Survival probability in the presence of a dynamic trap

Miguel A. Ré and Carlos E. Budde
Facultad de Matemática, Astronomía y Física, Universidad Nacional de Córdoba, Ciudad Universitaria, 5000 Córdoba, Argentina

Manuel O. Cáceres
Centro Atómico Bariloche and Instituto Balseiro, Comisión Nacional de Energía Atómica, Universidad Nacional de Cuyo, San Carlos de Bariloche, 8400 Bariloche, Argentina

(Received 30 October 1995; revised manuscript received 25 April 1996)

We present in this paper a theoretical study for the survival probability of a system of independent walkers in the presence of a dynamic trap by using the multistate continuous-time random-walk approach. The results presented are exact for any switching-time probability density controlling the dynamic of the trap, in the one-dimensional case without bias. The influence of a non-Markovian dynamic for the trap is presented and a comparison with a finite relaxation model is established for the long-time limit. [S1063-651X(96)07010-9]

PACS number(s): 05.40.+j, 05.60.+w, 02.50.+Ey, 82.20.Fd

I. INTRODUCTION

The survival probability (SP) is a magnitude of fundamental importance in many physical and chemical phenomena [1]. Blumen and co-workers [2] have considered the problem of the SP of one A and several B particles such that the A particle is annihilated at the encounter of a B particle. Depending on which of the species performs the motion, a distinction is made between the *trapping* (only the A particle moves), the *target* (only the B particles move), and the *moving target* (both species move) models.

As an important application of the *target* problem we mention the Glarum model for dipolar relaxation [3]. In this model each dipole is supposed to reorient itself in some manner leading to a single relaxation time. It is further assumed that there are a number of mobile defects also such that when a defect reaches a dipole, this relaxes instantly. The relaxation is described by the response function

$$\Psi(t)=\exp(-t/\tau)\Phi(t), \tag{1.1}$$

with $\Phi(t)$ the probability that no defect has reached the dipole position by time t (SP). On the other hand, the exponential contribution takes into account the relaxation of the dipole in a defect-free region with relaxation time τ. In his proposed solution, Glarum imposed the restriction of taking into account only the nearest defect at time $t=0$ for calculating $\Phi(t)$. Bordewijk [4] generalized this model by letting the dipole to be relaxed by any of the defects present in the system with concentration c.

A generalization of the Glarum model was proposed by Condat [5], eliminating the assumption of instantaneous relaxation by introducing a finite probability that the dipole is relaxed upon being reached by the defect. This problem was solved through the master-equation formalism. This formalism was also used by Condat to give an explanation for the closed-time distribution for ionic channels in cell membranes [6].

In a recent paper [7] we started with a generalization of the *target* model, which allows an encounter of A and B particles without annihilation depending on an internal state of particle A. Only if the A particle (which will be designed as ''the trap'') is active, the annihilation will take place. If the trap is inactive it behaves as a regular site. This problem is related to that of particles diffusing in the presence of a gate that opens and closes at stochastic times [8,9]. Szabo *et al.* have used this approach in order to study diffusion reactions where the reactivity of the species fluctuates in time, particularly when the accessibility of a binding site of a protein is modulated by a gate.

II. SURVIVAL PROBABILITY CALCULATION

Consider an infinite lattice with a dynamic trap in a given site, i.e., an absorbing site whose properties change in time. Assuming that at $t=0$ there is a random distribution of noniteracting walkers with a specified concentration c that are allowed to perform a Markovian random walk on the lattice, we have studied the problem of the absorption of these walkers by the dynamic trap [7,9].

In our model we characterize the changing properties of the trap by switching between a perfect trap state and a regular site state (no trap present). The process is controlled by two switching-time probability densities denoted by $f_{ij}(t)$, where $f_{ij}(t)dt$ is the probability that the trap, having acquired the state j at $t=0$, makes a transition to state i between t and $t+dt$. The subindices i,j $(i\neq j)$ can take the values 1 (active or perfect trap state) or 2 (inactive or regular site state). Upon arriving at the trap site, the walker may be absorbed (it leaves the lattice) if the trap is active or if the trap activates before the walker jumps to another site.

The absorption of a walker can model the relaxation of a target in the Glarum model. Of course, in a real material the defects modeled by the walkers are not absorbed, but continue their walk whether or not the target relaxes. However, from the point of view of the target under consideration, the process terminates when the relaxation occurs.

Following Bendler and Shlesinger [10], to calculate the survival probability we assume the trap situated at the origin of a lattice of V sites with N independent mobile walkers uniformly distributed, but initially excluded from the origin on this lattice (this picture corresponds to the dipole and defects in Bendler model). In this way the probability that a given walker is initially at a particular site $\mathbf{s}_0$ is V^{-1}.

We define SP as the probability that no walker has been absorbed by the trap by time t. As we are considering a dynamic trap, the first-passage time density in Eq. (38) in [10] must be replaced by the absorption probability density (APD) determined in [7], giving

$$\Phi(t)=\left\{1-V^{-1}\sum_{\mathbf{s}_0\neq\mathbf{0}}\int_0^t d\tau[R_{11}(\mathbf{0},\mathbf{s}_0;\tau)P_1+R_{12}(\mathbf{0},\mathbf{s}_0;\tau)P_2]\right\}^N. \tag{2.1}$$

In Eq. (2.1) we have considered both possibilities: the trap is initially active (with probability P_1) or inactive (with probability $P_2=1-P_1$). We assume a uniform probability distribution for the initial position of the walkers.

In the thermodynamic limit $N,V\to\infty$, with $c=N/V=\text{const}$, the walker concentration, the SP results

$$\Phi(t)=\exp\left\{-c\sum_{\mathbf{s}_0\neq\mathbf{0}}\int_0^t d\tau[R_{11}(\mathbf{0},\mathbf{s}_0;\tau)P_1+R_{12}(\mathbf{0},\mathbf{s}_0;\tau)P_2]\right\}. \tag{2.2}$$

Since our analytical expression for the APD is given in the Laplace representation, we continue the calculation, taking the Laplace transform of the exponent in (2.2)

$$s(u)=\mathcal{L}\left\{\sum_{\mathbf{s}_0\neq\mathbf{0};\ i=1,2}\int_0^t d\tau R_{1i}(\mathbf{0};\tau)P_i\right\}=\frac{1}{u}\sum_{\mathbf{s}_0\neq\mathbf{0};\ i=1,2}\frac{R^0_{1i}(-\mathbf{s}_0;u)}{R^0_{11}(\mathbf{0};u)}P_i, \tag{2.3}$$

where $\mathcal{L}$ stands for Laplace transform and we have used the solution as expressed in Eq. (21) of [7]. We wish to remark that this is a general result for a set of noninteracting walkers in any arbitrary D-dimensional lattice.

III. GENERALIZED GLARUM MODEL

In the previously cited papers [7,9] we have presented an explicit expression for the APD in the one-dimensional case without bias, characterized by the walker mean waiting time ($\langle t\rangle_w^{-1}=\lambda_w$) at any lattice site. The APD is given in terms of R_{1i_0}, which are, in this case,

$$R_{11}(\mathbf{0},\mathbf{s}_0;u)=\frac{g\dfrac{\rho(u_w)}{\rho(u_t)}[1+u_t-\rho(u_t)]^r+[1+u_w-\rho(u_w)]^r}{1+g\dfrac{\rho(u_w)}{\rho(u_t)}},$$

$$R_{12}(\mathbf{0},\mathbf{s}_0;u)=\frac{[1+u_w-\rho(u_w)]^r-\dfrac{\rho(u_w)}{\rho(u_t)}[1+u_t-\rho(u_t)]^r}{1+g\dfrac{\rho(u_w)}{\rho(u_t)}}, \tag{3.1}$$

where we have used the definitions

$$r=|\mathbf{0}-\mathbf{s}_0|,\quad \rho(x)=\sqrt{x(2+x)},$$
$$f_{12}\equiv f_{12}(u+\lambda_w),\quad f_{21}\equiv f_{21}(u+\lambda_w),$$
$$g=\frac{f_{21}}{f_{12}}\left(\frac{1-f_{12}}{1-f_{21}}\right),\quad \Theta=\frac{1-f_{12}f_{21}}{(1-f_{12})(1-f_{21})},$$
$$u_w=\frac{u}{\lambda_w},\quad u_t=\frac{\Theta}{\lambda_u}(u+\lambda_w)-1. \tag{3.2}$$

To obtain an explicit expression for the SP we substitute expression (3.1) into (2.3). In this situation $s(u)$ takes the form of a geometrical series, which may be evaluated to

$$s(u)=\frac{1}{u}\frac{2}{u_w+\rho(u_w)}\frac{1+\dfrac{\rho(u_w)}{\rho(u_t)}\dfrac{u_w+\rho(u_w)}{u_t+\rho(u_t)}\dfrac{Mg-1}{M+1}}{1+g\dfrac{\rho(u_w)}{\rho(u_t)}}, \tag{3.3}$$

with the definitions given in (3.2) and $M=P_1/P_2$. We wish to emphasize that formula (3.3) is exact for every switching-time density of the trap: $f_{ij}(t)$. The static trap [$P_1=1$, $f_{21}(u)=0$] and the always nonabsorbing site [$P_2=1$, $f_{12}(u)=0$] can be straightforwardly reobtained from (3.3).

A. Asymptotic limits

Here, we consider the behavior of the SP exponent in the limits: $t\to\infty$ and $t\to 0$. The calculation is carried out by using the exact expression given in (3.3) for $s(u)$ and considering the corresponding limits $u\to 0$ and $u\to\infty$. To study the long-time limit we approximate the Laplace transform of the shifted switching-time probability densities, as given in (3.2), in the $u\to 0$ limit, by

$$f_{12}\simeq a_2+b_2u,$$
$$f_{21}\simeq a_1+b_1u, \tag{3.4}$$

where we have defined

$$a_i=f_{ji}(\lambda_w),\quad b_i=\frac{df_{ji}}{du}(\lambda_w),\quad i\neq j. \tag{3.5}$$

This approximation is valid for any $f(u)$ since the shift introduced by the Laplace transform (see [7] and [9]) eliminates any possible anomalous behavior in the $u\to 0$ limit, inherent in the trap dynamic. Substituting (3.4) into (3.3) for $s(u)$ and keeping up to the third order of correction, we get

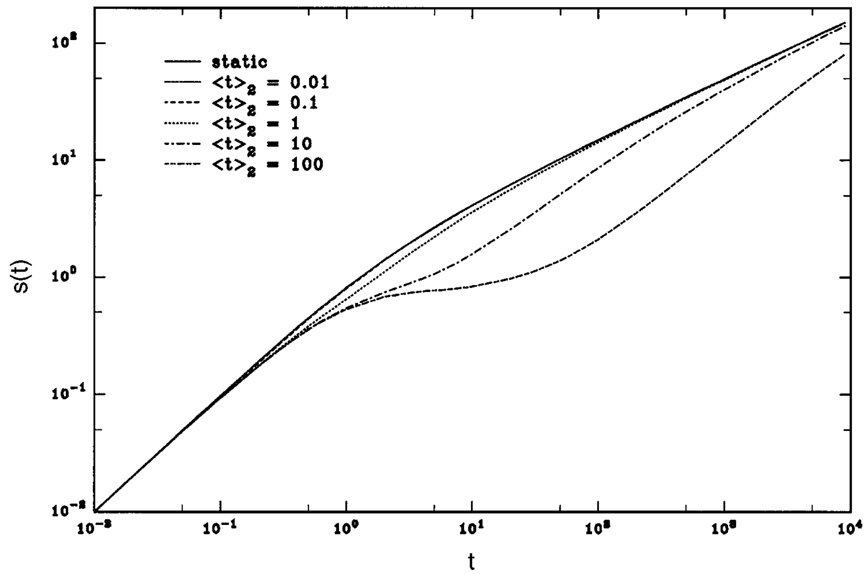

FIG. 1. Survival probability exponent vs time for the Markovian case (see the text). The walker mean time $\langle t\rangle_w=1$ and the mean active time $\langle t\rangle=1$ have been kept constant in all the cases presented. Here $\langle t\rangle_2=\int_0^\infty t f_{12}(t)dt$.

$$s(u)\simeq\frac{\sqrt{2\lambda_u}}{u^{3/2}}-\frac{1}{u}\left(1+2\frac{g_0}{\rho_0}\right)+\sqrt{\frac{2}{\lambda_w u}}\left[\frac{1}{4}+\frac{g_0}{\rho_0}\left(1+2\frac{g_0}{\rho_0}\right)+\frac{2}{\rho_0(u_0+\rho_0)}\frac{Mg_0-1}{M+1}\right],\tag{3.6}$$

with the new definitions

$$g_0\equiv g(u=0)=\frac{a_1(1-a_2)}{a_2(1-a_1)},$$

$$u_0\equiv u_t(u=0)=\frac{a_1}{1-a_1}+\frac{a_2}{1-a_2},\tag{3.7}$$

$$\rho_0\equiv\rho(u_t=u_0)=\sqrt{u_0(2+u_0)}.$$

From (3.6) and using a Tauberian theorem, we get, for $t\to\infty$,

$$s(t)\simeq\sqrt{\frac{8\lambda_w t}{\pi}}-\left(1+2\frac{g_0}{\rho_0}\right)+\sqrt{\frac{2}{\lambda_w\pi t}}\left[\frac{1}{4}+\frac{g_0}{\rho_0}\left(1+2\frac{g_0}{\rho_0}\right)+\frac{2}{\rho_0(u_0+\rho_0)}\frac{Mg_0-1}{M+1}\right].\tag{3.8}$$

This series expansion coincides with that of Condat (Eq. (4.5) in [5]) up to second order, identifying $\gamma=2\rho_0/g_0$, where γ is the absorption probability rate defined in [5]. In making the comparison it must be kept in mind that Condat's solution is expressed in the particular time scale $\lambda_w=2$. We wish to emphasize that this coincidence holds only in the long-time limit, differing both approaches in other time ranges, as will be shown for some particular cases.

On the other hand, the short-time behavior is calculated from the limit of (3.3) for $u\to\infty$. In general, we may only assume that in the limit $u\to\infty$ $f(u)\to 0$, which allows us to calculate the leading term of the series expansion for (3.3). Using an Abelian theorem, the short-time behavior is for $t\to 0$

$$s(t)\sim\lambda w P_1 t.\tag{3.9}$$

We can go no further without an explicit expression for the switching time of the trap. Expression (3.9) is valid in the limit $t\ll\langle t\rangle_w$ and $t\ll\langle t\rangle_j$, the mean time for the trap in state j. So the difference between (3.9) and the leading term in the static trap case is given by the appearance of P_1, the initial active state probability. But, of course, the transient behavior of $s(t)$ when the trap is dynamic has a nontrivial solution.

B. Particular cases

We now illustrate the exact transient, for the one-dimensional case, from (2.3), considering some typical switching time for the trap. The SP exponent $s(t)$ is plotted in the time domain. These values were numerically computed using the Laplace inversion algorithm LAPIN [11].

The first case presented in Fig. 1 corresponds to a Markovian dynamics for the switching time of the trap controlled by $f_{ij}(t)=\lambda_j\exp(-\lambda_j t)$ with $\lambda_j^{-1}=\langle t\rangle_j$, the mean time with the trap in state j. In this plot we show the $s(t)$ behavior for different values of $\langle t\rangle_2$ and we have included the static (always active) trap case. We have kept $\lambda_w=\lambda_1$ fixed and all times are expressed in units of $\langle t\rangle_w$.

The change of the mean inactive time, with $\langle t\rangle_1$ fixed, appears to have a greater influence in the $s(t)$ behavior than the change of the mean time $\langle t\rangle_j$ when $\langle t\rangle_1=\langle t\rangle_2$. Therefore an increase in the inactive mean time delays the $s(t)$ approach to the asymptotic limit. On the other hand, diminishing the inactive mean time makes $s(t)$, and consequently SP, get closer to the static case.

The other case, presented in Fig. 2, corresponds to a non-Markovian dynamics for the switching time, controlled by the family of functions

$$f_{ij}(t)=\frac{[\lambda_j(\nu+1)]^{\nu+1}}{\Gamma(\nu+1)}t^\nu\exp[-\lambda_j(\nu+1)t]\tag{3.10}$$

with $\lambda^{-1}=\langle t\rangle$.

The parameter ν gives a measure of the non-Markovianicity of the trap dynamics, such that the $\nu=0$ case corresponds to the Markovian dynamics previously discussed, while, on the

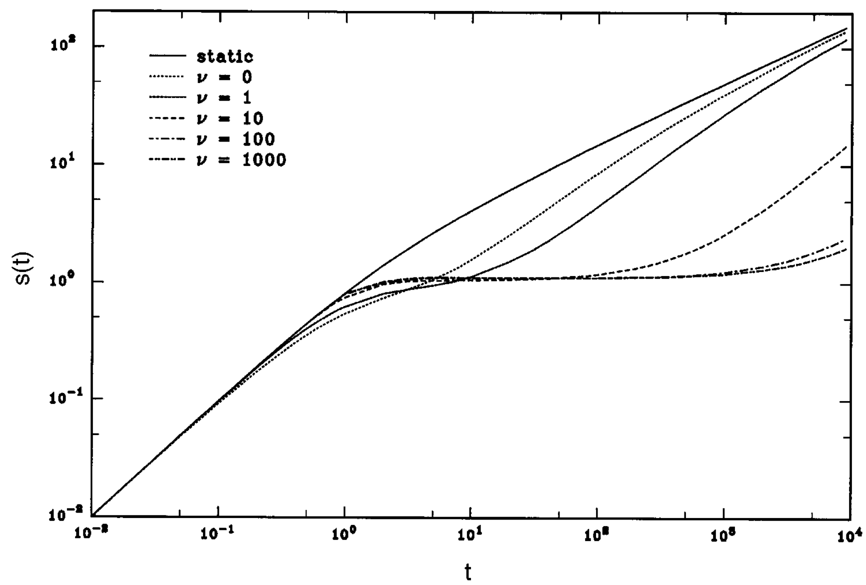

FIG. 2. Survival probability exponent vs time for the non-Markovian case. In this plot $\langle t \rangle_w = 1$, $\langle t \rangle_1 = 1$ and $\langle t \rangle_2 = 10$ have been chosen for all the curves.

other hand, in the $\nu \to \infty$ limit we get a deterministic periodic dynamics, i.e., $f_{ij}(t) \to \delta(t - \langle t \rangle_j)$.

The influence of ν on $s(t)$ is shown in Fig. 2. In this plot we keep fixed the parameters $\lambda_w = \lambda_1 = 10\lambda_2$. The variation of the parameters λ_j have an influence similar to that observed in the Markovian case, so these plots have not been included.

An important influence of the ν parameter variation on the $s(t)$ behavior is observed. Besides the crossing of the curves for $t \simeq 1$, there exists a region in the time domain of a nearly constant behavior for great values of ν. This constant behavior, in turn, delays the relaxation process (there is poor absorption of walkers in this time range). The static (always active) and Markovian ($\nu = 0$) dynamics have also been included for reference.

IV. CONCLUSION

In this paper we have presented a systematic approach to the SP calculation for a set of independent random walks in the presence of a dynamic trap. This model differs from the first-passage time approximation, denominated the static case in this presentation, in that the relaxation upon an encounter walker target is not necessarily instantaneous, but depends on an internal state of the dynamic trap. The solution is presented in an exponential form and the exponent is given by an exact analytical expression in the Laplace representation for any probability density function controlling the switching process of the trap.

We have explored the consequences of this generalization in the Glarum model for the one-dimensional, non-biased Markovian diffusion process. The asymptotic limits of $s(t)$ exhibit a behavior similar to that predicted by the static trap or the finite relaxation model [5], the difference being given by the coefficients of the series expansion (3.8). However, it can be concluded that the rate of the mean inactive time to the mean active time is the parameter to be taken into account, when departures from the the first-passage time approximation are to be considered. In fact, an increase in the mean inactive time, $\langle t \rangle_2$, delays the SP's decrease.

[1] J. W. Haus and K. W. Kehr, Phys. Rep. **150**, 263 (1987), and references therein.
[2] A. Blumen, J. Klafter, and G. Zumofen, in *Optical Spectroscopy of Glasses*, edited by I. Zschokke (Reidel, Dordrecht, 1986).
[3] S. H. Glarum, J. Chem. Phys. **33**, 1371 (1960).
[4] P. Bordewijk, Chem. Phys. Lett. **32**, 592 (1975).
[5] C. A. Condat, Z. Phys. B **77**, 313 (1989).
[6] C. A. Condat, Phys. Rev. A **39**, 2112 (1989).
[7] M. O. Cáceres, C. E. Budde, and M. A. Ré, Phys. Rev. E **52**, 3462 (1995).
[8] A. Szabo, D. Shoup, S. H. Northrup, and J. A. McCammon, J. Chem. Phys. **77**, 4484 (1982).
[9] C. E. Budde, M. O. Cáceres, and M. A. Ré, Europhys. Lett. **32**, 205 (1995).
[10] J. T. Bendler and M. F. Shlesinger, in *The Wonderful World of Stochastics*, edited by M. F. Shlesinger and G. H. Weiss (North-Holland, Amsterdam, 1985).
[11] G. Honig and U. Hirdes, J. Comput. Appl. Math. **10**, 113 (1984).