

Trapping reactions for mobile particles and a trap in the laboratory frame

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We have used a stochastic model to obtain the exact spatial particle density profile for the trapping process $A + B \rightarrow B$ in a one-dimensional lattice with a single trap, as seen from the laboratory frame. We obtain the profile for either perfect or imperfect reactions when A particles are immobile, but only for perfect absorption in the general case where both particles are mobile with different diffusivities. This profile is found to be similar to that seen from the reference system attached to the trap, the most noticeable difference being near the origin. [S1063-651X(99)08505-0]

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I. INTRODUCTION

The dynamics of elementary diffusion controlled reactions has been extensively studied [1], the main objective of such studies being the finding of theoretical models that describe correctly different chemical reactions. With the aim of obtaining a description of such kinds of phenomena including the probabilistic character of the reaction process, models, and techniques of analysis coming from the theory of nuclear reactors [2,3] have been adapted to model these reactions [4,5]. This framework turns out to be very adequate to describe different situations, making it possible to obtain results not only in the asymptotic, but also in the intermediate and short time regimes. The results yield excellent agreement with simulations [4–11], particularly when the model equation can be exactly solved. The reason is that the equation is the continuous limit of the master equation that describes the simulations exactly.

The trapping reaction $A + B \rightarrow B$ with a single trap and a uniform initial density of particles in a one-dimensional lattice is one of the simplest cases describing a certain kind of chemical reactions. However, there are some questions still open. A mathematically complex one is to find the statistics of the nearest-neighbor distance. This was completely solved only for the particular cases of immobile B particles [12–17] and immobile A particles [18,19]. The general case with both species mobile is still open [19,20]. In addition to that, the density profile, as seen from the trap frame was recently solved in Refs. [19,21]. In addition, in Ref. [21] the density profile as seen from the laboratory coordinate system was discussed, its scaling properties obtained, and an analytical expression was given for the case when the trap and particles have the same diffusivity.

In the present work we analyze the density profile when both species are mobile, within the framework of the stochastic model presented in Ref. [4]. We will show that it is possible to obtain the exact expression of $n(x,t)$, the distri-

bution of particles in the laboratory reference frame. The organization of the paper is as follows. The model is presented and we write the equation for our particular case. The exact solution is obtained in the Laplace-Fourier space for either perfect or imperfect reactions and arbitrary values of the diffusion constants D_A and D_B . When either of the diffusivities is zero we write the $n(x,t)$ in the space-time domain. Later we present the (arbitrary diffusivities) solution $n(x,t)$ but for perfect reactions. Finally we draw our conclusions while some details about the obtention of $n(x,t)$ are described in an appendix.

II. PARTICLE DISTRIBUTION FROM THE LABORATORY FRAME

The model considers two species of particles A and B , both mobile and independent, and having a given reaction probability when they meet. Here we will study only a one-dimensional trapping reaction in a system of diffusing A particles uniformly distributed 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 A particles, for a given realization of $\epsilon(t)$, the trap trajectory, is the following:

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

where γ is a constant measuring the reaction probability ($\gamma \rightarrow \infty$ for perfect reactions). In general we are interested in $n(x,t) = \langle N(x,t) \rangle$, the density averaged over realizations of $\epsilon(t)$.

The solution for the initial condition $n(x,0) = n_0$ and $\epsilon(0) = 0$ can be written [3,4] in the following form:

$$n(x,t) = n_0 - \gamma \int_0^t dt' \int_{-\infty}^{\infty} dx' G(x,t|x',t') \mathcal{A}(x',t'), \quad (2)$$

where the absorption function $\mathcal{A}(x,t)$ satisfies the following convolution equation:

$$\begin{aligned} \mathcal{A}(x,t) = & n_0 W(x,t|0,0) - \gamma \int_0^t dt' \int_{-\infty}^{\infty} dx' G(x,t|x',t') \\ & \times W(x,t|x',t') \mathcal{A}(x',t'). \end{aligned} \quad (3)$$

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Here $G(x,t|x',t')$ and $W(x,t|x',t')$ are the particle and trap propagator respectively. The use of a diffusive form for both propagators allows us to write the Laplace-Fourier transform of the density given by

$$\frac{n(w,s)}{n_0} = \frac{2\pi\delta(w)}{s} - \frac{\gamma}{(s+D_A w^2)(s+D_B w^2)[1+(s+\tilde{D}w^2)^{-1/2}\gamma/(2\sqrt{D})]}, \quad (4)$$

where

$$D = D_A + D_B, \quad (5)$$

$$\tilde{D} = \frac{D_A D_B}{D} = \frac{D_A D_B}{D_A + D_B}. \quad (6)$$

Note that by setting $w=0$ in the second term of Eq. (4), the total number of absorbed particles can be obtained. The resulting expression coincides with previous calculations performed on the trap frame [19,21].

Performing the inverse Laplace-Fourier transform of Eq. (4) is a difficult task. However, the expression simplifies considerably for two particular cases, $D_A=0$ and $D_B=0$, both having the same functional form. Taking the inverse transform we obtain the following expression:

$$\begin{aligned} \frac{n(x,t)}{n_0} &= \operatorname{erf}\left(\frac{|x|}{\sqrt{4D_{A,B}t}}\right) + e^{\gamma|x|/(2D_{A,B}) + \gamma^2 t/(4D_{A,B})} \\ &\times \operatorname{erfc}\left(\frac{|x|}{\sqrt{4D_{A,B}t}} + \gamma\sqrt{\frac{t}{4D_{A,B}}}\right). \end{aligned} \quad (7)$$

The fixed trap case is known [4] but here we obtain the case of immobile A particles. For a perfect absorption reaction the second term in Eq. (7) vanishes and the density at $x=0$ is null. This fact has different reasons in each case: while for $D_B=0$ the trap is at the origin in all the realizations, when $D_A=0$ the particles are immobile and they cannot migrate to fill the depletion left by the trap at $t=0$. The last remark is about the (in principle unexpected) fact that in the case of fixed A particles the density, as seen from the laboratory frame, is exactly the same as the one seen from the trap frame. This equality is only satisfied when $D_A=0$ (besides the $D_B=0$ case where it is trivially satisfied). We illustrate the indicated equality in Fig. 1. The agreement between simulations and the theoretical expression is apparent. Although simulation for different parameters can be included in the same graph using the dimensionless variables $x/\sqrt{D_B t}$ and $\gamma\sqrt{t/D_B}$, we use x and t to stress the equality between the densities from the two different frames.

From Eq. (4) we take the limit $\gamma \rightarrow \infty$ in order to obtain the mathematically simpler perfect reaction expression, resulting in

$$\frac{n(w,s)}{n_0} = \frac{2\pi\delta(w)}{s} - \frac{2\sqrt{D}\sqrt{s+\tilde{D}w^2}}{(s+D_A w^2)(s+D_B w^2)}. \quad (8)$$

Taking the inverse Laplace transform of Eq. (8) we obtain [24]

$$\begin{aligned} \frac{n(w,t)}{n_0} &= 2\pi\delta(w) - \frac{4}{\sqrt{\pi}} \frac{1}{(D_B - D_A)} \\ &\times \frac{e^{-\tilde{D}w^2 t}}{w} [D_B G(D_B \sqrt{t}w/\sqrt{D}) \\ &- D_A G(D_A \sqrt{t}w/\sqrt{D})], \end{aligned} \quad (9)$$

where $G(x) = \int_0^x \exp(t^2 - x^2) dt$ is the Dawson's integral [22]. The final result (see the Appendix) expressed in the dimensionless variables $\delta = D_B/D_A$ and $\xi = x/\sqrt{4D_B t}$ is

$$\hat{n}(\delta, \xi) = 1 + \frac{2}{\sqrt{\pi}} \frac{1}{\delta - 1} [\delta F(\delta, \xi) - F(1/\delta, \sqrt{\delta}\xi)], \quad (10)$$

$$F(\delta, \xi) = \int_{-\infty}^{\xi} \operatorname{erf}(\sqrt{\delta}x) \exp(-x^2) dx, \quad (11)$$

where we denote $n(x,t)/n_0$ expressed in δ and ξ variables by $\hat{n}(\delta, \xi)$. From Eq. (10) the limits $\delta \rightarrow 1$ ($D_A = D_B$) and $\xi \rightarrow 0$ ($x=0$) that were presented in Ref. [21] can be recovered (see the Appendix). In addition we can see that the density is an analytic function of ξ over the whole real axis, except for $\delta=0$ or $\delta \rightarrow \infty$ which were treated above, where there is a jump in its slope at $\xi=0$. Note that the density is still analytic for $\delta=1$ [Eq. (A13)]. The general aspect of $\hat{n}(\delta, \xi)$ is shown in Fig. 2. The curves were computed from

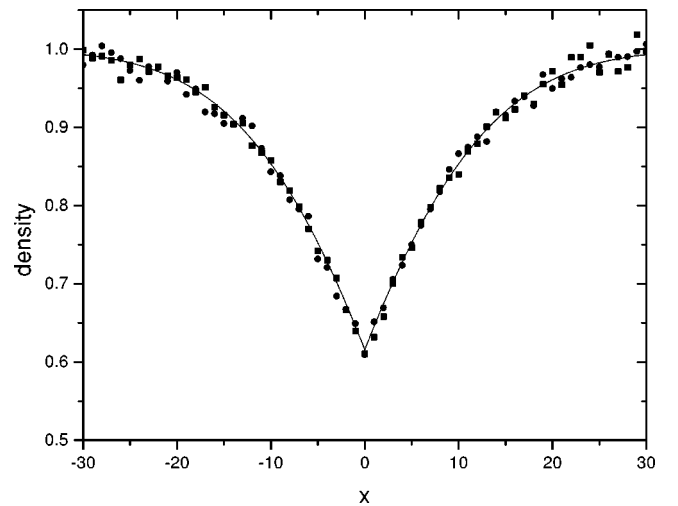


FIG. 1. Simulation for the density of A particles in the reference frame of the trap (circles) and from the laboratory coordinate system (squares) (in arbitrary units). The parameters are $L=480$, $D_B=1$, $\gamma=0.1$, $t=100$. The solid line is the theoretical value corresponding to both densities from Eq. (7).

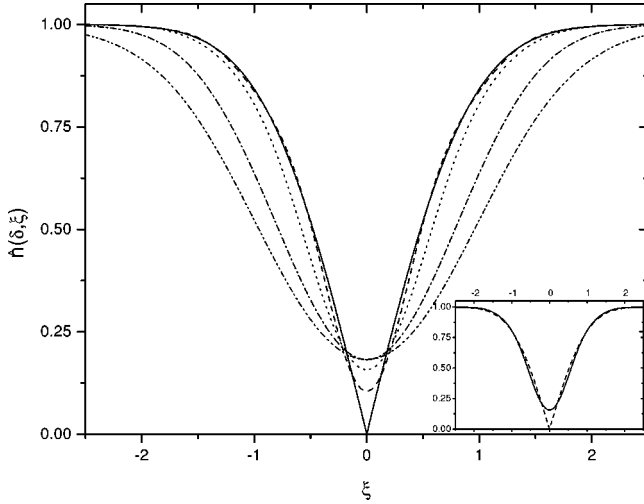


FIG. 2. Density of particles from Eq. (A4) in adimensional variables. The different curves correspond to $\delta=\infty$ (solid line), $\delta=100$ (dashed line), $\delta=5$ (dotted line), $\delta=1$ (dashed-dotted line), and $\delta=0.5$ (dashed-dotted-dotted line). The inset shows the density as seen from the laboratory frame (solid line) and from the trap frame (dashed line) for $\delta=5$.

Eq. (A4) which being equivalent to Eq. (10) is more convenient for numerical evaluation. In the inset we compare $\hat{n}(\delta, \xi)$ with the density as seen from a coordinate system attached to the trap ($\tilde{n}(\delta, \xi) = \text{erf}[\sqrt{\delta/(\delta+1)}|\xi|]$ [19,21]), where we can see that both densities are very close except for values near the origin. Finally, in Fig. 3 we compare simulations with $\hat{n}(\delta, \xi)$, where the good agreement is apparent.

The simulations were performed on a lattice of L sites, with periodic boundary conditions. We have used the same algorithm described in Ref. [19]. All results showed are the average over 10 000 realizations and with an initial density $n_0=1$.

III. FINAL REMARKS

Summarizing, we have shown that the stochastic model recently introduced for the description of diffusion limited reactions allows us to calculate the exact expression of $n(x, t)$, the distribution of particles in the laboratory frame, for perfect reactions. As noted in Ref. [21] the profile for imperfect trapping approaches that for perfect reactions as $t \rightarrow \infty$. The solution can be expressed either as a series of Hermite polynomials [Eq. (A4)] or through a definite integral [Eq. (10)]. While the series is appropriate for numerical evaluations due to its fast convergence, the integral is adequate for recovering the limits $D_A=D_B$ and $x=0$, previously reported in Ref. [21].

The expression obtained for $n(x, t)$ satisfies the scaling symmetries given in Ref. [21] and has an additional one: its invariance by exchange of diffusivities, i.e., $D_A \rightarrow D_B, D_B \rightarrow D_A$ or in the scaling variables $\delta \rightarrow 1/\delta, \xi \rightarrow \sqrt{\delta}\xi$. This symmetry is still valid for trap or A particles fixed and also for imperfect reactions, as we can see from Eq. (4). We have noted that in the case $D_A=0$ the resulting density has the same expression in a reference system attached to the trap [$\hat{n}(\delta, \xi)$] and in the laboratory coordinated system [$\tilde{n}(\delta, \xi)$].

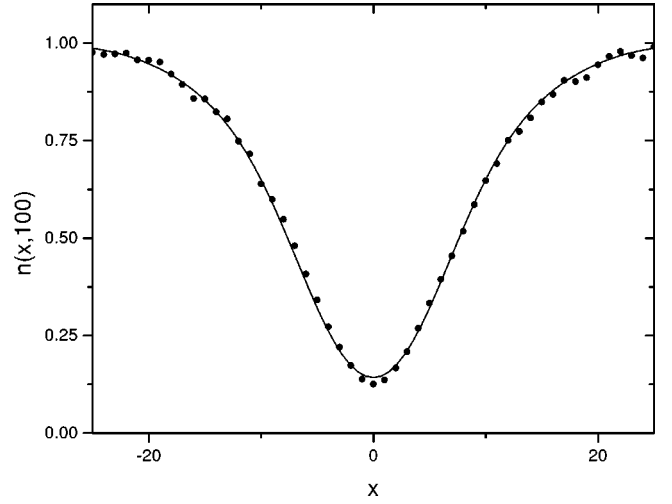


FIG. 3. Simulations for the particles density (dots) and theoretical value from Eq. (A3) (in arbitrary units). The parameters are $L=100$, $D_A=0.5$, $D_B=5$, $t=100$, and perfect absorption.

For arbitrary D_B/D_A the form of the solution was shown (Fig. 2). This can be contrasted with the known expression for the density in the trap frame; the result being that both expressions are similar. The largest difference is near $\xi=0$, where $\tilde{n}(\delta, \xi)$ is zero and has a discontinuity in its derivative while $\hat{n}(\delta, \xi)$ has a finite value and is a smooth function.

We note that Eq. (4), being an exact result, could be used to obtain the density $n(x, t)$ in the general case of an imperfect reaction, by numerically performing the inverse Laplace-Fourier transform. The simulations are in excellent agreement with the model. As was mentioned in the introduction, this is an expected result since the model has been solved exactly.

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APPENDIX

1. Calculation of the inverse transform

We expand Eq. (9) using

$$G(x) = x \exp(-x^2) \sum_{j=0}^{\infty} \frac{x^{2j}}{j!(2j+1)} \quad (\text{A1})$$

and after taking the inverse Fourier transform we obtain

$$\begin{aligned} \frac{n(x, t)}{n_0} = & 1 - \frac{2}{\pi} \frac{1}{(D_B - D_A)} \frac{1}{\sqrt{D}} \\ & \times \left[D_B^{3/2} \sum_{j=0}^{\infty} \left(\frac{D_B^2 t}{D} \right)^j \frac{(-1)^j}{j!(2j+1)} \partial_x^{2j} \exp\left(-\frac{x^2}{4D_B t}\right) \right. \\ & \left. - D_A^{3/2} \sum_{j=0}^{\infty} \left(\frac{D_A^2 t}{D} \right)^j \frac{(-1)^j}{j!(2j+1)} \partial_x^{2j} \exp\left(-\frac{x^2}{4D_A t}\right) \right]. \quad (\text{A2}) \end{aligned}$$

Applying the Rodrigues formula [22] now we finally obtain

$$\begin{aligned} \frac{n(x,t)}{n_0} &= 1 - \frac{2}{\pi} \frac{1}{(D_B - D_A)} \frac{1}{\sqrt{D}} \\ &\times \left[D_B^{3/2} e^{-x^2/(4D_B t)} \sum_{j=0}^{\infty} \left(\frac{D_B}{4D} \right)^j \frac{(-1)^j}{j!(2j+1)} \right. \\ &\times H_{2j} \left(\frac{x}{\sqrt{4D_B t}} \right) - D_A^{3/2} e^{-x^2/(4D_A t)} \\ &\times \left. \sum_{j=0}^{\infty} \left(\frac{D_A}{4D} \right)^j \frac{(-1)^j}{j!(2j+1)} H_{2j} \left(\frac{x}{\sqrt{4D_A t}} \right) \right] \quad (\text{A3}) \end{aligned}$$

or in dimensionless variables

$$\begin{aligned} \hat{n}(\delta, \xi) &= 1 - \frac{2}{\pi} \frac{1}{(\delta-1)} \frac{1}{\sqrt{\delta+1}} \\ &\times \left[\delta^{3/2} e^{-\xi^2} \sum_{j=0}^{\infty} \left(\frac{\delta}{\delta+1} \right)^j \frac{(-1)^j}{j!(2j+1)2^j} H_{2j}(\xi) \right. \\ &- e^{-\delta\xi^2} \sum_{j=0}^{\infty} \left(\frac{1}{\delta+1} \right)^j \frac{(-1)^j}{j!(2j+1)2^j} H_{2j}(\sqrt{\delta}\xi) \left. \right], \quad (\text{A4}) \end{aligned}$$

where $H_i(x)$ is the Hermite polynomial of degree i . This series is adequate for evaluating the density profile numerically due to its rapid convergence.

2. Series sum and F function

We expand the $\text{erf}(\sqrt{\delta}x)$ in a Hermite polynomial series

$$\text{erf}(\sqrt{\delta}x) = \frac{1}{\sqrt{\pi}} \sum_{j=0}^{\infty} \frac{(-1)^j}{j!(2j+1)2^{2j}} \left(\frac{\delta}{1+\delta} \right)^{j+1/2} H_{2j+1}(x), \quad (\text{A5})$$

that after multiplying by the Gaussian function and integrating gives

$$\begin{aligned} F(\delta, \xi) &= \int_{-\infty}^{\xi} \text{erf}(\sqrt{\delta}x) \exp(-x^2) dx \\ &= -\sqrt{\frac{\delta}{\pi(1+\delta)}} \exp(-\xi^2) \\ &\times \sum_{j=0}^{\infty} \frac{(-1)^j}{j!(2j+1)2^{2j}} \left(\frac{\delta}{1+\delta} \right)^j H_{2j}(\xi). \quad (\text{A6}) \end{aligned}$$

Some particular values of the function $F(\delta, \xi)$ are

$$F(1, \xi) = \frac{\sqrt{\pi}}{4} [\text{erf}^2(\xi) - 1], \quad (\text{A7})$$

$$F(\delta, 0) = \frac{1}{\sqrt{\pi}} \arctan(1/\sqrt{\delta}) - \frac{\sqrt{\pi}}{2}, \quad (\text{A8})$$

$$F(\delta, \infty) = 0, \quad (\text{A9})$$

$$\frac{\partial}{\partial \delta} F(\delta, \xi) \Big|_{\delta=1} = -\frac{1}{4\sqrt{\pi}} \exp(-2\xi^2), \quad (\text{A10})$$

$$\frac{\partial}{\partial \xi} F(\delta, \xi) = \text{erf}(\sqrt{\delta}\xi) \exp(-\xi^2). \quad (\text{A11})$$

The integral defined for Eq. (A8) can be found in Ref. [23]. Using this equation and after some algebra the density in $\xi = 0$ is

$$\hat{n}(\delta, 0) = \frac{1}{2} - \frac{1}{\pi} \frac{\delta+1}{\delta-1} \arctan\left(\frac{\delta-1}{2\sqrt{\delta}}\right), \quad (\text{A12})$$

while from Eq. (A9) $\hat{n}(\delta, \infty) = 1$. The l'Hôpital's rule applied to Eq. (10) yields

$$\begin{aligned} \hat{n}(1, \xi) &= 1 + \frac{2}{\sqrt{\pi}} \left[F(1, \xi) + 2 \frac{\partial}{\partial \delta} F(\delta, \xi) \Big|_{\delta=1} - \frac{\xi}{2} \frac{\partial}{\partial \xi} F(1, \xi) \right] \\ &= \frac{1}{2} + \frac{1}{2} \text{erf}^2(\xi) - \frac{1}{\pi} \exp(-2\xi^2) \\ &\quad - \frac{1}{\sqrt{\pi}} \xi \exp(-\xi^2) \text{erf}(\xi), \quad (\text{A13}) \end{aligned}$$

the explicit expression for the $D_A = D_B$ case.

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