

Survival probability of a ballistic tracer particle in the presence of diffusing traps

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(Received 20 May 2003; published 2 October 2003)

We calculate the survival probability $P_S(t)$ up to time t of a tracer particle moving along a deterministic trajectory in a continuous d -dimensional space in the presence of diffusing but mutually noninteracting traps. In particular, for a tracer particle moving ballistically with a constant velocity c , we obtain an exact expression for $P_S(t)$, valid for all t , for $d < 2$. For $d \geq 2$, we obtain the leading asymptotic behavior of $P_S(t)$ for large t . In all cases, $P_S(t)$ decays exponentially for large t , $P_S(t) \sim \exp(-\theta t)$. We provide an explicit exact expression for the exponent θ in dimensions $d \leq 2$ and for the physically relevant case, $d = 3$, as a function of the system parameters.

DOI: 10.1103/PhysRevE.68.045101

PACS number(s): 05.70.Ln, 05.40.Jc, 02.50.-r

The calculation of the survival probability of a tracer particle moving in the presence of diffusing traps is a problem of long standing interest as it appears, in various guises, in a wide variety of contexts such as reaction-diffusion systems [1], chemical kinetics [2–4], predator-prey models [5], and “walker persistence” problems [6]. The tracer particle dies instantly upon meeting any of the diffusing traps. Perhaps the simplest of all these problems is the case when the diffusing traps are *noninteracting* and the motion of the tracer particle is governed by its own intrinsic dynamics that depends on the specific problem. For example, if the tracer particle is static, this problem is known as the *target annihilation* problem [7]. Of particular interest is the case when the tracer particle itself has a diffusive motion, a problem that was first studied by Bramson and Lebowitz [8] and has recently seen a flurry of activity [9–13]. It is, however, somewhat frustrating that, despite various new developments, this *diffusive target annihilation* problem has defied a *direct* exact solution. In contrast, we show in this paper that the *ballistic target annihilation* problem, where the tracer particle moves ballistically with a constant velocity, is exactly solvable.

A precise definition of the general problem is as follows. Consider a set of particles initially (at time $t = 0$) distributed randomly in a continuous d -dimensional space with average density ρ . Each of these particles subsequently undergoes independent diffusive motion with the same diffusion constant D . A tracer particle is introduced into the system at $t = 0$ at the origin and subsequently moves according to its own prescribed equation of motion. This motion can be either deterministic or stochastic, depending on the problem. For a given trajectory $\vec{R}_0(t)$ of the tracer particle, we ask: what is the probability $P_S(t)$ that none of the random walkers hits the tracer particle up to time t ? Evidently $P_S(t)$ depends implicitly on the trajectory $\vec{R}_0(t)$. For a deterministic motion of the tracer particle where the trajectory $\vec{R}_0(t)$ is prescribed, its survival probability is precisely $P_S(t)$. On the other hand, for stochastic motion of the tracer particle the survival probability is obtained by subsequently averaging $P_S(t)$ over all possible trajectories of the tracer particle. Thus the basic step, in either case, is to compute $P_S(t)$ for a given deterministic trajectory $\vec{R}_0(t)$. In this paper we limit

ourselves to the study of this general deterministic trajectory problem and, in particular, present explicit exact results when the trajectory is ballistic (see Fig. 1).

For a given fixed trajectory $\vec{R}_0(t)$, this problem can be formally reduced to a single-particle problem as follows. Let $Q(\vec{r}_i, t)$ be the probability that the i th random walker, starting from the initial position \vec{r}_i , does not meet the trajectory $\vec{R}_0(t)$ up to time t . Note that $Q(\vec{r}_i, t)$ depends implicitly on the trajectory $\vec{R}_0(t)$. The initial position \vec{r}_i of the i th walker is a random variable distributed over a volume V of a d -dimensional space with uniform probability density $1/V$. We assume that there are N such walkers. Eventually we will take the limit $N \rightarrow \infty$, $V \rightarrow \infty$ keeping the density $\rho = N/V$ fixed. Since the random walkers are independent, one immediately gets $P_S(t) = \langle \prod_{i=1}^N Q(\vec{r}_i, t) \rangle$ where the angular brackets denote the average over the initial positions \vec{r}_i of the random walkers. We next write $Q(\vec{r}_i, t) = 1 - P(\vec{r}_i, t)$ and use the product measure of the initial condition to write $P_S(t) = [1 - 1/V \int P(\vec{r}, t) d\vec{r}]^N$. Taking the $V \rightarrow \infty$ limit at fixed ρ gives

$$P_S(t) = \exp\left[-\rho \int P(\vec{r}, t) d\vec{r}\right] = \exp[-\mu(t)], \quad (1)$$

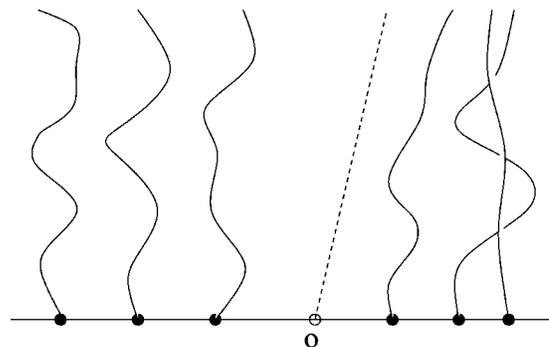


FIG. 1. A schematic picture of the space(horizontal)-time(vertical) trajectories of the diffusing traps (solid curves) and that of the ballistic tracer particle (dashed line) in $d = 1$. The diffusing trajectories are allowed to cross each other.

where $\mu(t) = \rho \int P(\vec{r}, t) d\vec{r}$ and $P(\vec{r}, t)$ is the probability that a single random walker starting at \vec{r} hits the trajectory $\vec{R}_0(t)$ before time t . Note that the calculation of $P(\vec{r}, t)$ and hence that of $\mu(t)$ is, in general, very hard even for this single-particle problem due to the *moving* boundary $\vec{R}_0(t)$. Such problems, generally termed Stefan problems, are well known to be formidable to solve [14]. In some simple cases one can derive the asymptotic behaviors of $P(\vec{r}, t)$ for large t [5]. Unfortunately, this asymptotic form of $P(\vec{r}, t)$ cannot be used to perform the integral over \vec{r} in Eq. (2) since this integral usually diverges. One therefore needs an alternative approach.

Fortunately, a technique for computing $\mu(t)$ for a general trajectory $\vec{R}_0(t)$ has recently been developed [13]. It was shown that, for $d < 2$, $\mu(t)$ satisfies the exact integral equation [13]

$$\rho = \int_0^t dt' \dot{\mu}(t') G(\vec{R}_0(t), t | \vec{R}_0(t'), t'), \quad (2)$$

where $\dot{\mu} = d\mu/dt$ and $G(\vec{R}_0(t), t | \vec{R}_0(t'), t') = [4\pi D(t-t')]^{-d/2} \exp\{-[\vec{R}_0(t) - \vec{R}_0(t')]^2/4D(t-t')\}$ is the standard d -dimensional diffusion propagator. For the marginal dimension $d=2$, Eq. (2) is still valid, though one has to introduce an ultraviolet cutoff in the diffusion propagator. The derivation of this integral equation has been detailed in Ref. [13]. Note that for continuous space with $d > 2$, if the tracer is a point particle then the random walkers will never meet the point particle trajectory. This is, however, not true on a lattice. So, if one sticks to a continuous space, the problem is sensible for $d > 2$ provided the tracer particle has a finite size. The formula in Eq. (2) assumes a point particle trajectory and hence is valid only for $d \leq 2$. For $d > 2$, there is no equivalent formula and one has to use other methods (see later in the paper).

For a general trajectory $\vec{R}_0(t)$ it is not easy to invert the integral equation (2) to obtain an explicit expression for $\mu(t)$. However, the advantage of Eq. (2) is that in many cases it can be exploited to derive exact asymptotic results. For example, for the ‘‘diffusive target annihilation’’ problem, Eq. (2) has been used to derive asymptotically exact bounds for the survival probability [13]. Note, however, that in the diffusive case, one had to average over all trajectories of the tracer particle weighted with the Wiener measure [13]. Another solvable case is in $d=1$ when the tracer particle moves deterministically as $R_0(t) = c\sqrt{t}$. For this case an exact expression for $\mu(t)$ for large t was obtained [13].

The purpose of this paper is to present another solvable case where the tracer particle moves ballistically through the system. For $d \leq 2$, we will consider the tracer to be a point particle with a trajectory $\vec{R}_0(t) = ct\hat{z}$, where c denotes the velocity of the particle and \hat{z} denotes the unit vector along the direction of motion, which we choose to be the z axis. For $d > 2$, we will consider the tracer particle to be a ball of finite radius a . For $d \leq 2$, we show how Eq. (2) can be exploited to derive an explicit exact result for $P_S(t)$ for all t .

For $d > 2$, we use a different method. We will present an explicit result for $\mu(t)$ in the physically relevant dimension $d=3$, though our method can, in principle, be used for any $d > 2$. Note that this problem has an alternative physical description. In terms of the relative coordinates $\vec{R}_i = \vec{r}_i - \vec{R}_0$, it represents a system of noninteracting particles diffusing in the presence of a constant drift velocity in the negative z direction. The physical origin of this drift could be, for example, an external field such as gravity or an electric field. The survival probability $P_S(t)$ of the tracer particle, in this alternative formulation, is simply the probability that none of the particles hits the origin up to time t .

We consider first the case $d < 2$. The substitution $\vec{R}_0(t) = ct\hat{z}$ in Eq. (2) reduces it to a convolution form,

$$\rho = \int_0^t dt' \dot{\mu}(t') \frac{\exp[-c^2(t-t')/4D]}{[4\pi D(t-t')]^{d/2}}, \quad (3)$$

which can, subsequently, be solved by the Laplace transform method. We denote $\alpha = c^2/4D$ and define the Laplace transform $\tilde{\mu}(s) = \int_0^\infty \mu(t) e^{-st} dt$. Taking Laplace transforms on both sides of Eq. (3) and using $\mu(0) = 0$, we obtain $\tilde{\mu}(s) = A[(\alpha + s)^{1-d/2}/s^2]$, where $A = \rho(4\pi D)^{d/2}/\Gamma(1-d/2)$ is a constant. To invert the Laplace transform, we write $\tilde{\mu}(s) = A(1/s + \alpha/s^2)(\alpha + s)^{-d/2}$. The inverse Laplace transform of the first factor $(1/s + \alpha/s^2)$ is simply $(1 + \alpha t)$ and that of the second factor $(\alpha + s)^{-d/2}$ can be easily found to be $e^{-\alpha t} t^{d/2-1}/\Gamma(d/2)$. We then use the convolution theorem again to write $\mu(t)$ as

$$\mu(t) = \frac{A}{\Gamma(d/2)} \int_0^t [1 + \alpha(t-t_1)] e^{-\alpha t_1} t_1^{d/2-1} dt_1. \quad (4)$$

The integral on the right-hand side can be expressed in closed form as

$$\mu(t) = B[(1 + \alpha t) \gamma(d/2, \alpha t) - \gamma(d/2 + 1, \alpha t)], \quad (5)$$

where $B = \rho(4\pi D)^{d/2} \sin(\pi d/2)/[\pi \alpha^{d/2}]$ and $\gamma(\nu, x) = \int_0^x \exp(-y) y^{\nu-1} dy$ is the incomplete gamma function. Note that the exact expression for $\mu(t)$ in Eq. (5) is valid for all t and $d < 2$.

Let us consider some limiting cases of the general result in Eq. (5). In the limit when the velocity $c \rightarrow 0$ at fixed t , our problem reduces to the static ‘‘target annihilation’’ problem for which exact results are already available [7,10]. Expanding Eq. (5) for small $\alpha = c^2/4D$ we find, to leading order, $\mu(t) = A_1 t^{d/2}$ where $A_1 = 2\rho(4\pi D)^{d/2} \sin(\pi d/2)/\pi d$. This indicates a stretched exponential decay for the survival probability $P_S(t) = \exp(-A_1 t^{d/2})$ and the constant A_1 matches exactly that of the static case derived earlier [7,10]. Note that the limit $c \rightarrow 0$ for fixed t is equivalent to the limit $t \rightarrow 0$ with c fixed, since in Eq. (5) the time t appears only in the scaling combination αt . Thus the result $P_S(t) = \exp(-A_1 t^{d/2})$ also holds for small t with c fixed. We now consider the opposite limit of $t \rightarrow \infty$ at fixed c . In this case we find, from Eq. (5), $\mu(t) \rightarrow A_2 t$ as $t \rightarrow \infty$ where $A_2 = \rho(4\pi D)^{d/2} \sin(\pi d/2) \Gamma(d/2)/[\pi \alpha^{(d-2)/2}]$. This indicates

an exponential decay for the survival probability at late times, $P_S(t) \rightarrow \exp(-\theta t)$ where the decay exponent $\theta = A_2$ is given by the following exact expression:

$$\theta = \rho \pi^{d/2-1} (4D)^{d-1} \sin(\pi d/2) \Gamma(d/2) c^{2-d}, \quad (6)$$

as a function of the four physical parameters ρ , c , D , and d .

The marginal dimension $d=2$ is a special case. The integral equation (2) is still valid, provided one introduces an ultraviolet cutoff reflecting the necessity of a lattice structure. Alternatively, a short time cutoff t_0 can be introduced in the diffusion propagator:

$$\begin{aligned} G(\vec{R}_0(t), t | \vec{R}_0(t'), t') \\ = \exp\{-[\vec{R}_0(t) - \vec{R}_0(t')]^2 / 4D(t-t') \\ + t_0\} / [4\pi D(t-t'+t_0)], \end{aligned}$$

where we consider t_0 to be small. To extract the leading asymptotic behavior, one can put $t_0=0$ inside the exponential and retain it only in the denominator of the propagator. Using this propagator in Eq. (2), substituting $\vec{R}_0(t) = ct\hat{z}$ and then taking the Laplace transform as for $d < 2$ gives $\tilde{\mu}(s) = 4\pi\rho D / [s^2 \tilde{g}(s)]$ where $\tilde{g}(s) = \int_0^\infty dt \exp[-(\alpha+s)t] / (t+t_0)$. Unlike the $d < 2$ case, it is now difficult to invert the Laplace transform. However, the large- t behavior of $\mu(t)$ can be easily extracted from the $s \rightarrow 0$ behavior of the Laplace transform. As $s \rightarrow 0$, $\tilde{g}(s) \rightarrow F(\alpha t_0)$ where $F(x) = \int_0^\infty du \times \exp(-u)/(u+x)$. Inverting $\tilde{\mu}(s)$, one then gets $\mu(t) \rightarrow [4\pi\rho D / F(\alpha t_0)] t$ as $t \rightarrow \infty$. In the limit $t_0 \ll 1/\alpha$, one gets $F(\alpha t_0) \approx -\ln(\alpha t_0)$. Thus, the survival probability again decays exponentially for large t , $P_S(t) = \exp(-\theta t)$, where θ is now nonuniversal, $\theta = 4\pi\rho D / [-\ln(\alpha t_0)]$.

We turn now to the case $d > 2$. We consider a spherical tracer particle of radius a moving ballistically with constant velocity c in the z direction. Unfortunately, for $d > 2$ we do not yet have an analog of Eq. (2). Thus one has to resort to the original single-particle formulation in Eq. (1). Fortunately, for the ballistic case in $d > 2$, the exact asymptotic behavior of $P_S(t)$ for large t can be derived even within this formulation. It turns out to be advantageous in this case to consider the alternative description of the problem in terms of the relative coordinates $R_i(t) = r_i(t) - \vec{R}_0(t)$ where the traps diffuse independently in the presence of an external drift along the negative z direction. Upon shifting to this relative coordinate, one finds from Eq. (1),

$$P_S(t) = \exp\left[-\rho \int P(\vec{R}, t) d\vec{R}\right] = \exp[-\mu(t)], \quad (7)$$

where $P(\vec{R}, t) = 1 - Q(\vec{R}, t)$ and $Q(\vec{R}, t)$ is the probability that a trap, diffusing in the presence of an external drift and starting at the initial position \vec{R} outside the sphere of radius a , does not hit the surface of the sphere before time t . The integral in Eq. (7) is now restricted to the region $|\vec{R}| \geq a$.

It is easy to see that the probability $Q(\vec{R}, t)$ satisfies a backward Fokker-Planck equation,

$$\frac{\partial Q}{\partial t} = D \nabla^2 Q - c \hat{z} \cdot \vec{\nabla} Q, \quad (8)$$

which takes the form of a diffusion equation with drift. This is a backward equation since we are varying the initial position \vec{R} of the trap. Equation (8) holds in the region $|\vec{R}| \geq a$ with the boundary conditions $Q(\vec{R}, t) = 0$ for $|\vec{R}| = a$ and $Q(\vec{R}, t) \rightarrow 1$ as $|\vec{R}| \rightarrow \infty$. This is because if the particle starts at the surface of the sphere at $t=0$, the probability that it does not hit the surface before time t vanishes for all $t > 0$. Similarly, if the particle starts at infinity, with probability 1 it will not hit the sphere in any finite time t . Evidently the probability $P(\vec{R}, t) = 1 - Q(\vec{R}, t)$ also satisfies the same backward Fokker-Planck equation in Eq. (8) (with Q replaced by P) but with a reversal of boundary conditions, $P(\vec{R}, t) = 1$ for $|\vec{R}| = a$ and $P(\vec{R}, t) \rightarrow 0$ as $|\vec{R}| \rightarrow \infty$.

Note that this Fokker-Planck equation can be written as a continuity equation, $\partial_t P + \vec{\nabla} \cdot \vec{J} = 0$ with a current $\vec{J} = -D \vec{\nabla} P + c \hat{z} P$. Before solving this equation, we first make a simple observation. We have, from Eq. (7), $\mu(t) = \rho \int_{|\vec{R}| \geq a} P(\vec{R}, t) d\vec{R}$. Therefore, $\dot{\mu}(t) = \rho \int_{|\vec{R}| \geq a} \partial_t P d\vec{R}$. Using the continuity equation and Gauss's divergence theorem, we obtain

$$\dot{\mu}(t) = -\rho D \int_{|\vec{R}|=a} \vec{\nabla} P \cdot d\vec{S}, \quad (9)$$

where the surface integral is over the sphere of radius a . In deriving Eq. (9) we have used the boundary conditions on P and the identity $\int_{|\vec{R}|=a} \hat{z} \cdot d\vec{S} = 0$.

It turns out that, for $d > 2$, Eq. (8) has a stationary solution. This is because the particle always has a finite probability to escape the sphere for $d > 2$. Thus, in order to extract the leading asymptotic behavior of $\mu(t)$ for $t \rightarrow \infty$, one can replace $P(\vec{R}, t)$ by its stationary solution $P_{st}(\vec{R})$ on the right hand side of Eq. (9). A subsequent integration over t , using $\mu(0) = 0$, shows that, to leading order for large t , $\mu(t) = \theta t$ where

$$\theta = -\rho D \int_{|\vec{R}|=a} \vec{\nabla} P_{st} \cdot d\vec{S}. \quad (10)$$

Note that while Eq. (9) is valid for all d , the result in Eq. (10) is valid only for $d > 2$. This is because the trick of replacing $P(\vec{R}, t)$ by its stationary solution $P_{st}(\vec{R})$ does not work for $d \leq 2$ since there is no stationary solution in that case.

Thus for $d > 2$ the survival probability also decays exponentially for large t , $P_S(t) \sim \exp(-\theta t)$ with the exponent θ given by the general formula in Eq. (10). Obtaining an explicit expression for θ requires knowledge of the stationary solution of Eq. (8) which we now provide for the physically relevant dimension $d=3$. The stationary solution satisfies the equation

$$D \nabla^2 P_{st} = c \hat{z} \cdot \vec{\nabla} P_{st} \quad (11)$$

with the boundary conditions $P_{st}(\vec{R})=1$ for $|\vec{R}|=a$ and $P_{st}(\vec{R})\rightarrow 0$ as $|\vec{R}|\rightarrow\infty$. This problem does not have a radial symmetry. Fortunately, the substitution $P_{st}(\vec{R})=\exp(\beta z)\psi(\vec{R})$, with $\beta=c/2D$, restores the radial symmetry since $\psi(\vec{R})$ satisfies the Poisson equation $\nabla^2\psi=\beta^2\psi$. The general solution satisfying the boundary condition at infinity can be obtained by standard techniques, to give

$$P_{st}(\vec{R})=R^{-1/2}e^{\beta R \cos \phi} \sum_{l=0}^{\infty} b_l P_l(\cos \phi) K_{l+1/2}(\beta R), \quad (12)$$

where $R=|\vec{R}|$, ϕ is the angle between \vec{R} and the z axis, $P_l(x)$ is the Legendre polynomial of degree l , and $K_\nu(x)$ is the modified Bessel function of index ν . The unknown coefficients b_l are determined from the boundary condition $P_{st}(R=a)=1$. Substituting $R=a$ in Eq. (12) and using the orthogonality properties of the functions $P_l(x)$ gives, after some algebra,

$$P_{st}(\vec{R})=\sqrt{\frac{a}{R}}e^{\beta R \cos \phi} \sum_{l=0}^{\infty} \left(l+\frac{1}{2}\right) a_l P_l(\cos \phi) \frac{K_{l+1/2}(\beta R)}{K_{l+1/2}(\beta a)}, \quad (13)$$

where $a_l=\int_{-1}^1 P_l(x)e^{-\beta ax}dx=(-1)^l\sqrt{2\pi/\beta a}I_{l+1/2}(\beta a)$.

Substituting the stationary solution, Eq. (13), into Eq. (10) and performing the surface integral, we finally obtain, after a

few steps of algebra, the following rather nontrivial expression for θ in terms of the physical parameters ρ , D , a , and c :

$$\theta=2\pi a\rho D\left[1-2\pi\sum_{l=0}^{\infty}(-1)^l \times\left(l+\frac{1}{2}\right)\frac{K'_{l+1/2}(\beta a)}{K_{l+1/2}(\beta a)}I_{l+1/2}^2(\beta a)\right], \quad (14)$$

where $K'_\nu(x)=dK_\nu(x)/dx$ and $\beta=c/2D$. The series in Eq. (14) can be summed numerically. If $H(\beta a)$ is the function in the square brackets, then $H(x)$ is monotonically increasing, with $H(0)=2$ and $H(x)/x\rightarrow 1$ for $x\rightarrow\infty$. The former result, corresponding to $c=0$, recovers the known result, $\theta=4\pi a\rho D$, for a static target [11]. The latter, corresponding to $c\rightarrow\infty$, can be understood by noting that in this limit the probability that the sphere has not been hit by a trap is given by $\exp(-\rho V)$, where $V=\pi a^2 ct$ is the volume swept out by the sphere in time t and we require that this volume initially contains no traps. Hence $\theta\rightarrow\pi a^2 c\rho$ in this limit, corresponding to $H(x)\rightarrow x$.

In summary, we have studied the general problem of calculating the survival probability of a tracer particle moving along a deterministic trajectory in the presence of diffusing traps. In particular, when the tracer particle moves ballistically we have shown that its survival probability $P_S(t)\sim\exp(-\theta t)$ for large t in all dimensions. We have derived exact expressions for the exponent θ in terms of the system parameters for $d\leq 2$ and for $d=3$.

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