_0 = D/(1 - \lambda)$. Then

$$\frac{P(t)}{P_0(t)} = \frac{\langle \exp(S_1[\vec{y}])\rangle_R}{\langle \exp(S_1[\vec{y}])\rangle}, \tag{17}$$

where the average in both cases is over paths weighted by $\exp(-S_0[\vec{y}])$.

The final step is to expand the numerator and denominator using the cumulant expansion. To first order in λ (i.e., first order in S_1) one has

$$P(t)/P_0(t) = \exp(\langle S_1\rangle_R - \langle S_1\rangle). \tag{18}$$

Since the different values of i decouple in S_0 we have

$$\langle S_1\rangle_R = (\lambda/2D)\sum_{i<j}\int_0^t dt'\,\langle \dot{y}_i(t')\rangle_R \langle \dot{y}_j(t')\rangle_R. \tag{19}$$

The corresponding expression for the unrestricted paths vanishes, since $\langle \dot{y}_i(t')\rangle = 0$ by symmetry. The quantity $\langle \dot{y}_i(t')\rangle_R$ is independent of i apart from the sign: $\langle \dot{y}_i(t')\rangle_R > 0$ (< 0) for traps that stay to the right (left) of the particle. The calculation of $\langle \dot{y}_i(t')\rangle_R$ is straightforward. We require the result only in the regime $t_0 \ll t' \ll t$, where $t_0 = y_{i0}^2/D$ and y_{i0} is the initial value of trap i. In this regime one finds (for traps which start on the right of the particle) [11]

$$\langle \dot{y}_i(t')\rangle_R = 2(D_0/\pi t')^{1/2}, \qquad t_0 \ll t' \ll t. \tag{20}$$

We now insert this result into Eq. (19). Let there be N_L (N_R) traps to the left (right) of the particle. Then the $[N_L(N_L - 1)/2 + N_R(N_R - 1)/2]$ pairs (i, j) of traps whose members are on the *same* side of the particle contribute with positive weight to (19) while the $N_L N_R$ pairs whose members are on *opposite* sides enter with negative weight. Defining $\Delta = N_L - N_R$ (and $N = N_L + N_R$) this gives

$$\langle S_1\rangle_R = \frac{\lambda D_0}{\pi D}(\Delta^2 - N)\ln t \tag{21}$$

to leading logarithmic accuracy for large t. The factor $\ln t$ comes from the integral $\int_{t_0}^t (dt'/t')$ that appears when Eq. (20) is substituted into Eq. (19). Using the form (20) for all t', with t and t_0 as upper and lower cutoffs, is correct to leading logarithmic accuracy [11]. Note that the contributions from the lower cutoff, which depend on the initial positions of the traps, do not contribute to the leading logarithm. Using (21) in (18), recalling that $\langle S_1\rangle = 0$ and $P_0(t) \sim t^{-N/2}$, and noting that, to leading order in D', $\lambda = D'/D$ and $D_0 = D$, one finds $P(t) \sim t^{-\theta}$ with θ given by Eq. (4). The power-law decays hold when $t \gg y_{0i}^2/D$ for all i. The magnitudes of the initial coordinates y_{0i} determine the *amplitude* of the power law, while their signs determine the *exponent* through the value of Δ.

Equation (3) can be compared with the exactly solved cases $N_L = N_R = 1$ ("surrounded prey") and $N_L = 0, N_R = 2$ ("chased prey") [9,10], for which $\theta = \pi/2\alpha$ and $[\pi/2(\pi - \alpha)]$, respectively, where $\alpha = \cos^{-1}[D'/(D + D')]$. Expanding these to first order in D' gives agreement with Eq. (4).

In summary, we have obtained the exact asymptotic form of the survival probability of a particle moving in an infinite background of mobile traps. The asymptotic form is independent of the diffusion constant of the particle. A perturbation expansion in the ratio of the particle and trap diffusion constants has been developed for the case of a finite number of traps.

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