Diffusion in the presence of partial absorbers

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We analyze two models of partially absorbing media: one with a trapping reaction at static sites, and one with a single absorber driven by a dichotomic process. Our goal is to investigate the effect of the correlation time in the motion of the trap on the trapping dynamics. For fixed traps, we show different time behaviors arising from different distributions of traps. Analytical and simulated results of the mean distance from a trap to the nearest nonabsorbed particle, and of the mean number of particles between traps, are shown. For a quasidynamical trap, we show how the dynamics of the absorption depends on the correlation time of the absorber.

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I. INTRODUCTION

In recent years considerable effort has been devoted to the study of diffusion-controlled reactions, which play an important role in diverse branches of chemistry, physics, and biology. These processes include coalescence and annihilation reactions in one- or two-species systems [1–5]. However, much less work has been done in systems of partially absorbing media, which are of particular interest in many problems of attenuation in biological and physical systems [6,7].

In this paper we study a trapping reaction (symbolically written $A + B \to B$) in two systems of diffusing A particles: one with static B traps, and another with a single trap that performs a dichotomic motion. Our main goal is to describe the effects of the correlation time in the dynamics of the trap on the trapping process. We chose, as a paradigm of a stochastic process with correlation time, a dichotomic process known as "telegraphic" noise. This is the simplest process with a finite correlation time, and it can be used to model more complex processes, such as Ornstein-Uhlenbeck's, which has the same two-times correlation function.

The model equations include a Dirac δ-function potential for the reaction term, which is a limiting case of a model developed by us in previous papers [9]. We show how the distribution function of particles can be calculated exactly and how to obtain the different velocities of depletion produced by finite or infinite distributions of traps.

We will briefly review the central concepts of the model, as it was presented in [9]. The model equation for the evolution of the probability density of the diffusing particles is the following:

$$\frac{\partial}{\partial t} P_A(x,t) = D_A \frac{\partial^2}{\partial x^2} P_A(x,t) - \gamma \delta(x-\epsilon(t)) P_A(x,t), \tag{1}$$

where γ is a constant representing the probability per time unit for the reaction to take place in each event, and $\epsilon(t)$ is a stochastic process that models the position of the absorber. The only necessary hypothesis to solve this equation is that the process $\epsilon(t)$ is Markovian.

We first take the mean value of Eq. (1) with respect to the process ϵ, that is, over realizations of the trap motion. We obtain

$$\frac{\partial}{\partial t} \langle P_A(x,t) \rangle = D_A \frac{\partial^2}{\partial x^2} \langle P_A(x,t) \rangle - \gamma \mathcal{A}(x,t), \tag{2}$$

where $\mathcal{A}(x,t) = \langle \delta(x-\epsilon(t)) P_A(x,t) \rangle$ is an *absorption function* that contains all the effect of B on A. We now look for an equation for $\mathcal{A}(x,t)$ whose solution allows one to get the averaged density $\langle P_A(x,t) \rangle$. To start with, we take the integral form of Eq. (1):

$$\begin{aligned} P_A(x,t) = & \int_{-\infty}^{+\infty} dx' G(x,t|x',0) P_A(x',0) \\ & -\gamma \int_0^t dt' \int_{-\infty}^{+\infty} dx' G(x,t|x',t') \\ & \times \delta(x'-\epsilon(t')) P_A(x',t'), \end{aligned} \tag{3}$$

where $G(x,t|x',t')$ is the evolution operator or Green function of the diffusion equation $[(\partial_t - D\partial_{xx}) G(x,t|x',t') = \delta(x-x')\delta(t-t')]$.

We solve Eq. (3) by iterating, to get the series

$$\begin{aligned} P_A(x,t) = & \int_{-\infty}^{+\infty} dx' G(x,t|x',t') P_A(x',0) \\ & -\gamma \int_0^t dt' \int_{-\infty}^{+\infty} dx' G(x,t|x',t') \delta(x'-\epsilon(t')) \\ & \times \int_{-\infty}^{+\infty} dx'' G(x',t'|x'',t'') P_A(x'',0) + \cdots . \end{aligned} \tag{4}$$

After multiplying Eq. (4) by $\delta(x-\epsilon(t))$ and taking averages, we obtain the absorption function

$$\begin{aligned}\mathcal{A}(x,t) &= \langle \delta(x-\epsilon(t))P_A\rangle \\ &= \int_{-\infty}^{+\infty} dx' G(x,t|x',t')\,\langle\delta(x-\epsilon(t))\rangle\, P_A(x',0) \\ &\quad -\gamma\int_0^t dt'\int_{-\infty}^{+\infty}dx'\int_0^t dt''\int_{-\infty}^{+\infty}dx'' G(x,t|x',t')G(x',t'|x'',t'') \\ &\quad \times\langle\delta(x-\epsilon(t))\delta(x'-\epsilon(t'))\rangle\, P_A(x'',t'')+\cdots . \end{aligned} \tag{5}$$

The Markovian property of the process ϵ can now be used to write the averages of δ functions of Eq. (5) in terms of $W(x,t|x',t')$, the transition probability of the process. A new series is obtained, which can be cast again in integral form:

$$\begin{aligned}\mathcal{A}(x,t) = &\int_0^t dt'\int_{-\infty}^{+\infty}dx' G(x,t|x',t')P(x',t')\delta(t') \\ &\times\int_{-\infty}^{+\infty} W(x,t|x_0,0)P_B(x_0)dx_0 \\ &-\gamma\int_0^t dt'\int_{-\infty}^{+\infty}dx' G(x,t|x',t') \\ &\times W(x,t|x',t')\mathcal{A}(x',t'). \end{aligned} \tag{6}$$

Once Eq. (6) is solved the solution of Eq. (2) can be expressed as

$$\begin{aligned}\langle P_A(x,t)\rangle = &\int_{-\infty}^{+\infty}dx' G(x,t|x',0)P_A(x',0) \\ &-\gamma\int_0^t dt'\int_{-\infty}^{+\infty}dx' G(x,t|x',t')\mathcal{A}(x',t'). \end{aligned} \tag{7}$$

II. FIXED TRAPS

Consider the reaction process $A+B\rightarrow B$, in which the A species performs a discrete random walk on a one-dimensional lattice, and the B species is a set of N imperfect traps at sites j_k. The discrete equation governing the evolution of the probability density of A particles is

$$\begin{aligned}P_i(n+1)-P_i(n) &= p_\pm P_{i-1}(n)+p_\pm P_{i+1}(n) \\ &\quad -2p_\pm P_i(n) - p\sum_{k=1}^{N}\delta_{i,j_k}P_i(n), \end{aligned} \tag{8}$$

where i is the lattice site, n is the time index, $p_\pm$ is the jumping probability, p is the reaction (absorption) probability, and the sum is performed over the set of traps. The continuous limit of Eq. (8) is obtained by defining the variables $t=n\tau$ and $x=i\Delta$, and letting the time and space steps, τ and Δ, go to zero. The resulting equation is a reaction-diffusion one:

$$\frac{\partial}{\partial t}P(x,t) = D\frac{\partial^2}{\partial x^2}P(x,t) - \gamma\sum_{k=1}^{N}\delta(x-x_k)P(x,t), \tag{9}$$

where

$$\begin{aligned} D &= \lim_{\tau,\Delta\to 0}\Delta^2 p_\pm/\tau, \\ \gamma &= \lim_{\tau,\Delta\to 0} p/\tau, \\ \delta(x-x_k) &= \lim_{\tau,\Delta\to 0}\delta_{i,j_k}/\Delta. \end{aligned} \tag{10}$$

This exact limit, which allows direct comparison between analytical and simulated results, has been considered before for a single trapping particle [9,7,8], and its connection with the diffusion equation with an albedo (radiation) boundary condition has been discussed there. In a previous paper [9] we have studied several situations in which the traps are also allowed to diffuse.

Equation (9) can be cast in integral form with the aid of the Green function $G(x,t|x',t')$:

$$\begin{aligned}P(x,t) = &\int_{-\infty}^{+\infty}dx' G(x,t|x',0)P(x',0) \\ &-\gamma\sum_{j=1}^{N}\int_0^t dt'\int_{-\infty}^{+\infty}dx' G(x,t|x',t') \\ &\times\delta(x-x_j)P(x',t'). \end{aligned} \tag{11}$$

For a uniform initial distribution of the species A, integrating the second term of Eq. (11) we have

$$P(x,t) = P_0 - \gamma\sum_{j=1}^{N}\int_0^t dt' G(x,t|x_j,t')P(x_j,t'), \tag{12}$$

which can be solved using the Laplace transform

$$P(x,s) = \frac{P_0}{s} - \gamma\sum_{j=1}^{N}\frac{\exp(-|x-x_j|\sqrt{s/D})}{\sqrt{4sD}}P(x_j,s). \tag{13}$$

For specific distributions of the traps, Eq. (13) provides an algebraic system of equations in the unknown $P(x_j,s)$, which give the general solution. In the following we consider some possibilities.

In the presence of a single trap at the origin the solution, after inverse Laplace transforming, is

$$\begin{aligned}P(x,t) = P_0\Bigg[&\mathrm{erf}\left(\frac{|x|}{\sqrt{4\tau}}\right)+\exp\left(|x|\frac{\gamma}{2D}+\frac{\gamma^2}{4D^2}\tau\right) \\ &\times\mathrm{erfc}\left(\frac{|x|}{\sqrt{4\tau}}+\frac{\gamma}{2D}\sqrt{\tau}\right)\Bigg], \end{aligned} \tag{14}$$

where $\tau=Dt$. We can calculate the time dependence of the mean distance of the nearest A particle to the trap from Eq. (14), which provides a description of the depletion of the A system. If $Q(y,t) = \exp\left[-\int_0^y P(x,t)dx\right]$ is the probability that the nearest A particle is at a distance equal to or greater than y from the trap, then the mean distance of the nearest neighbor is $\langle y\rangle = \int_0^\infty Q(y,t)dy$ [10]. In this case we have the following long time behavior:

$$\langle y\rangle = \frac{\pi^{3/4}}{\sqrt{2P_0}}\tau^{1/4}\exp\left(\frac{2DP_0}{\sqrt{\pi}\gamma^2}\tau^{-1/2}\right) \times\text{erfc}\left(\frac{\sqrt{2DP_0}}{\gamma\pi^{1/4}}\tau^{-1/4}\right), \qquad (15)$$

which tends slowly to the known $\tau^{1/4}$ asymptotic behavior [10]. In Fig. 1 we show this result and the result of a simulation of the process. (For a description of the simulations, see below.)

In the presence of several traps, a quantity of interest for the analysis of the depletion of the A particles and the formation of an aggregate of traps is the integral of the probability density between two inner traps. Its time dependence shows the path that the system follows to segregate the two species. With two traps at positions $x_1 = -L$ and $x_2 = L$, Eq. (13) ($N = 2$) is solved as a system of two equations in the unknowns $P(-L,s)$ and $P(L,s)$, which, using the symmetry, gives

$$P(x,s) = \frac{P_0}{s}\left[1-\gamma\frac{\exp\left(-|x+L|\sqrt{s/D}\right)+\exp\left(-|x-L|\sqrt{s/D}\right)}{\gamma+\gamma\exp\left(-2L\sqrt{s/D}\right)+2\sqrt{s/D}}\right]. \qquad (16)$$

This distribution, integrated between the traps, has the following long time behavior:

$$\int_{-L}^{L} P(x,t)dx = 2P_0L^2\left(\pi\tau\right)^{-1/2}. \qquad (17)$$

In Fig. 2 we show the result of the simulation performed in this situation.

This power law of the decay of the number of particles between the inner traps of a multitrap system persists (with varying prefactors) for any *finite* number of traps. But for an infinite number of trapping sites, a situation possibly realized in a real physical system—such as quasiparticles diffusing in a defective crystal—the behavior is quite different. Let the trap sites be $x_j = jL$; then the densities $P(jL,s)$ are all equal for an infinite number of traps due to the symmetry of the system. Equation (13) then implies

$$P(jL,s) = P(0,s) = \frac{P_0}{s} - \frac{\gamma P(0,s)}{\sqrt{4Ds}} \times \sum_{j=-N/2}^{N/2}\exp\left(-|jL|\sqrt{s/D}\right). \qquad (18)$$

The geometric sum in Eq. (18) can be done exactly, and for $N\to\infty$ one obtains

$$P(0,s) = \frac{P_0}{s}\left[1+\frac{\gamma}{\sqrt{4Ds}}\frac{1+\exp(-L\sqrt{s/D})}{1-\exp(-L\sqrt{s/D})}\right]^{-1}, \qquad (19)$$

which, in (13), gives

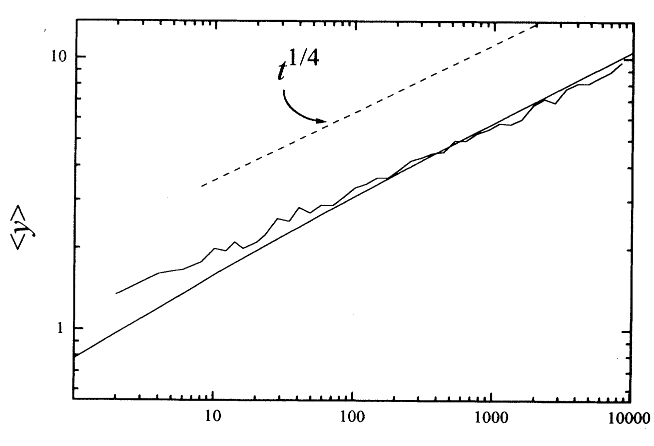

FIG. 1. Distance of the nearest surviving A particle to the trap vs time, in a system consisting of a single trap and 100 initial A particles uniformly distributed. The unbroken line is the plot of Eq. (7). The parameters are $\tau = 0.005$, $\Delta = 0.1$, $D = 1$, $\gamma = 1$, grid sites=100, 200 realizations.

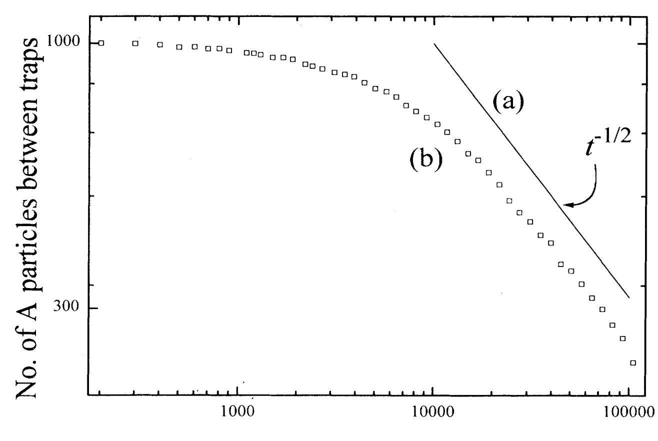

FIG. 2. (b) Log-log plot of the number of surviving particles between traps vs time, in a system of 10 000 initial A particles uniformly distributed and two traps. The straight line (a) has step one-half. The parameters are $\tau = 0.005$, $\Delta = 0.1$, $D = 1$, $\gamma = 1$, grid sites=1000, 6 realizations.

$$P(x,s) = \frac{P_0}{s} - \frac{P_0}{s}\left[\frac{\sqrt{4Ds}}{\gamma} + \frac{1+\exp(-L\sqrt{s/D})}{1-\exp(-L\sqrt{s/D})}\right]^{-1} \times \sum_{j=-\infty}^{\infty} \exp\left(-|x-jL|\sqrt{s/D}\right). \quad (20)$$

Now the sum in Eq. (20) can be split into two geometric sums, one from $j=-\infty$ to 0 and another from $j=1$ to ∞. The resulting expression can be integrated in x giving

$$\int_0^L P(x,s)dx = \frac{P_0 L}{s} - \frac{P_0\sqrt{4D}}{s^{3/2}}\left[\frac{\sqrt{4Ds}}{} \times\gamma + \frac{1+\exp(-L\sqrt{s/D})}{1-\exp(-L\sqrt{s/D})}\right]^{-1}. \quad (21)$$

At large time, the behavior of (21) is exponential (Fig. 3):

$$\int_0^L P(x,s)dx \sim P_0 L \exp\left(-\gamma t/L\right). \quad (22)$$

The simulations were performed on a circular lattice of M sites. We initially distributed N particles at random over the circle, and allowed them to perform a discrete random walk. In each time step, all the particles were moved one site to either side at random with probability $p_\pm = 1/2$. Also, in each step, all the particle positions were checked and compared with the fixed trap(s) site(s). If they coincided, the particle was immediately removed from the system with probability p. These steps were repeated up to a time far shorter than the one required for a mean particle to complete a round trip along the circle [$\sim$(circumference)$^2/p_\pm$], except for the simulation of the infinitely-many-traps system. This was simulated by two traps diametrically opposed in the circle, and letting the particles diffuse many times around it. The distance from a specified trap to the nearest surviving particle and the number of surviving particles between two specified traps were evaluated by simple algorithms at some predefined times and stored to be averaged. The whole process was repeated many times with the same parameters to obtain mean values of the interesting quantities.

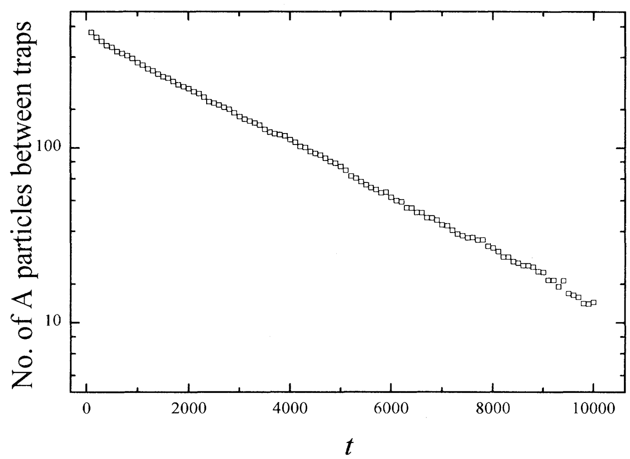

FIG. 3. Log-linear plot of the number of surviving A particles between two adjacent traps vs time, in a system with an infinite number of equally spaced traps, showing the exponential behavior of Eq. (14). The parameters are $\tau = 0.005$, $\Delta = 0.1$, number of initial A particles=2000, $D = 1$, $\gamma = 1$, grid sites=100, 10 realizations.

The problem of particles diffusing in a random distribution of traps can also be solved in this framework, with an extra effort. However, this problem has been previously solved in Ref. [5].

III. QUASIDYNAMICAL TRAP

In this section we study a one-dimensional trapping system with a single trap, subject to a dichotomic process with finite correlation time (or "telegraphic noise"). We aim to analyze the effect of the correlation time on the trapping dynamics. The telegraphic noise is the simplest process with a finite correlation time, and can be used to model more complex processes, such as Ornstein-Uhlenbeck's, which has the same two-time correlation function.

We have the absorption function localized on two points, $\mathcal{A}(x,t) = \mathcal{A}_a(t)\delta(x-a) + \mathcal{A}_{-a}(t)\delta(x+a)$, and the integral in space of (6) is a two-term sum:

$$\mathcal{A}_a(t)\delta(x-a) + \mathcal{A}_{-a}(t)\delta(x+a) = \int dx' G(x-x',t)P_A(x',0)\left[W(x,t|a,0)P_B(a,0) + W(x,t|a,0)P_B(a,0)\right] -\gamma\int dt' G(x-a,t-t')W(x,t|a,t')\mathcal{A}_a(t') -\gamma\int dt' G(x+a,t-t')W(x,t|-a,t')\mathcal{A}_{-a}(t'). \quad (23)$$

The transition probability of a telegraphic process with correlation time λ^{-1} is

$$W(x,t|a,t') = \frac{1}{2}\{1+\exp\left[-2\lambda(t-t')\right]\}\delta_{x,a} + \frac{1}{2}\{1+\exp\left[-2\lambda(t-t')\right]\}\delta_{x,-a}. \quad (24)$$

Let us suppose a localized initial distribution of the diffusing particles, and a symmetric initial distribution of the absorber: $P_A(x,0) = \delta(x-x_0)$, $P_B(a,0) = P_B(-a,0) = 1/2$. Substituting these and Eq. (24) into Eq. (23), and using the symmetry $\mathcal{A}_a(t) = \mathcal{A}_{-a}(t)$, we found the following equation for the temporal part of the absorption function:

$$\mathcal{A}_a(t) = \left(2\sqrt{4\pi Dt}\right)^{-1} \exp\left[-(a-x_0)^2/4Dt\right] -\gamma \int dt'[G(0,t-t')w_1(t-t') +G(2a,t-t')w_2(t-t')]\mathcal{A}_a(t'). \tag{25}$$

Equation (25) is a convolution that can be solved by Laplace transforming:

$$\mathcal{A}_a(s) = \frac{\exp\left(-|a-x_0|\sqrt{s/D}\right)}{4\sqrt{sD}} \frac{1}{1+\gamma\left[F_1(s)+F_2(s)\right]}, \tag{26}$$

where

$$F_1(s) \equiv \mathcal{L}\left[G(0,t)w_1(t),s\right] = \frac{1}{2}\left[(4Ds)^{-1/2} + (4D(s+2\lambda))^{-1/2}\right]$$
$$F_2(s) \equiv \mathcal{L}\left[G(2a,t)w_2(t),s\right] = \frac{1}{2}\exp\left(-2|a|\sqrt{s/D}\right)(4Ds)^{-1/2} + \exp\{-2|a|\sqrt{(s+2\lambda)/D} \times [4D(s+2\lambda)]^{-1/2}\}. \tag{27}$$

In a general situation the inverse transform can be very difficult, but the extreme cases of infinite and zero correlation time are easy. If $\lambda = 0$, we have

$$\mathcal{A}_a(s) = \frac{1}{4}\exp\left(-|a-x_0|\sqrt{s/D}\right)\left(\sqrt{s/D}+\gamma/2\right)^{-1}, \tag{28}$$

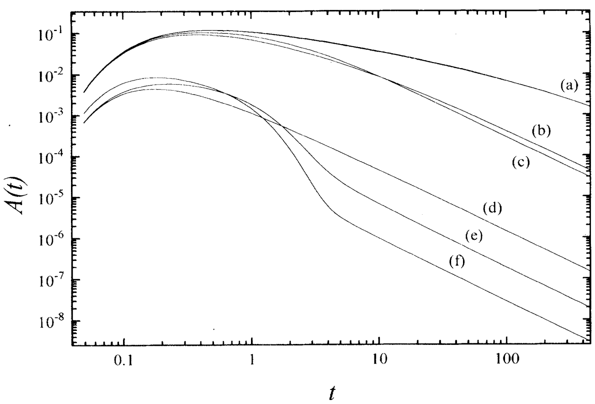

FIG. 4. Number of A particles absorbed vs time. The parameters are (a) $\gamma = 0.1, \lambda = 0, 10, \infty$ (the three curves almost coincide); (b) $\gamma = 1, \lambda = 0$; (c) $\gamma = 1, \lambda = \infty$; (d) $\gamma = 100, \lambda = 0$; (e) $\gamma = 100, \lambda = 10$; (f) $\gamma = 100, \lambda = \infty$.

and if $\lambda \to \infty$

$$\mathcal{A}_a(s) = \frac{1}{4}\exp\left(-|a-x_0|\sqrt{s/D}\right) \times \left[\gamma/4 + \sqrt{s/D} + (\gamma/4)\exp\left(-2|a|\sqrt{s/D}\right)\right]^{-1}. \tag{29}$$

This, in turn, has simple forms at short and long times:

$$\mathcal{A}_a(s) = \begin{cases} \frac{1}{4}\exp\left(-|a-x_0|\sqrt{s/D}\right)\left(\sqrt{s/D}+\gamma/2\right)^{-1} & \text{(long time, } \lambda\to\infty) \\ \frac{1}{4}\exp\left(-|a-x_0|\sqrt{s/D}\right)\left(\sqrt{s/D}+\gamma/4\right)^{-1} & \text{(short time, } \lambda\to\infty). \end{cases} \tag{30}$$

The distribution of the diffusing particles can be obtained from the absorption function:

$$\langle P_A(x,t)\rangle = \int dx' G(x-x',t-t')P_A(x',0) -\gamma\int_0^t dt'[G(x-a,t-t') +G(x+a,t-t')]\mathcal{A}(t'). \tag{31}$$

For an initial distribution of the form $P_A(x,0) = \delta(x-x_0)$ we finally have

$$\langle P_A(x,s)\rangle = \frac{\exp\left(-|x-x_0|\sqrt{s/D}\right)}{\sqrt{4Ds}} -\gamma\left(e^{-|x-a|\sqrt{s/D}} + e^{-|x+a|\sqrt{s/D}}\right) \times\frac{\exp\left(-a\sqrt{s/D}\right)}{8\sqrt{s}\left(\sqrt{s}+\gamma/2\right)}. \tag{32}$$

This results can be compared with those for a system with two *fixed* traps. The absorption function [Eq. (26)] and its limit cases Eqs. (28) and (29) will serve. A simple calculation with a single trap at the origin shows the same absorption function as in the dichotomic case with infinite correlation time ($\lambda = 0$). Likewise, two symmetric traps at both sides of the origin have the same absorption function as the dichotomic absorber with null correlation time ($\lambda \to \infty$). In Fig. 4 we show the absorption function (number of particles absorbed) for these two limits and for a finite correlation time. These curves were obtained via a numerical inverse transformation of Eqs. (28), (29), and (26), and clearly show the different behaviors produced for a correlation time in the dynamics of the traps. We can conclude that this affects the system for a time depending on the ratio $\gamma/D^{1/2}$, and that this dependence disappears at long times.

IV. CONCLUSIONS

In conclusion, we have shown that the behavior of a system with an infinite number of traps cannot be inferred from that of a system with a finite number of traps. Both the analytical results and the simulations show that the density between two traps in the former case decays exponentially in time. In the latter, regardless of the number of traps (but finite), the behavior follows a power law. In fact, this behavior can be understood by noting that in an infinite system with a finite number of traps, the diffusing particles can travel arbitrarily far from the trapping region. In any *finite* system this cannot happen, and the exponential contribution to the integrated density should persist. Consider, for instance, a finite system with perfect reflecting boundary conditions. The Green function corresponding to this case will have an infinite sum of Gaussian contributions (arising from an imagelike method), similar to the sum appearing in Eq. (20) in the context of an infinite periodic system. Clearly, the asymptotic behavior for long times will also be exponential.

We have presented a simple model of a quasidynamical absorber driven by a dichotomic process, shown how a finite-time correlated process can be taken into account, and how the correlation time affects the dynamics. It is worth stressing the adequacy of the present scheme to yield straightforward results in a variety of situations—as long as the subjacent dynamics is Markovian, as in the present case. We stress that this is the simplest example of diffusion in the presence of traps with a correlated dynamics. We can expect a stronger effect in the case of annihilation reactions ($A+B \to 0$) if both reactants have a correlated dynamics. Their study will be the subject of further work.

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