Results in trapping reactions for mobile particles and a single trap

A. D. Sánchez,[1,*] M. A Rodriguez,[2,†] and H. S. Wio[1,‡]
[1]*Centro Atómico Bariloche, Instituto Balseiro, Comisión Nacional de Energía Atómica, Universidad Nacional de Cuyo, 8400 San Carlos de Bariloche, Rio Negro, Argentina*
[2]*Consejo Superior de Investigaciones Científicas, Instituto de Física de Cantabria, and Universidad de Cantabria, Santander, Spain*
(Received 10 December 1997)

We have exploited a stochastic model for the description of diffusion controlled reactions for trapping processes with a single trap in a one-dimensional lattice in order to describe in an exact way the particle distribution as ''seen'' from the trap, being fixed or mobile, as well as for perfect or imperfect reactions. From this we have obtained the exact result for the total number of absorbed particles. Moreover, we have a formal expression for the nearest-neighbor particle distribution that gives the known results in both limits (fixed trap and fixed particles) and also present an approximate expression that works quite well when the particle diffusivity is greater than the trap diffusivity.
[S1063-651X(98)00106-8]

PACS number(s): 05.40.+j, 82.20.−w, 05.20.−y, 02.50.−r

I. INTRODUCTION

The dynamics of diffusion controlled reactions has been extensively studied in recent years due to its relevance in the most diverse areas of physics, chemistry, and biology. These processes include coalescence and annihilation reactions in one- and two-species systems [1]. One of the objectives of such studies was to find theoretical models that describe the different possible situations correctly. Since the pioneering contribution of Smoluchowski [2], many different models have been proposed [3]. However, most of them do not give correct results because the effects of fluctuations and/or correlations were not taken into account. A complete description of this kind of phenomenon must include the probabilistic character of the reaction process. More recent studies have been reviewed in Refs. [4] and [5]. Among other aspects, the anomalous kinetics associated with the formation of segregates of particles in low-dimensional systems has attracted considerable attention. There is a remarkable sensitivity of such segregation phenomena to changes in initial conditions, the presence of sources, disorder, external forces, etc. A large part of the recent literature is devoted to the analysis of these phenomena under the assumption that some kind of rate equations are valid [4,5].

With the objective of obtaining a more complete description of such kind of phenomena including the probabilistic character of the reaction process, we have recently introduced a model that is the continuous limit of the master equation usually employed in simulations of these processes. This model has provided a very adequate framework in which to describe these processes, offering the possibility of describing not only the asymptotic, but also intermediate- and short-times regime, yielding excellent agreement with simulations both in one- and two-species trapping ($A+B \rightarrow B$ and $A+B \rightarrow B$, $B+C \rightarrow C$) and annihilation ($A+B \rightarrow 0$) reactions as well as in several different situations [6–13].

One quantitative measure of the tendency of low-dimensional reacting systems to segregate is the distance d (in a trapping system $A+B \rightarrow B$, with several A and one B) of the B particle (or trap) to the nearest unreacted A particle, that is, the generalization of the Hertz distribution [14] that is valid when neither the trap nor the particles are mobile. Several authors have studied this problem of a fixed trap by analyzing different models and schemes including perfect [15,16] and imperfect [17,18] reactions, the hard-core potential [19] and external fields [20,21]. In these works it was established that the average nearest-neighbor distance grows asymptotically as $\langle d \rangle \sim t^{1/4}$ for perfect and imperfect reactions, even for the hard-core potential case. Also, the other limit case, that is, with A particles stationary and B mobile, has been analyzed [22] yielding $\langle d \rangle \sim t^{1/2}$. The much more complicated intermediate situation, with both the particles and the trap mobile, has received less attention. There are simulations [23] indicating that $\langle d \rangle \sim t^{\alpha}$, where α is some value that interpolates between 1/2 and 1/4 and is a function of the ratio between D_A and D_B (the diffusivities of the particles and the trap, respectively). The empirical relation obtained from the simulations is $\alpha = (1/\pi)\tan^{-1}\sqrt{1+2(D_B/D_A)}$.

In the present work we analyze this problem within the framework of our model. We will show that it is possible to obtain the exact expression of $\tilde{n}(z,t)$, the distribution of particles in the reference frame of the trap, and from this N_{ABS}, the total number of absorbed particles. Moreover, we derive a formal expression for the probability distribution function (PDF) of d in the general case.

The organization of the paper is as follows. In Sec. II we obtain the expressions for $\tilde{n}(z,t)$ and N_{ABS}. In Sec. III we compute the finite-size effect for both quantities. In Sec. IV we derive a formal expression for the nearest-neighbor particle distribution and we extract from it the limiting cases of a stationary trap and mobile particles and stationary particles and mobile trap. An approximated explicit form for the d's PDF is presented in Sec. V. Section VI describes the way we have performed the simulations and shows the comparison of simulations with theoretical results. Section VII is devoted to

*Electronic address: sanchez@cab.cnea.edu.ar
†Electronic address: rodrigma@besaya.unican.es
‡Electronic address: wio@cab.cnea.edu.ar

some conclusions. We show in the Appendix an independent derivation of the one-sided nearest-neighbor particle distribution in the fixed particles case, using the renewal theory approach.

II. PARTICLE DISTRIBUTION FROM THE TRAP

The model, as was presented in Ref. [6], considers two species of particles A and B, both mobile, independent, and having a given reaction probability when they meet. Here we will study only a one-dimensional trapping reaction (symbolically written $A+B\rightarrow B$) in a system of diffusing A particles and a single trap B that also performs a diffusive motion.

The model equation for the evolution for $N(x,t)$, the density of the diffusing A particles, for a given trap realization $\epsilon(t)$ is

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

where γ is a constant that measures the reaction probability. As was shown in Ref. [6], the perfect reaction case corresponds to taking $\gamma\rightarrow\infty$ in the resulting expressions.

We start by considering the integral form of Eq. (1)

$$N(x,t)=n_0-\gamma\int_0^t dt'\int_{-\infty}^{+\infty}dx'\,G(x,t|x',t') \times\delta(x'-\epsilon(t'))N(x',t'), \quad (2)$$

where $G(x,t|x',t')$ is the propagator (or conditional probability) of the diffusive A particles. The first term in Eq. (2) appears from the propagation of the initial condition, which we assume to be uniform and equal to n_0.

Instead of repeating the procedure of Ref. [6] and in order to change our reference system from the laboratory to other one fixed to the trap, we make the change of variable

$$x=\epsilon(t)+z. \quad (3)$$

The form of the equation, using the new variable, is

$$\mathcal{N}(z,t)=n_0-\gamma\int_0^t dt'\,G(\epsilon(t)+z,t|\epsilon(t'),t')\mathcal{N}(0,t'), \quad (4)$$

where $\mathcal{N}(z,t)=N(\epsilon(t)+z,t)$. Here, and in order to find a closed equation for $\mathcal{N}$, we have also performed a similar change in the integration variable $[x'=\epsilon(t')+z']$.

Iterating Eq. (4), we obtain the series

$$\mathcal{N}(z,t)=n_0(1-\gamma\int_0^t dt'\,G(\epsilon(t)+z,t|\epsilon(t'),t') +\gamma^2\int_0^t dt'\int_0^{t'}dt''G(\epsilon(t)+z,t|\epsilon(t'),t') \times G(\epsilon(t'),t'|\epsilon(t''),t'')-\cdots). \quad (5)$$

The use of a diffusive form for the trap propagator $[W(x,t|x',t')]$ allows us to write averages over realizations of the process $\epsilon(t)$ (indicated by angular brackets) as

$$\langle G(\epsilon(t)+z,t|\epsilon(t')+z',t')\rangle=\mathcal{G}(z,t|z',t'), \quad (6)$$

$$\langle G(\epsilon(t)+z,t|\epsilon(t')+z',t')G(\epsilon(t')+z',t'|\epsilon(t'')+z'',t'')$$
$$=\mathcal{G}(z,t|z',t')\langle G(\epsilon(t')+z',t'|\epsilon(t'')+z'',t'')\rangle,\ldots$$

where $\mathcal{G}(z,t|z',t')$ is a diffusion propagator with a diffusivity that is the sum of both particle and trap diffusivities

$$\mathcal{G}(z,t|z',t')=\frac{1}{\sqrt{4\pi(D_A+D_B)(t-t')}} \times\exp\left[-\frac{(z-z')^2}{4(D_A+D_B)(t-t')}\right]. \quad (7)$$

Keeping this in mind, we perform the average and Eq. (5) finally becomes

$$\tilde{n}(z,t)=n_0-\gamma\int_0^t dt'\int_{-\infty}^{+\infty}dz'\,\mathcal{G}(z,t|z',t')\,\delta(z')\tilde{n}(z',t'), \quad (8)$$

where $\tilde{n}(x,t)=\langle\mathcal{N}(x,t)\rangle$.

A comparison of Eq. (8) with Eq. (2) clearly indicates that the form of the distribution $\tilde{n}(x,t)$ is analogous to the distribution $N(x,t)$ from a fixed trap at the origin [6] but replacing D_A by $D=D_A+D_B$, i.e.,

$$\tilde{n}(x,t)=n_0\left[\mathrm{erf}\left(\frac{|x|}{\sqrt{4Dt}}\right)+\exp\left(\frac{\gamma|x|}{2D}+\frac{\gamma^2t}{4D}\right) \times\mathrm{erfc}\left(\frac{|x|}{\sqrt{4Dt}}+\gamma\sqrt{\frac{t}{4D}}\right)\right]. \quad (9)$$

This is an exact result that is valid for all cases. For a perfect absorption reaction the second term of Eq. (9) vanishes.

An interesting aspect could be to quantify the width of depletion zone. With this aim, we linearize the density $\tilde{n}$ near the origin and look for the value w where it reaches the initial density n_0. The resulting expression is

$$w(t)=\frac{2D}{\gamma}\left[\frac{\exp\left(\frac{-\gamma^2t}{4D}\right)}{\mathrm{erfc}\left(\gamma\frac{\sqrt{t}}{4D}\right)}-1\right], \qquad w(t)\cong\sqrt{\pi Dt}, \quad (10)$$

where the last equation is an approximate expression that is valid in the long-time limit for imperfect absorption but is the exact solution for perfect absorption at all times.

We can also calculate the number of absorbed particles N_{ABS}, integrating $n_0-\tilde{n}(x,t)$. The result is

$$N_{ABS}(t)=4n_0\left[\sqrt{\frac{Dt}{\pi}}+\frac{D}{\gamma}\exp\left(\frac{\gamma^2 t}{4D}\right)\operatorname{erfc}\left(\gamma\sqrt{\frac{t}{4D}}\right)-\frac{D}{\gamma}\right], \tag{11}$$

where the last two terms vanish for perfect trapping, rendering the $t^{1/2}$ dependence in the complete time regime. This result agrees with previous simulations of the flux at the trap with perfect absorption [23], which is given by $(d/dt)\,N_{ABS}=2n_0\sqrt{D/\pi}t^{-1/2}$.

III. FINITE-SIZE EFFECTS

In order to obtain the correction corresponding to finite-size effects, we present now an approach similar to the problem of obtaining the density profile from the trap frame, but in a finite lattice with periodic boundary conditions. This system is similar to a periodic arrangement of traps that all move rigidly without varying the distances among them. Proceeding in a similar way to Sec. II, the result for the density as seen from the trap is the same as the density with a fixed periodic arrange of traps, replacing D_A by $D=D_A+D_B$. This problem has been solved in Refs. [9] and [11] in the Laplace domain. Unfortunately, it is not possible to perform the exact inverse transform and we can only obtain the short- and long-time behaviors.

A way of obtaining an analytic correction to $\tilde{n}$ and N_{ABS} due to finite-size effects is to perform the difference between the respective quantity in an infinite system and a finite one in the Laplace domain and to look for an approximate result for short times. We call $\tilde{n}^{(d)}(x,t)$ and $N_{ABS}^{(d)}(t)$ these respective differences, which are given by

$$\tilde{n}^{(d)}(x,s)=\frac{n_0}{s}\left[\frac{\exp\left(-\frac{\sqrt{s}}{D}|x|\right)+\exp\left(-\frac{\sqrt{s}}{D}(L-|x|)\right)}{2\frac{\sqrt{Ds}}{\gamma}\left[1-\exp\left(-\frac{\sqrt{s}}{D}L\right)\right]+1+\exp\left(-\frac{\sqrt{s}}{D}\right)L}-\frac{\exp\left(-\frac{\sqrt{s}}{D}|x|\right)}{2\frac{\sqrt{Ds}}{\gamma}+1}\right], \tag{12}$$

$$N_{ABS}^{(d)}(s)=2\frac{n_0\sqrt{D}}{s^{3/2}}\left[\frac{1}{2\left(\frac{\sqrt{Ds}}{\gamma}\right)+1}-\frac{1}{2\left(\frac{\sqrt{Ds}}{\gamma}\right)+\coth\left(\frac{L\sqrt{s}}{2\sqrt{D}}\right)}\right]. \tag{13}$$

These expressions can be expanded for large values of s in powers of the small quantity $\exp(-\sqrt{s/D}L)$. Closing up the expansion to first order we obtain

$$\tilde{n}^{(d)}(x,s)\cong\frac{n_0}{s}\left[\frac{\exp\left(-\frac{\sqrt{s}}{D}(L-|x|)\right)}{2\left(\frac{\sqrt{Ds}}{\gamma}\right)+1}+\left(2\frac{\sqrt{Ds}}{\gamma}-1\right)\frac{\exp\left(-\frac{\sqrt{s}}{D}(L+|x|)\right)}{\left(2\frac{\sqrt{Ds}}{\gamma}+1\right)^2}\right], \tag{14}$$

$$N_{ABS}^{(d)}\cong 4n_0\sqrt{D}\frac{\exp\left(\frac{\sqrt{s}}{D}L\right)}{s^{3/2}\left(2\frac{\sqrt{Ds}}{\gamma}+1\right)^2}. \tag{15}$$

Finally, the corrections for finite-size effect can be obtained, resulting in

$$\begin{aligned}\tilde{n}^{(d)}(x,t)\cong n_0\Bigg\{&2\gamma\sqrt{\frac{t}{\pi D}}\exp\left(\frac{-(L+|x|)^2}{4Dt}\right)\\&+\operatorname{erfc}\left(\frac{L-|x|}{\sqrt{4Dt}}\right)-\operatorname{erfc}\left(\frac{L+|x|}{\sqrt{4Dt}}\right)\\&+\left[1-\frac{\gamma}{D}(L+|x|)-\frac{\gamma^2 t}{D}\right]\\&\times\exp\left(\frac{\gamma}{2D}(L+|x|)+\frac{\gamma^2 t}{4D}\right)\\&\times\operatorname{erfc}\left(\frac{L+|x|}{\sqrt{4Dt}}+\gamma\sqrt{\frac{t}{4D}}\right)\\&-\exp\left(\frac{\gamma}{2D}(L-|x|)+\frac{\gamma^2 t}{4D}\right)\\&\times\operatorname{erfc}\left(\frac{L-|x|}{\sqrt{4Dt}}+\gamma\sqrt{\frac{t}{4D}}\right)\Bigg\},\end{aligned} \tag{16}$$

$$N_{ABS}^{(d)}(t)\cong 4n_0\left[4\sqrt{\frac{Dt}{\pi}}\exp\left(-\frac{L^2}{4Dt}\right)-\left(\frac{4D}{\gamma}+L\right)\times\operatorname{erfc}\left(\frac{L}{\sqrt{4Dt}}\right)+\left(\frac{4D}{\gamma}-L-\gamma t\right)\times\exp\left(\frac{\gamma}{2D}L+\frac{\gamma^2 t}{4D}\right)\operatorname{erfc}\left(\frac{L}{\sqrt{4Dt}}+\gamma\sqrt{\frac{t}{4D}}\right)\right]. \tag{17}$$

These expressions simplify considerably for perfect absorption, yielding

$$\tilde{n}^{(d)}(x,t)\cong n_0\left[\operatorname{erfc}\left(\frac{L-|x|}{\sqrt{4Dt}}\right)-\operatorname{erfc}\left(\frac{L+|x|}{\sqrt{4Dt}}\right)\right], \tag{18}$$

$$N_{ABS}^{(d)}(t)\cong 4n_0\left[2\sqrt{\frac{Dt}{\pi}}\exp\left(-\frac{L^2}{4Dt}\right)-L\operatorname{erfc}\left(\frac{L}{\sqrt{4Dt}}\right)\right]. \tag{19}$$

IV. NEAREST-NEIGHBOR DISTRIBUTION

A general expression for the PDF of the nearest-neighbor particle has not been obtained until now. In fact, only two limiting cases corresponding to keeping fixed either the trap or particles have been analytically treated in the literature. Both approaches, which at least in principle are not connected, give a different asymptotic behavior. In this section we derive a general expression for this PDF, obtaining the known results in the above-mentioned limiting cases.

We consider a particular realization of the process $\epsilon(t)$ and an average over the particle random walks. The density, as viewed from the trap, is $\mathcal{N}(x,t)$. Thus, following Ref. [16], the probability of not finding any particle in $(-d,d)$ is given by

$$Q(d,t)=\left[1-\frac{\int_{-d}^{d}\mathcal{N}(x,t)dx}{\int_{-L/2}^{L/2}\mathcal{N}(x,t)dx}\right]^{\left[\int_{-L/2}^{L/2}\mathcal{N}(x,t)dx\right]}, \tag{20}$$

where L is the lattice length. Here it is worth remarking that the essential assumption of statistical independence in the processes of diffusion and survival of each particle holds whenever we consider the same realization. On the contrary, by considering several realizations of $\epsilon(t)$, the independence assumption would fail, as noted in Ref. [22]. Then it is clear that averages over $\epsilon(t)$ must be taken at the end. After taking $L\to\infty$, we have the PDF differentiating $Q(d,t)$ with respect to d and averaging. The final result is

$$p(d,t)=-\frac{\partial}{\partial d}\left\langle\exp\left[-\int_{-d}^{d}\mathcal{N}(x,t)dx\right]\right\rangle=\left\langle[\mathcal{N}(d,t)+\mathcal{N}(-d,t)]\exp\left[-\int_{-d}^{d}\mathcal{N}(x,t)dx\right]\right\rangle, \tag{21}$$

where $\mathcal{N}(x,t)$ is given by Eq. (4). A similar procedure renders the one-sided PDF, that is,

$$f_{x_1}(d,t)=\left\langle\mathcal{N}(d,t)\exp\left[-\int_0^d\mathcal{N}(x,t)dx\right]\right\rangle. \tag{22}$$

Equations (21) and (22) are exact in all range of diffusivities, as well as for perfect and imperfect reactions. However, so far they are only formal results.

We can compute from Eqs. (21) and (9) the exact result

$$p(0,t)=2\tilde{n}(0,t)=2n_0\exp\left(\frac{\gamma^2 t}{4D}\right)\operatorname{erfc}\left(\gamma\sqrt{\frac{t}{4D}}\right). \tag{23}$$

This expression is null for perfect absorption, whereas the asymptotic behavior for imperfect reactions is $p(0,t)\simeq 4(n_0/\gamma)\sqrt{D/(\pi t)}$.

One of the limit cases of Eq. (21) is when B is a fixed trap ($D_B=0$). Since all realizations correspond to $\epsilon(t)=0$, we have $\mathcal{N}(x,t)=\tilde{n}(x,t)=N(x,t)$ and

$$p(d,t)=2N(d,t)\exp\left[-2\int_0^d N(x,t)dx\right]. \tag{24}$$

The factor 2 appearing in both the prefactor and the exponent is due to considering the smaller of the right and the left nearest-particle distances. Consideration of the one-sided distribution from Eq. (22) results in the Redner–Ben-Avraham formula [16]. Within our model these PDFs can be obtained exactly. We give here the value of the integral that appears in the exponent. It is

$$\int_0^x N(z,t)dz=n_0\left\{\sqrt{\frac{4D_A t}{\pi}}\left[\exp\left(-\frac{x^2}{4D_A t}\right)-1\right]+\left(x+\frac{2D_A}{\gamma}\right)\operatorname{erf}\left(\frac{x}{\sqrt{4D_A t}}\right)+\frac{2D_A}{\gamma}\exp\left(\frac{\gamma^2 t}{4D_A}\right)\times\left[\exp\left(\frac{\gamma x}{2D_A}\right)\operatorname{erfc}\left(\frac{x}{\sqrt{4D_A t}}+\gamma\sqrt{\frac{t}{4D_A}}\right)-\operatorname{erfc}\left(\gamma\sqrt{\frac{t}{4D_A}}\right)\right]\right\}. \tag{25}$$

The asymptotic expression for the PDF is the skewed Gaussian

$$p(d,t\to\infty)=2n_0\left(\frac{d}{\sqrt{D_A}}+\frac{2\sqrt{D_A}}{\gamma}\right)\frac{1}{\sqrt{\pi t}}\times\exp\left[-n_0\left(\frac{d^2}{\sqrt{D_A}}+\frac{4\sqrt{D_A}}{\gamma}d\right)\frac{1}{\sqrt{\pi t}}\right], \tag{26}$$

which allows us to calculate the mean value of d in the asymptotic time regime

$$\langle d\rangle = \frac{(\pi^3 D_A t)^{1/4}}{2\sqrt{n_0}} \exp\left(\frac{4n_0 D_A^{3/2}}{\gamma^2\sqrt{\pi t}}\right) \operatorname{erfc}\left[\frac{2\sqrt{n_0} D_A^{3/4}}{\gamma(\pi t)^{1/4}}\right] \cong \frac{(\pi^3 D_A t)^{1/4}}{2\sqrt{n_0}}. \quad (27)$$

Equations (26) and (27) were obtained in Ref. [17], where the partial reflection coefficient κ is related with γ through $\kappa = \gamma/(2D_A)$ [6].

The opposite limit of immobile particles is less trivial but also possible to obtain in the perfect absorption case. Instead of solving Eq. (4) using that $G(\epsilon(t)+z,t|\epsilon(t'),t') = \delta(\epsilon(t)+z-\epsilon(t'))$, we can directly guess the solution as

$$\mathcal{N}(z,t) = n_0\{1-\theta(z-\epsilon_{min}(t))+\theta(z-\epsilon_{max}(t))\}, \quad (28)$$

$\epsilon_{min}(t)$ and $\epsilon_{max}(t)$ being the minimum and maximum values reached by the trap until time t in the trap frame. Although we can obtain $p(d,t)$, for simplicity we only present the derivation of $f_{x_1}(d,t)$. Substituting this expression in Eq. (22), we obtain

$$f_{x_1}(d,t) = n_0 \int_0^d h(x,t) e^{-n_0(d-x)} dx, \quad (29)$$

where $h(x,t)$ is the PDF of $\epsilon_{max}(t)$. This convoluted form corresponds to a PDF of a sum of two independents variables: $\epsilon_{max}(t)$ and the distance from the maximum excursion to the nearest particle (exponentially distributed). This approach is the one used in [22], where the expression was explicitly computed. We do not repeat the calculations here, but we note that this result is contained in Eq. (A4) by taking $\gamma \to \infty$.

V. A SIMPLE APPROXIMATION

As we have seen in the preceding section, the calculation of the PDF in a general situation involves the averaging of $\exp[-2\int_0^d \mathcal{N}(x,t)dx]$, $\mathcal{N}(x,t)$ being a functional of the process $\epsilon(t)$. The explicit form of $\mathcal{N}(x,t)$ in terms of $\epsilon(t)$ could be obtained solving the integral equation (4). Both calculations, the averaging and the inversion of Eq. (4), would be analytically performed only in very few cases. In general, one should resort to approximations. In this section we show a simple approximation leaving more sophisticated methods based on path integrals for a future work.

In our approximation we will take the averages of Eq. (21) using the method of cumulants. Hence we have

$$\ln\left\langle \exp\left[-\int_{-d}^{d}\mathcal{N}(x,t)dx\right]\right\rangle = -2\int_0^d \tilde{n}(x,t)dx + \frac{1}{2}\left\{\int_{-d}^{d}\int_{-d}^{d}\langle \mathcal{N}(x,t)\mathcal{N}(x',t)\rangle \times dx\, dx' - 4\left[\int_0^d \tilde{n}(x,t)dx\right]^2\right\} + \cdots. \quad (30)$$

The lower-order approximation consist on closing the expansion up to first order. In this case the PDF can be written as

$$p(d,t) = 2\tilde{n}(d,t)\exp\left[-2\int_0^d \tilde{n}(x,t)dx\right] \quad (31)$$

and an explicit expression can be given since $\tilde{n}$ and the integral involved have been exactly calculated previously [Eqs. (9) and (25), substituting D_A by D]. Within this approximation the absorption of diffusing particles with a coefficient D_A due to a diffusing trap of coefficient D_B is equivalent to the case of diffusing particles with the coefficient D_A+D_B absorbed by a fixed trap and hence Eqs. (26) and (27) are valid (again substituting D_A by D) and then we have $\langle d\rangle \sim t^{1/4}$ in the long-time regime.

VI. SIMULATIONS

To test our results we have performed simulations for different values of parameters. The simulations were performed on a lattice of L sites with periodic boundary conditions. We have initially distributed N_0 particles at random over the lattice and allowed them to perform a continuous-time random walk (characterized by the jump frequency at each neighbor site q). In each site we can have any number of A particles and when two particles (A and B) coincide in the same site, the A particle disappears with a rate p.

This algorithm is implemented in the following way. At the start we assign a diffusion time for each particle and a reaction time for each A particle in the same site as the trap. Then we perform the event corresponding to the earlier time. If it is a reaction process the A particle disappears; if it is a diffusion process the particle moves to one of the neighboring sites. Then we generate a new diffusion and eventually new reaction times. The algorithm follows, choosing the event corresponding again to the earlier time and repeating the same steps until the desired final time is reached. Finally, it is not difficult to see that diffusion and reaction times must be generated by adding to the present time a new time with the following PDFs: $f(t) = 2q\exp(-2qt)$ for diffusion times and $f(t) = p\exp(-pt)$ for reaction times. The connections between simulation parameters and the model ones are given by $D = q\Delta x^2$ and $\gamma = p\Delta x$, where Δx is the jump length. All simulations are the result of 10 000 realizations and they were performed in a lattice of 101 sites with an initial density of particles $n_0 = 1$.

To test the theoretical expression for $\tilde{n}(x,t)$ [Eq. (9)] we have performed simulations for different values of D_A and D_B. In Fig. 1 we show those comparisons for different values of γ. In addition, we also compare with the results of the model considering a finite-size lattice. Curves for different values of γ are similar, with the notable difference that for perfect absorption the density at the trap position is null and reaches a finite value for imperfect absorption, which is larger for smaller γ. The agreement between the model and the simulations is excellent.

In Fig. 2 we show the comparison between simulations and our model results for N_{ABS} for different values of γ. The agreement between the model and the simulations is again excellent up to times where finite-size effects are noticeable. In the inset we show the lower-order correction to the model due to these effects.

Figure 3 shows the comparison of our approximation to

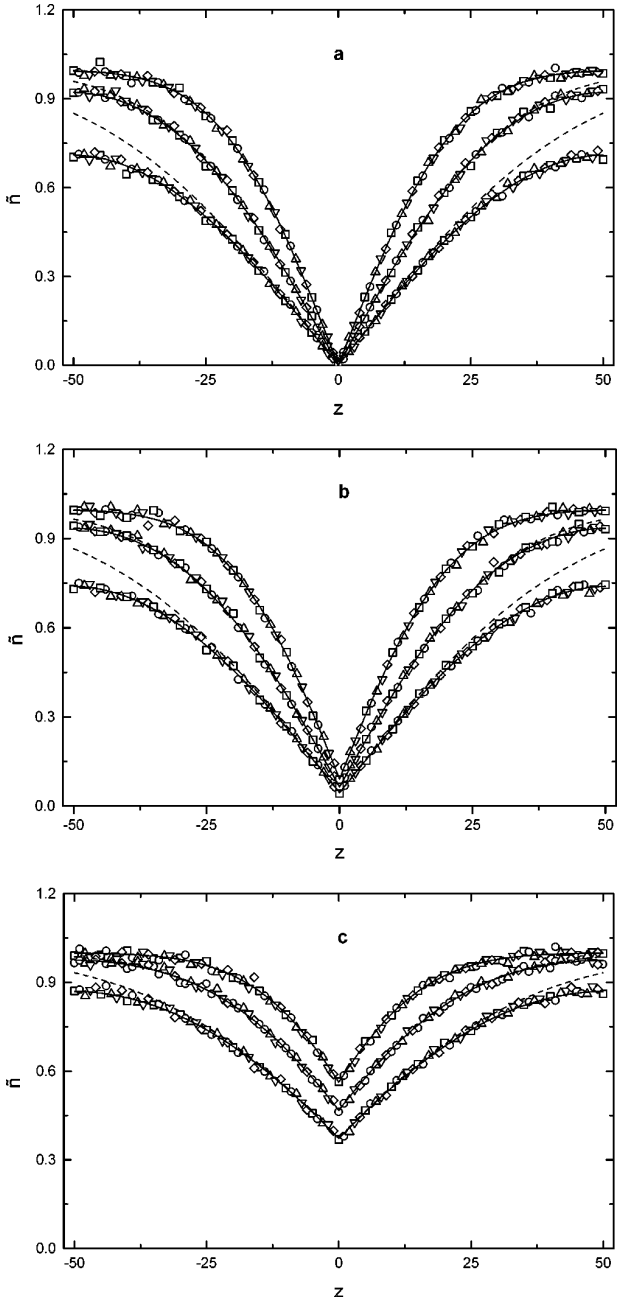

FIG. 1. Density of A particles in the reference frame of the trap for different values of γ: (a) $\gamma\to\infty$ (perfect reaction), (b) $\gamma=1$, and (c) $\gamma=0.1$. The solid line corresponds to our model finite-size results, the dashed line to the infinite lattice, and the points are the results of simulations for different D_A values: $D_A=1$ (squares), 0.75 (circles), 0.5 (up triangles), 0.25 (down triangles), and 0 (diamonds), in such way that $D=1$ in all cases. The different curves corresponds to times (from top to bottom) $t=150$, 300, and 600. The values of w in ascending order of time are (a) 21.7, 30.7, and 43.4; (b) 20, 28.9, and 41.6; and (c) 15.6, 22.8, and 33.6.

the PDF [Eq. (31)] with simulations. We note that the mentioned expression is exact for $D_B=0$ for the whole time regime. We can see that the approximation works better for smaller values of trap diffusivity and for shorter times. For $d=0$, the theoretical value given by Eq. (31) is the exact one and coincides with Eq. (23). However, the values of the PDF at the origin coming from simulations, even though all of them reach the same value independent of D_B, do not agree with the theoretical one.

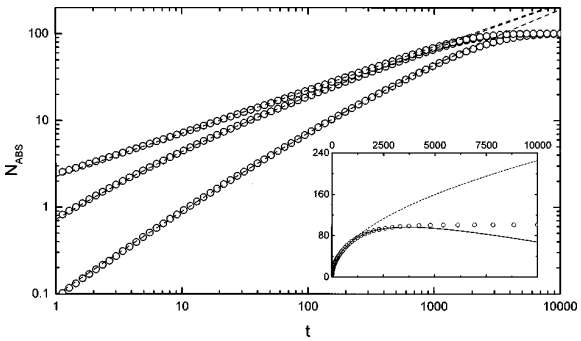

FIG. 2. A log-log plot of absorbed particles for different values of absorption. From top to bottom $\gamma\to\infty$, $\gamma=1$, and $\gamma=0.1$. The points are the result of simulations, while the dashed line corresponds to our model for an infinite lattice. The inset shows the same curves for $\gamma=1$ in a linear plot, where the finite-size corrections (solid line) have been added. The diffusivities used are $D_A=D_B=0.5$.

VII. CONCLUSIONS

In conclusion, we have shown that the stochastic model we have recently introduced for the description of diffusion limited reactions allows us to calculate the exact expression of $\tilde{n}(z,t)$, the distribution of particles in the reference frame of the trap. The resulting density depends only on diffusivities through the sum of trap and particle ones. Setting $D=D_A+D_B$, $\tilde{n}(z,t)$ can be obtained changing D_A to D in the density $N(x,t)$ of the simpler problem of a fixed trap at the origin and mobile particles. Integrating the density, we have computed the absorbed particle number given an analytical expression rendering a $t^{1/2}$ dependence, in accord with previous simulations [23]. Moreover, we have calculated the finite-size corrections to both quantities, showing excellent agreement with simulations, and also obtained an estimation for the depletion width that in the long-time limit goes as $w(t)\sim\sqrt{\pi Dt}$.

A general (formal) expression for the PDF of the nearest-neighbor particle in the general case has been derived. From this expression we have reobtained the known cases of fixed trap and fixed particles, which in principle have shown no connections between them until now. Although the general expression is a formal one, through a cumulant expansion we have obtained a simple approximation that works quite well for small D_B. This PDF is normalized and yields the exact value for $d=0$ given by Eq. (23). This approximation yields, in the asymptotic limit, $\langle d\rangle\sim t^{1/4}$. Instead, in Ref. [23], an exponent depending on the ratio D_A/D_B has been proposed, but without a clear argument supporting such a result, which nevertheless does work well.

The form of Eq. (21), together with the assumption of the trap's diffusion motion, preluded a path integral treatment (which is yet to be fully exploited in the context of diffusion limited reactions [24]), which suggests better approximations for the entire regime of values of D_A and D_B. Such an analysis will be the subject of a future work.

We remark here that it is not difficult to obtain the PDF

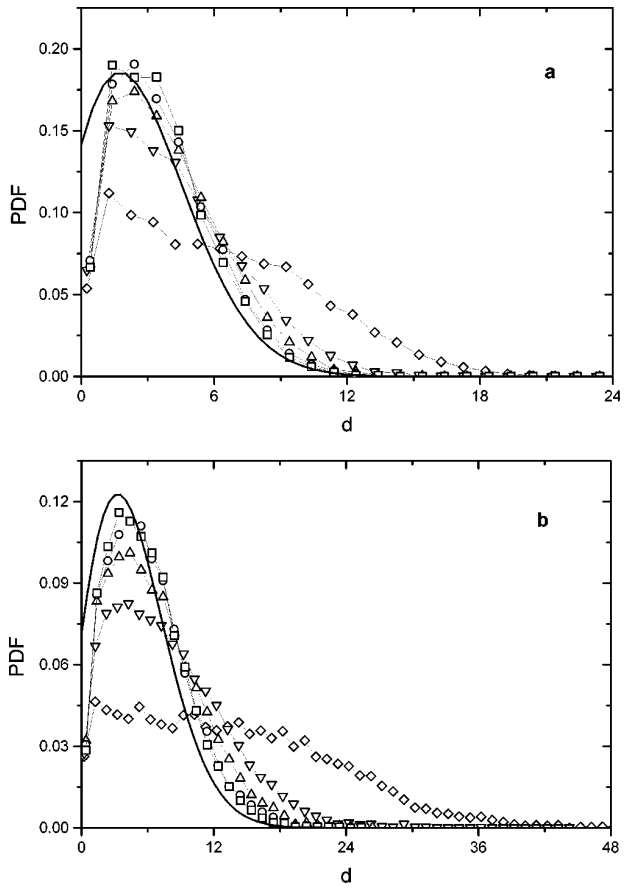

FIG. 3. PDF for (a) $t=250$ and (b) $t=1000$. The solid line corresponds to our approximation, while points correspond to simulations with different values of diffusivities. The parameter values and the code for diffusivities used are the same as those in Fig. 1(b).

for the nearest-neighbor distance for a finite lattice following a procedure similar to that in Sec. IV, but without taking $L\to\infty$. It renders a formal equation similar to Eq. (21). However, such an equation will still have, for $d=0$, the same value given by Eq. (23). Hence the discrepancy for small values of d between theory and simulations cannot be explained as a finite-size effect, but can arise from the discreteness of the simulations compared with the continuous character of the theory. Moreover, we can do an approximation similar to those in Sec. V by replacing $\mathcal{N}$ by $\tilde{n}$ in Eq. (21), but the corrections are negligible for the parameter range used in the simulations.

The results indicated above, as well as previous ones [6–13], clearly indicate the flexibility and adequacy of our stochastic model to describe situations related with the kinetics of diffusion limited reactions.

ACKNOWLEDGMENTS

The authors want to thank G. Sibona for calling their attention to relevant references. Financial support from the Ministerio de Educación y Ciencia, Spain (DGICyT Project No. PB93-0054-C02-02) and from CONICET, Argentina (Project No. PIP-4953/96) are greatly acknowledged. H.S.W. thanks the ICTP, Trieste, Italy, and H.S.W. and A.D.S. thank the Instituto de Física de Cantabria, Santander, Spain for the kind hospitality extended to them during their respective stays.

APPENDIX: A RENEWAL APPROACH FOR FIXED PARTICLES

We consider here the case when the particles are fixed and the trap is a mobile one. We call x_1 the distance between the trap and the nearest particle, x_2 the distance between it and the following particle, etc. Then we consider this situation as a modified renewal process [25], where $x_2, x_3, \ldots$, all have the same exponential PDF given by

$$f_{x_i}(x)=f(x)=n_0\exp(-n_0x), \tag{A1}$$

with $i=2,3,\ldots$. Note that this assumption is exact for perfect absorption, but only a good approximation for the case of imperfect reactions. Then we can write the relation

$$\tilde{n}^*(p,t)=f^*_{x_1}(p,t)\sum_{j=0}^{\infty}[f^*(p)]^j, \tag{A2}$$

where the asterisk to a function indicates the Laplace transform in the spatial variable. From Eq. (A2) one immediately obtains the nearest-neighbor particle distribution in the Laplace domain $f^*_{x_1}(p,t)$, which results

$$f^*_{x_1}(p,t)=\frac{n_0}{p+n_0}\left\{e^{D_Btp^2}\mathrm{erfc}(\sqrt{D_Bt}p)+\frac{p}{p-\gamma/(2D_B)}\times\left[e^{\gamma^2t/(4D_B)}\mathrm{erfc}\left(\gamma\sqrt{\frac{t}{4D_B}}\right)-e^{D_Btp^2}\mathrm{erfc}(\sqrt{D_Bt}p)\right]\right\}. \tag{A3}$$

This expression can be inverted to give the one-sided PDF

$$f_{x_1}(x,t)=\frac{n_0\gamma}{2n_0D_B+\gamma}e^{-n_0x+n_0^2D_Bt}\left[\mathrm{erf}\left(\frac{x}{\sqrt{4D_Bt}}-n_0\sqrt{D_Bt}\right)+\mathrm{erf}(n_0\sqrt{D_Bt})\right]+\frac{n_0}{n_0+\frac{\gamma}{2D_B}}e^{\gamma^2t/(4D_B)}\times\left[n_0e^{-n_0x}\mathrm{erfc}\left(\gamma\sqrt{\frac{t}{4D_B}}\right)+\frac{\gamma}{2D_B}e^{\gamma x/(2D_B)}\mathrm{erfc}\left(\frac{x}{\sqrt{4D_Bt}}+\gamma\sqrt{\frac{t}{4D_B}}\right)\right]. \tag{A4}$$

However, to obtain the mean value, it is easier to compute it from Eq. (A3), taking $\langle d\rangle=-(\partial/\partial p)f^*_{x_1}(p,t)|_{p=0}$, which gives

$$\langle d\rangle=\frac{1}{n_0}+\sqrt{\frac{4D_Bt}{\pi}}+\frac{2D_B}{\gamma}\left[e^{\gamma^2t/(4D_B)}\mathrm{erfc}\left(\gamma\sqrt{\frac{t}{4D_B}}\right)-1\right]. \tag{A5}$$

This result generalizes the one obtained in Ref. [22], where only perfect absorption was considered.

[1] D. Avnir and Kagan, Nature (London) **307**, 717 (1984); G. T. Dee, Phys. Rev. Lett. **57**, 275 (1986); R. E. Liesegang, Naturwiss. Wochensch. **11**, 353 (1896); T. A. Witten and L. M. Sander, Phys. Rev. Lett. **47**, 1400 (1981); K. F. Mueller, Science **225**, 1021 (1984).
[2] M. V. Smoluchowski, Z. Phys. Chem. **92**, 129 (1917).
[3] See, e.g., S. A. Rice, *Diffusion-Limited Reactions* (Elsevier, Amsterdam, 1985).
[4] S. Havlin and D. Ben-Avraham, Adv. Phys. **36**, 695 (1987); Y. B. Zeldovich and A. S. Mikhailov, Usp. Fiz. Nauk. **153**, 469 (1987) [Sov. Phys. Usp. **30**, 246 (1987)]; K. Lindenberg, B. J. West, and R. Kopelman, in *Noise and Chaos in Nonlinear Dynamical Systems*, edited by F. Moss, L. Lugiato, and W. Schleich (Cambridge University Press, Cambridge, England, 1990), p. 142; D. Ben-Avraham, M. A. Burschka, and C. R. Doering, J. Stat. Phys. **60**, 695 (1990).
[5] S. Redner and F. Leyvraz, in *Fractals in Science*, edited by A. Bunde and S. Havlin (Springer-Verlag, Berlin, 1994), p. 197, and references cited therein; see also several articles in the Raoul Kopelman Festschrift issue of J. Phys. Chem. **98**, No. 30 (1994).
[6] M. A. Rodriguez, G. Abramson, H. S. Wio, and A. Bru, Phys. Rev. E **48**, 829 (1993).
[7] G. Abramson, A. Bru Espino, M. A. Rodriguez, and H. S. Wio, Phys. Rev. E **50**, 4319 (1994).
[8] H. S. Wio, G. Abramson, M. A. Rodriguez, and A. Bru, Chaos Solitons Fractals **6**, 575 (1995).
[9] G. Abramson and H. S. Wio, Chaos Solitons Fractals **6**, 1 (1995).
[10] A. D. Sánchez, E. M. Nicola, and H. S. Wio, Phys. Rev. Lett. **78**, 2244 (1997).
[11] G. Abramson and H. S. Wio, Phys. Rev. E **53**, 2265 (1996).
[12] A. D. Sánchez and H. S. Wio, Physica A **237**, 452 (1997).
[13] G. Abramson, Ph.D. thesis, Instituto Balseiro, Universidad Nacional de Cuyo, 1995 (unpublished); A. Bru, Ph.D. thesis, Universidad Complutense de Madrid, 1995 (unpublished).
[14] S. Chandrasekhar, Rev. Mod. Phys. **15**, 1 (1943).
[15] G. H. Weiss, R. Kopelman, and S. Havlin, Phys. Rev. A **39**, 466 (1989).
[16] S. Redner and D. Ben-Avraham, J. Phys. A **23**, L1169 (1990).
[17] H. Taitelbaum, R. Kopelman, G. H. Weiss, and S. Havlin, Phys. Rev. A **41**, 3116 (1990).
[18] H. Taitelbaum, Phys. Rev. A **43**, 6592 (1991).
[19] H. Taitelbaum, S. Havlin, and G. H. Weiss, Chem. Phys. **146**, 351 (1990).
[20] C. A. Condat, G. Sibona, and C. E. Budde, Phys. Rev. E **51**, 2839 (1995).
[21] G. Sibona, C. E. Budde, and C. A. Condat, Phys. Rev. E **54**, 6232 (1996).
[22] D. Ben-Avraham and G. H. Weiss, Phys. Rev. A **39**, 6436 (1989).
[23] R. Schoonover, D. Ben-Avraham, S. Havlin, R. Kopelman, and G. H. Weiss, Physica A **171**, 232 (1991).
[24] H. S. Wio and F. G. Nicolini, in *Path Integration: Trieste 1991*, edited by H. A. Cerdeira, S. Lundqvist, D. Mugnai, A. Ranfagni, V. Sa-yakanit, and L. S. Schulman (World Scientific, Singapore, 1993), p. 582.
[25] D. R. Cox, *Renewal Theory* (Methuen, London, 1970).