Theory of the absorption probability density of diffusing particles in the presence of a dynamic trap

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There have been a number of recent investigations of diffusing particles in the presence of traps. Among many applications of this process, we find phenomena such as reaction rates, biological models, and dielectric relaxation. In this paper we present a theory for the absorption probability density for a walker in the presence of a dynamic trap by using the multistate continuous-time random-walk approach. The results are exact for every switching-time probability density of the trap. The deterministic and Markovian cases can be obtained by selecting the appropriate switching-time density for the trap. Siegert's result is reobtained in the static case. We perform Monte Carlo simulations, and compare these results with our analytical prediction, finding excellent agreement for symmetric and nonsymmetric switching-time densities.

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I. INTRODUCTION

A well established method for studying reaction rates [1], biological problems [2], solid state transport [3,4], dielectric relaxation [5], etc. is developed through random walk (RW) modeling. The magnitude of interest in these models is the absorption probability density (APD) of the walker by a trap [which coincides with the first passage time density (FPTD) in presence of a static trap]. Different generalizations have been proposed for continuous time RW (CTRW) on lines such as the study of the presence of an imperfect trap [6]. The authors have started with the study of the influence in the APD by the presence of a dynamic trap due to the problem of a gate which opens and closes at random times [7]. In these generalizations, the APD does not coincide with the FPTD because a path of the walker through the trap position does not mean that it will be absorbed.

The problem is solved using the multistate CTRW (MCTRW) [3,8–10] technique in a similar way as applied to the problem of non-Markovian global dynamic disorder [11,12]. The method proceeds by using the internal state scheme, which is mathematically equivalent to non-Markovian local dynamic disorder. The deterministic, static, and Markovian cases are particular situations included in our solution, and may be calculated by selecting the appropriate switching-time density of the trap.

In Sec. II we solve the problem of a CTRW in an infinite homogeneous medium with an impurity. This is achieved by generalizing a technique developed by Montroll and West in his study of the effect of traps on lattice walks [3]. The dynamic trap is introduced in Sec. III through the MCTRW scheme, where internal states are given by the *activation* or *deactivation* of the trap. In Sec. IV we present an explicit analytical solution for the one-dimensional case in the Laplace representation. Markovian and non-Markovian situations are analyzed by selecting appropriate functions for the switching-time probability density of the trap. In Sec. V the asymptotic behavior of the APD in the limits for $t \to 0$ and $t \to \infty$ are presented.

The results in the time domain are numerically calculated from the analytical results in the Laplace representation, and then compared with the output of Monte Carlo simulations. Both approaches show a very good agreement.

The solution obtained can be extended to higher dimensions or to the problem of diffusion with bias. The APD will also be used in a generalization of the Glarum model to the case of a dynamic relaxation rate. Work along these lines will be presented in a future paper.

II. RANDOM WALK IN THE PRESENCE OF AN IMPURITY

Let us start with the problem of a particle that does a random walk in an infinite homogeneous medium. Let $H_0(\mathbf{s},\mathbf{s}';t)$ be the probability density for the hopping so that $H_0(\mathbf{s},\mathbf{s}';t)=H_0(\mathbf{s}-\mathbf{s}';t)$. If in the site $\mathbf{s}_1$ there is an impurity, we can characterize the jump from this site by the hopping probability density $H_1(\mathbf{s},\mathbf{s}_1;t)$.

Let $R(\mathbf{s},t)dt$ be the probability to arrive at site $\mathbf{s}$ just at the time between t and $t+dt$. From its definition it is clear that $R(\mathbf{s},t)dt$ is different from $P(\mathbf{s},t)$, the probability to be at site $\mathbf{s}$ at time t. Therefore $R(\mathbf{s},t)$ satisfies the following integral equation (here we assume that the random walk starts at $\mathbf{s}_0$ in $t=0$):

$$R(\mathbf{s},t)-\sum_{\mathbf{s}'}\int_0^t R(\mathbf{s}',\tau)H(\mathbf{s},\mathbf{s}';t-\tau)d\tau=\delta_{\mathbf{s},\mathbf{s}_0}\delta_{t,0^+}\ , \qquad (1)$$

where $H(\mathbf{s},\mathbf{s}';t)$ is given by

$$H=\begin{cases}H_0(\mathbf{s}-\mathbf{s}';t) & \text{if } \mathbf{s}'\neq\mathbf{s}_1\\ H_1(\mathbf{s},\mathbf{s}_1;t) & \text{if } \mathbf{s}'=\mathbf{s}_1\ .\end{cases} \tag{2}$$

We write Eq. (1) in the Laplace representation as

$$\begin{aligned}R(\mathbf{s},u)&=\sum_{\mathbf{s}'\neq\mathbf{s}_1} H_0(\mathbf{s}-\mathbf{s}';u)R(\mathbf{s}',u)\\&\quad+H_1(\mathbf{s},\mathbf{s}_1;u)R(\mathbf{s}_1;u)+\delta_{\mathbf{s},\mathbf{s}_0}\\&=\sum_{\mathbf{s}'}H_0(\mathbf{s}-\mathbf{s}';u)R(\mathbf{s}',u)+H_1(\mathbf{s},\mathbf{s}_1;u)R(\mathbf{s}_1,u)\\&\quad-H_0(\mathbf{s}-\mathbf{s}_1;u)R(\mathbf{s}_1,u)+\delta_{\mathbf{s},\mathbf{s}_0}\ .\end{aligned} \tag{3}$$

$R(\mathbf{s},u)$ and $H(\mathbf{s},\mathbf{s}';u)$ are the Laplace transform functions calculated by

$$R(\mathbf{s},u)=\int_0^\infty e^{-ut}R(\mathbf{s},t)dt \tag{4}$$

for the function R, and in a similar way for function H.

The solution of Eq. (3) is as follows:

$$\begin{aligned}R(\mathbf{s},u)&=R_0(\mathbf{s}-\mathbf{s}_0;u)-R(\mathbf{s}_1,u)[R_0(\mathbf{s}-\mathbf{s}_1;u)-\delta_{\mathbf{s},\mathbf{s}_1}]\\&\quad+R(\mathbf{s}_1;u)\left[\sum_{\mathbf{s}'}H_1(\mathbf{s}',\mathbf{s}_1;u)R_0(\mathbf{s}-\mathbf{s}';u)\right]\ ,\end{aligned} \tag{5}$$

where we have used the homogeneous Green function

$$R_0(\mathbf{s},u)=\sum_{\mathbf{s}'}H_0(\mathbf{s}-\mathbf{s}';u)R_0(\mathbf{s}';u)+\delta_{\mathbf{s},0}\ . \tag{6}$$

As the solution (5) is valid for every $\mathbf{s}$, if we take the particular value $\mathbf{s}=\mathbf{s}_1$ we get

$$R(\mathbf{s}_1;u)=\frac{R_0(\mathbf{s}_1-\mathbf{s}_0;u)}{R_0(0;u)-\sum_{\mathbf{s}'}H_1(\mathbf{s}',\mathbf{s}_1;u)R_0(\mathbf{s}_1-\mathbf{s}';u)}\ . \tag{7}$$

With this result we have got an explicit expression for $R(\mathbf{s};u)$. We obtain $P(\mathbf{s};u)$ in terms of $R(\mathbf{s};u)$ as

$$P(\mathbf{s};u)=R(\mathbf{s};u)V(\mathbf{s};u)\ . \tag{8}$$

$V(\mathbf{s};u)$ is the Laplace transform of the probability that no jump occurs in a given time interval. This function may be calculated by

$$V(\mathbf{s};t)=1-\int_0^t\sum_{\mathbf{s}'}H(\mathbf{s}',\mathbf{s};t')dt' \tag{9}$$

in the time domain.

The particular case of a static trap at site $\mathbf{s}_1$ is included in our solution by taking $H_1(\mathbf{s},\mathbf{s}_1;t)$ as

$$H_1(\mathbf{s},\mathbf{s}_1;t)=0,\quad \forall t,\mathbf{s}\ . \tag{10}$$

With this choice replaced in (7), we find that the Laplace transform of the probability density for the walker to arrive at site $\mathbf{s}$, just at time t, is given by

$$R(\mathbf{s}_1;u)=\frac{R_0(\mathbf{s}_1-\mathbf{s}_0;u)}{R_0(0;u)}\ . \tag{11}$$

Multiplying and dividing by $V(0;u)$, which may be obtained from (9) by replacing $H(\mathbf{s}',\mathbf{s},t)$ by $H_0(\mathbf{s}'-\mathbf{s},t)$, and then calculating its Laplace transform we get

$$R(\mathbf{s}_1;u)=\frac{P_0(\mathbf{s}_1-\mathbf{s}_0;u)}{P_0(0;u)}\ . \tag{12}$$

We wish to remark that $R(\mathbf{s}_1;t)$ is the FPTD from $\mathbf{s}_0$ to $\mathbf{s}_1$. When the impurity corresponds to a static trap, $R(\mathbf{s}_1;u)$ should be interpreted as the APD by the trap or the equivalent FPTD. This is the Siegert formula [13,14] for a homogeneous RW. Thus we have proved the Siegert theorem in the framework of the CTRW theory.

By means of the CTRW approach, we will be able to tackle the problem when the trap is dynamic by introducing the internal state scheme. We will use a method largely inspired in a recently developed one to study diffusion in the presence of external anomalous noise [12].

III. DYNAMIC TRAP

We represent a dynamic trap as a place on the lattice (the impurity in the previous section) whose properties change in time. This change in time will be characterized by a 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 $f_{ij}(t)$, which in principle could be nonsymmetric, where $f_{ij}(t)dt$ is the probability that the impurity, having acquired the state j at $t=0$, makes a transition to state i between t and $t+dt$. The subindex i,j $(i\neq j)$ can take the values 1 (active or perfect trap state) or 2 (inactive or regular site state). In order to use the MCTRW approach, we have to introduce a generalization of the probability density for the hopping function $H(\mathbf{s},\mathbf{s}';t)$, as was given in [9].

Let $\mathcal{H}(\mathbf{s},\mathbf{s}';t)$ be the (2×2) probability density matrix in such a way that this matrix takes into account the hopping of the random walk and also independently the change of the states of the dynamic trap. This matrix must reflect the fact that $\mathbf{s}_1$ (where the impurity is located) is an absorbent site when the trap is active (state $j=1$), and $\mathbf{s}_1$ is an indistinguishable site of the lattice when the trap is inactive (state $j=2$). This condition is achieved by requiring that if the walker falls in $\mathbf{s}_1$, it cannot leave that site if it has been absorbed:

$$\mathcal{H}_{i,1}(\mathbf{s},\mathbf{s}_1;t)=0,\quad \forall\ \mathbf{s};i=1,2,\text{ and } t\ . \tag{13}$$

The condition of *independent processes* imposes a decoupled structure similar to the one used in [12]. Let us consider that the particle does a Markovian random walk (i.e., the waiting time of the walker is exponential). Therefore, we can define the bulk matrix $\mathcal{H}^0(\mathbf{s},\mathbf{s}';t)$ in the following way:

$$\mathcal{H}^0(\mathbf{s},\mathbf{s}';t)=\begin{bmatrix}M_{11}(\mathbf{s},\mathbf{s}';t)\phi_{11}(t) & M_{12}(\mathbf{s};t)f_{12}(t)\\ M_{12}(\mathbf{s};t)f_{21}(t) & M_{11}(\mathbf{s},\mathbf{s}';t)\phi_{22}(t)\end{bmatrix}\ , \tag{14}$$

where

$$M_{11}(\mathbf{s},\mathbf{s}';t)\equiv M_{11}(\mathbf{s}-\mathbf{s}';t)=B(\mathbf{s},\mathbf{s}')\exp\left[-\sum_{\mathbf{s}'}B(\mathbf{s}',\mathbf{s})t\right], \quad (15)$$

$$M_{12}(\mathbf{s},t)\equiv M_{12}(t)=\exp\left[-\sum_{\mathbf{s}'}B(\mathbf{s}',\mathbf{s})t\right]. \quad (16)$$

The elements of the matrix $\mathcal{H}^0(\mathbf{s},\mathbf{s}';t)=\mathcal{H}^0(\mathbf{s}-\mathbf{s}';t)$ have to be interpreted in the following forms:

(i) $B(\mathbf{s},\mathbf{s}')\exp[-\sum_{\mathbf{s}'}B(\mathbf{s},\mathbf{s}')t]$ is the waiting-time probability density for the walker, where $B(\mathbf{s},\mathbf{s}')=B(\mathbf{s}-\mathbf{s}')$ is the walker hopping structure in a generic d-dimensional regular lattice.

(ii) $f_{ij}(t)$ is the switching-time probability density of the trap defined above.

(iii) $\phi_{ii}(t)$ is the probability that the impurity is still in the state i after a time t since it has got that state.

Therefore the matrix $\mathcal{H}(\mathbf{s},\mathbf{s}';t)$, with one impurity, which characterizes the MCTRW can be written as

$$\mathcal{H}(\mathbf{s},\mathbf{s}';t)=\begin{Bmatrix}\mathcal{H}^0(\mathbf{s}-\mathbf{s}';t) & \text{if } \mathbf{s}'\neq\mathbf{s}_1\\ \mathcal{H}^1(\mathbf{s},\mathbf{s}_1;t) & \text{if } \mathbf{s}'=\mathbf{s}_1\end{Bmatrix}, \quad (17)$$

where the elements of $\mathcal{H}(\mathbf{s}',\mathbf{s}_1;u)$ are given in terms of (13) and (14) as

$$\begin{aligned}&\mathcal{H}^1_{i2}(\mathbf{s}',\mathbf{s}_1;u)=\mathcal{H}^0_{i2}(\mathbf{s}',\mathbf{s}_1;u),\\&\mathcal{H}^1_{i1}(\mathbf{s}',\mathbf{s}_1;u)=0.\end{aligned} \quad (18)$$

Now the multistate generalization of (1), in the Laplace representation, acquires the form [9]

$$R_i(\mathbf{s},u)=\sum_{\mathbf{s}'j}\mathcal{H}_{ij}(\mathbf{s},\mathbf{s}';u)R_j(\mathbf{s}';u)+\delta_{\mathbf{s},\mathbf{s}_0}\delta_{i,i_0}. \quad (19)$$

Using (17) and (19) in a similar way as we did to get (5), and introducing the homogeneous Green matrix $\mathcal{R}^0_{ij}(\mathbf{s};u)$, we obtain for the solution of $R_1(\mathbf{s};u)$:

$$R_i(\mathbf{s};u)=\mathcal{R}^0_{ii_0}(\mathbf{s}-\mathbf{s}_0;u)+\sum_l R_l(\mathbf{s}_1;u)\left[\sum_{\mathbf{s}'j}\mathcal{R}^0_{ij}(\mathbf{s}-\mathbf{s}';u)\mathcal{H}^1_{jl}(\mathbf{s}',\mathbf{s}_1;u)-\mathcal{R}^0_{il}(\mathbf{s}-\mathbf{s}_1;u)+\delta_{\mathbf{s},\mathbf{s}_1}\delta_{il}\right]. \quad (20)$$

This expression is valid for every $\mathbf{s}$ and i; thus, if we take $\mathbf{s}=\mathbf{s}_1$ we get a system of linear equations for $R_i(\mathbf{s}_1;t)$. Obviously, the number of equations is equal to the number of internal states. The solution of this problem gives the probability to arrive at site $\mathbf{s}_1$ as a function of the homogeneous Green matrix $\mathcal{R}^0_{ij}(\mathbf{s};t)$. As before, the vector probability $P_i(\mathbf{s};u)$ can be written in terms of the vector $R_i(\mathbf{s};u)$ [9], [12] by using the generalization of (8) and (9) to the MCTRW scheme. The solution of (20), for $\mathbf{s}=\mathbf{s}_1$, can be written in the form

$$\begin{aligned}R_1(\mathbf{s}_1;u)&=\mathcal{R}^0_{1i_0}(\mathbf{s}_1-\mathbf{s}_0;u)[\mathcal{R}^0_{11}(\mathbf{0};u)]^{-1},\\R_2(\mathbf{s}_1;u)&=[\mathcal{R}^0_{11}(\mathbf{0};u)\mathcal{R}^0_{2i_0}(\mathbf{s}_1-\mathbf{s}_0;u)\\&\quad-\mathcal{R}^0_{21}(\mathbf{0};u)\mathcal{R}^0_{1i_0}(\mathbf{s}_1-\mathbf{s}_0;u)]\\&\quad\times[\mathcal{R}^0_{11}(\mathbf{0};u)]^{-1},\end{aligned} \quad (21)$$

where the initial position of the walker is $\mathbf{s}_0$, and the initial state of the trap is i_0. $R_1(\mathbf{s}_1;u)$, the Laplace representation of APD, is the main goal of our work. This probability is expressed in terms of the known functions of the problem: the waiting time of the walker and the switching-time probability density for the change of states of the trap. Obviously, this APD is expressed in terms of the homogeneous Green matrix. In the Fourier representation ($\mathbf{s}\to\mathbf{k}$) this Green matrix can be written as $\mathcal{R}^0_{ij}(\mathbf{k};u)=[\mathcal{I}-\mathcal{H}^0(\mathbf{k};u)]^{-1}_{ij}$, which, in principle, can be solved in any dimension and for any lattice structure (with or without bias). Due to the structure of the matrix $\mathcal{H}^0(\mathbf{s}-\mathbf{s}';t)$ [see Eqs. (14)–(16)], its Fourier and Laplace transforms will be

$$\mathcal{H}^0(\mathbf{k};u)=\begin{bmatrix}B(\mathbf{k})\phi_{11}(u+B(\mathbf{k}=0)) & f_{12}(u+B(\mathbf{k}=0))\\ f_{21}(u+B(\mathbf{k}=0)) & B(\mathbf{k})\phi_{22}(u+B(\mathbf{k}=0))\end{bmatrix}. \quad (22)$$

Using the definition of $\phi_{ii}(t)$ [see the remarks after Eq. (16)], we get its Laplace transform

$$\phi_{11}(u)=[1-f_{21}(u)]/u,\quad \phi_{22}(u)=[1-f_{12}(u)]/u. \quad (23)$$

In this way, all the elements of $\mathcal{H}^0(\mathbf{k};u)$ are given in terms of an arbitrary walker structure function $B(\mathbf{k})$, and a general dynamic for the trap: $f_{21}(u)$ and $f_{12}(u)$.

IV. THE DYNAMIC TRAP IN A ONE-DIMENSIONAL RANDOM WALK

As an example of our theory, we present here the solution for the one-dimensional case without bias, determined by the walker's hopping structure of the bulk,

$$B(\mathbf{s}-\mathbf{s}')=\lambda_w(\tfrac{1}{2}\delta_{\mathbf{s},\mathbf{s}'-1}+\tfrac{1}{2}\delta_{\mathbf{s},\mathbf{s}'+1}), \quad (24)$$

where $\lambda_w=\sum_{\mathbf{s}'}B(\mathbf{s}-\mathbf{s}')$ is the inverse of the walker mean waiting-time ($\langle t\rangle_w$) at any site of the lattice. In this case $B(\mathbf{k})=\lambda_w\cos(\mathbf{k})$. Then $\mathcal{R}^0_{ij}(\mathbf{k};u)$ is obtained straightforwardly using (22) to (24). Taking the inverse Fourier transform of $\mathcal{R}^0_{ij}(\mathbf{k};u)$, formula (21) gives the desired quantity. $R_1(\mathbf{s}_1;u)$ gives the probability density to be absorbed by the dynamic trap located at $\mathbf{s}_1$ (the APD in the Laplace representation).

Because there is not bias, the result will only depend on the distance $r=|\mathbf{s}_1-\mathbf{s}_0|$. Assuming that the initial condition of the trap is *active* we have to use $i_0=1$ in (21); thus, the expression for $R_1(\mathbf{s}_1;u)$ is

$$R_1(\mathbf{s}_1;u)=\left[1+\frac{u}{\lambda_w}\right]^r\frac{C(u)[A(u)]^r+D(u)[B(u)]^r}{C(u)+D(u)}\ , \tag{25}$$

where we have defined the auxiliary functions

$$\begin{aligned} C(u)&=\frac{f_{21}}{\sqrt{\alpha(u)}}\frac{1-f_{12}}{1-f_{21}}\ ,\\ D(u)&=\frac{f_{12}}{\sqrt{\beta(u)}}\ ,\\ A(u)&=\frac{1-f_{12}f_{21}}{(1-f_{12})(1-f_{21})}-\sqrt{\alpha(u)}\ ,\\ B(u)&=1-\sqrt{\beta(u)}\ , \end{aligned} \tag{26}$$

and we have used the notation

$$\begin{aligned} &f_{12}\equiv f_{12}(u+\lambda_w);\ f_{21}\equiv f_{21}(u+\lambda_w)\ ,\\ &\alpha(u)=\left[\frac{1-f_{12}f_{21}}{(1-f_{12})(1-f_{21})}\right]^2-\left[\frac{\lambda_w}{\lambda_w+u}\right]^2, \\ &\beta(u)=1-\left[\frac{\lambda_w}{\lambda_w+u}\right]^2 . \end{aligned} \tag{27}$$

Formula (25) is exact for every switching-time density of the trap: $f_{ij}(t)$. The case when the trap is always *active* can easily be reobtained by taking $f_{21}(u)\equiv 0$ (remember that the trap was assumed to be active in $t=0$). In the rest of this section we illustrate the result obtained in (25), presenting some typical situations.

(i) The first case that is analyzed corresponds to a Markovian dynamic for the trap, with symmetric switching-time probability density; i.e., the activation and deactivation of the trap are controlled by the same probability density function

$$f_{12}(t)=f_{21}(t)=\lambda_t\exp(-\lambda_t t)\quad\text{with } \lambda_t^{-1}=\langle t\rangle_t\ .$$

In this expression $\langle t\rangle_t$ corresponds to the impurity mean time in a given state (1=active trap state; 2=regular site state). The results for different values of $\langle t\rangle_t$ are shown in Fig. 1. These were numerically computed from (25), using the Laplace inversion program LAPIN [15].

The inset of this figure shows a comparison with the values obtained from Monte Carlo simulation of the process for two particular cases: the static trap (no deactivation) and the Markovian dynamic trap with $\langle t\rangle_t=1$. The agreement between both approaches is very good at any time, as expected because (25) is an exact result.

(ii) The following case presented corresponds to a Markovian dynamic trap, where we have relaxed the symmetric condition. So the switching-time probability densities are given by

$$f_{ij}(t)=\lambda_j\exp(-\lambda_j t)\quad\text{with } \lambda_j^{-1}=\langle t\rangle_j\ .$$

In this expression $\langle t\rangle_j$ corresponds to the impurity mean time in the state j with $j=1$ (active trap state), and $j=2$ (regular site state). The results for the different values of the parameter λ_j ($j=1,2$) are shown in Fig. 2. Figure 2(a) shows the influence of the value of $\lambda_1^{-1}\equiv\langle t\rangle_a$ in the APD, keeping a constant value for λ_2. However, Fig.

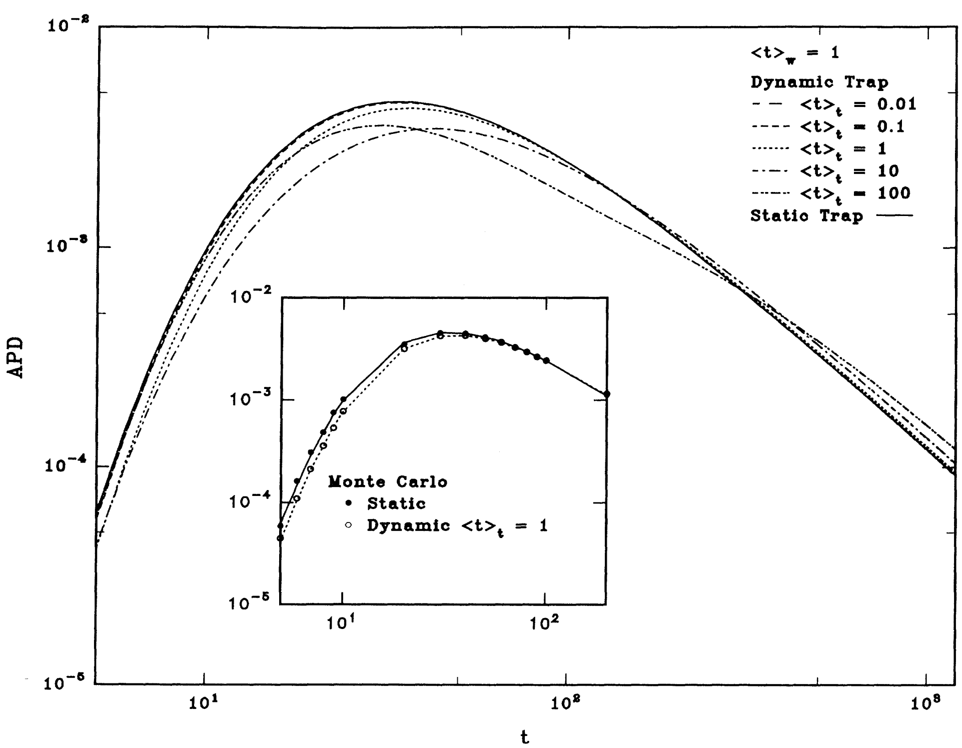

FIG. 1. Absorption probability density vs time for the symmetric Markovian case. In all cases the walker mean waiting time and its initial separation $r=10$ are kept constant. The inset shows a comparison with Monte Carlo simulations.

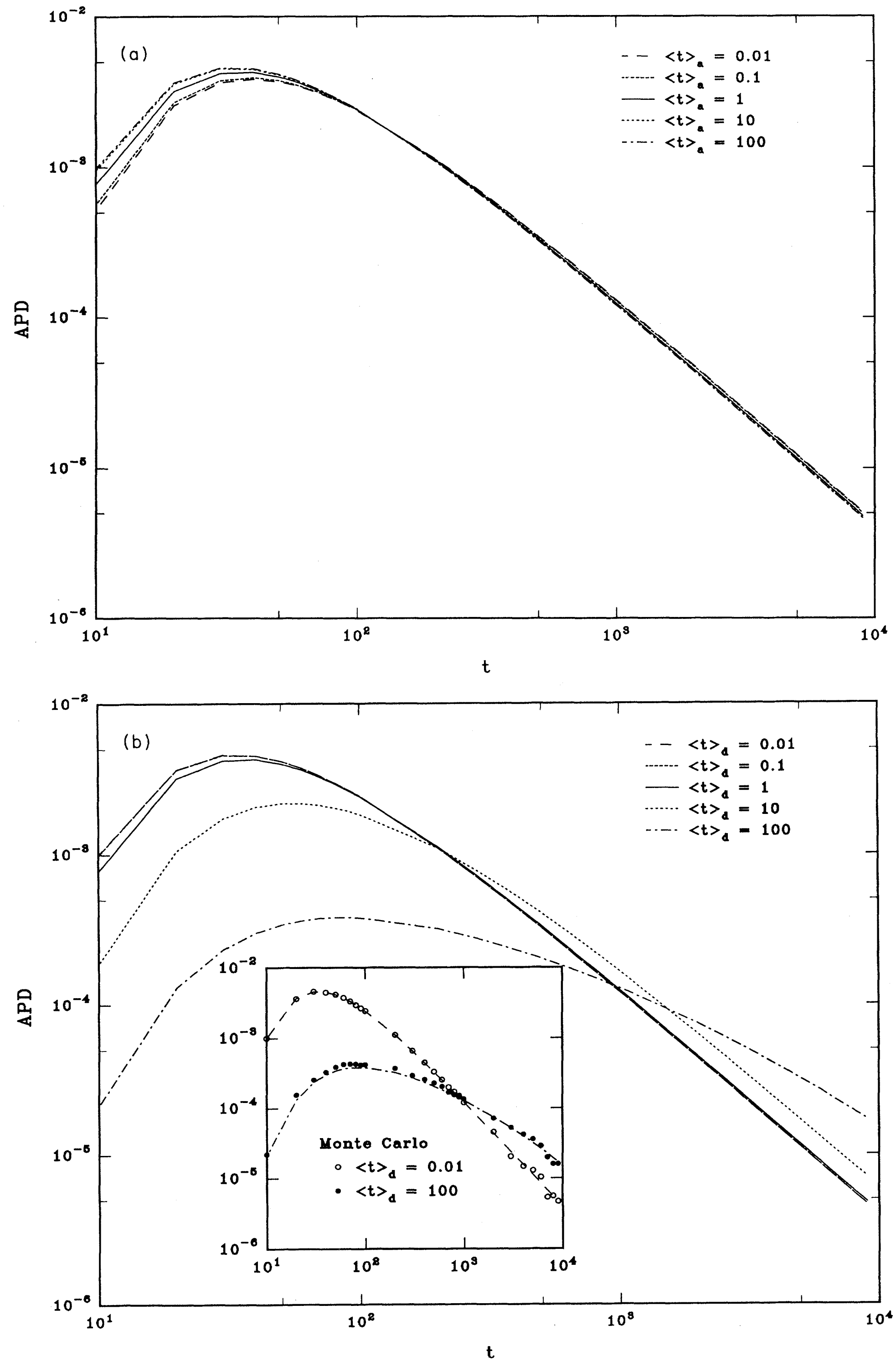

FIG. 2. Absorption probability density vs time for the more general Markovian case, without the symmetric condition (see text). (a) shows the influence in the APD of the variation of the mean active time for the trap, keeping constant $\langle t \rangle_d \equiv \lambda_2^{-1} = 1$. (b) shows the dependence with the variation of the mean inactive time, with $\langle t \rangle_a \equiv \lambda_1^{-1} = 1$. In both cases the initial separation is $r = 10$.

2(b) shows the influence of the value of $\lambda_2^{-1} \equiv \langle t \rangle_d$. In both plots we have included the symmetric case $(\lambda_1 = \lambda_2 = \lambda_w = 1)$ for reference.

The greater influence of the mean inactive time on the APD functions can be appreciated, showing this fact (during the transient) an intuitively expected result, i.e., the peak value of the APD is a decreasing function of the mean inactive time $\langle t \rangle_d$. However, the most probable value (for the RW to be trapped) moves to later times for increasing $\langle t \rangle_d$. What is clearly important about this analysis is the possibility of having analytically the whole transient behavior of the APD for any kind of switching

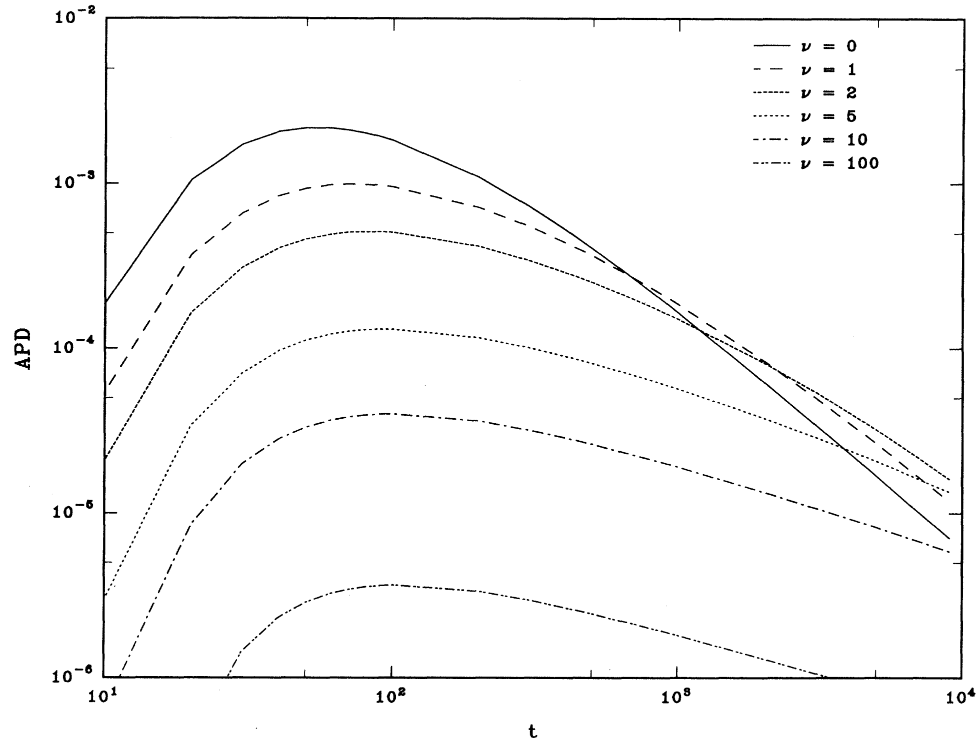

FIG. 3. Absorption probability density vs time for the non-Markovian case presented. The APD dependence with the family parameter ν is shown. All other parameters are kept constant: $\langle t\rangle_a=1$; $\langle t\rangle_d=10$; $r=10$.

time. We have also included an inset in Fig. 2(b) to show the comparison between the analytical results (through numerical Laplace inversion) and Monte Carlo simulations.

(iii) Finally, in Fig. 3, we show the results for a non-Markovian case, with a nonsymmetric switching-time probability density given by the family of functions

$$f_{ij}(t)=\frac{[\lambda_j(\nu+1)]^{\nu+1}}{\Gamma(\nu+1)}t^{\nu}\exp[-\lambda_j(\nu+1)t] \quad \text{with } \lambda_j^{-1}=\langle t\rangle_j$$

and ν the index of the family function. The variation of the APD can be observed with this family parameter. The variation of the λ_j parameters have a similar influence as shown for the Markovian case, so these figures have not been included for this trap dynamic. Note that in the limit $\nu\to\infty$ the deterministic (periodic) case is obtained, i.e., $f_{ij}(t)\to\delta(t-\langle t\rangle_j)$. Thus, if the trap behaves (opens and closes) in a deterministic way, the APD decreases its value at the early stage and the most probable value remains approximately at the same place.

V. ASYMPTOTIC LIMITS

In this section, we consider the behavior of the APD in the limits $t\to 0$ and $t\to\infty$. The calculation may be carried out starting with the exact expression given in (25) (the APD Laplace transform) in the corresponding limits $u\to\infty$ and $u\to 0$, by using a Tauberian theorem [16].

In order to study the long-time limit, we assume that the Laplace transform of the shifted switching-time probability densities can be approximated, for $u\to 0$, by

$$f_{12}\simeq f_{01}+f_{11}u, \quad f_{21}\simeq f_{02}+f_{12}u \; , \tag{28}$$

with the definitions

$$f_{0i}=f_{ij}(\lambda_w) \text{ and } f_{1i}=\frac{df_{ij}}{du}(u=0) \quad i\neq j \; .$$

This approximation is valid for any function $f(u)$ since the shift introduced in the Laplace transform, as indicated in (27), eliminates any possible anomalous behavior in the limit $u\to 0$, inherent in the dynamic of the trap. Substituting the approximations (28) in the general expression (25), and keeping just the first power of u we get

$$R_1(s_1,u)\simeq 1+\vartheta_l u^{1/2} \; , \tag{29}$$

with

$$\vartheta_l=\sqrt{2/\lambda_w}\left\{\frac{f_{02}}{f_{01}}\frac{(1-f_{01})^2}{\sqrt{\xi}}\times\left[\left[\frac{1-f_{01}f_{02}-\sqrt{\xi}}{(1-f_{01})(1-f_{02})}\right]^r-1\right]-r\right\} ,$$

$$\xi=(1-f_{01}f_{02})^2-(1-f_{01})^2(1-f_{02})^2 \; . \tag{30}$$

From Eq. (29) and using a Tauberian theorem [16], we get for the long-time limit of the APD, in one dimension,

$$R_1(s_1,t)\simeq\frac{1}{\sqrt{2\pi\lambda_w}}\vartheta_l t^{-3/2} \; . \tag{31}$$

All the time scales of the system appear in a nontrivial form in this expression, but the asymptotic behavior remains the same whatever the non-Markovian dynamic of the trap is.

The short-time behavior is obtained by taking the limit $u \to \infty$ in (25). Therefore, using an Abelian theorem we get

$$R_1(\mathbf{s}_1,t) \simeq \left[\frac{\lambda_w}{2}\right]^r \frac{1}{\Gamma(r)} t^{r-1} \,. \tag{32}$$

In this expression we have used $t \ll \langle t \rangle_w$ and $t \ll \langle t \rangle_j$, so in this short-time limit the time scale of the absorption is controlled by the time scale of the walker.

VI. CONCLUSIONS

In this paper, we have presented a systematic approach to the problem of diffusion in the presence of a dynamic trap by using a Green matrix technique. In particular, we have worked out the case where the trap has only two internal states (i.e., *active* or *deactive);* therefore, the problem was reduced to solve a 2×2 matrix system. As a particular example we have shown the explicit expression for the APD in a one-dimensional RW in the presence of a trap with arbitrary switching-time probability density. It is important to remark that the long-time behavior of the APD is essentially the same as that of a static trap with a prefactor that depends on the statistics of the trap dynamic. We recall that our analytical approach is very useful for obtaining the transient behavior of the APD. For example, the case where there are several independent RW's can also be treated, within our theory, analytically, in the Laplace domain. The agreement between the theory and Monte Carlo simulations is very good for any kind of dynamic of the trap, as expected.

The figures in this paper show the dependence of the APD with different switching-time probability densities of the trap, including asymmetric and non-Markovian cases. The decreasing of the APD in the peak zone with greater values of $\langle t \rangle_d$ in asymmetric cases is of particular importance. Applications of the present approach to the study of biomembrances and Glarum model with dynamic relaxation rates are in progress and will be reported elsewhere.

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[1] G. H. Weiss, J. Stat. Phys. **42**, 3 (1986).
[2] N. S. Goel and N. Richter-Dyn, in *Stochastic Models in Biology* (Academic, New York, 1974).
[3] E. W. Montroll and B. J. West, in *Fluctuation Phenomena,* edited by E. W. Montroll and J. L. Lebowitz (Elsevier, Amsterdam, 1987).
[4] E. Hernandez-García and M. O. Cáceres, Phys. Rev. A **42**, 4503 (1990).
[5] J. T. Bendler and M. F. Shlesinger, in *The Wonderful World of Stochastics,* edited by M. F. Shlesinger and G. H. Weiss (Elsevier, Amsterdam, 1985).
[6] C. A. Condat, Z. Phys. B **77**, 313 (1989).
[7] A. Szabo, D. Shoup, S. H. Northrup, and J. A. McCammon, J. Chem. Phys. **77**, 4484 (1982).
[8] U. Landman, E. W. Montroll, and M. F. Shlesinger, Phys. Rev. Lett. **38**, 285 (1977).
[9] M. O. Cáceres, Phys. Rev. A **33**, 647 (1986).
[10] C. B. Briozzo, C. E. Budde, O. Osenda, and M. O. Cáceres, J. Stat. Phys. **65**, 167 (1991).
[11] P. A. Alemany, M. O. Cáceres, and C. E. Budde, Phys. Rev. A **38**, 3664 (1988).
[12] C. E. Budde and M. O. Cáceres, Phys. Rev. Lett. **60**, 2712 (1988).
[13] A. J. F. Siegert, Phys. Rev. **81**, 617 (1951).
[14] Van Kampen; in *Stochastic Processes in Physics and Chemistry,* 2nd ed. (North Holland, Amsterdam, 1993).
[15] G. Honig and U. Hirdes, J. Comp. Appl. Math. **10**, 113 (1984).
[16] W. Feller, *An Introduction to Probability Theory and Its Applications* (Wiley, New York, 1966) Vol. 2, p. 424.