Diffusion in Fluctuating Media: The Resonant Activation Problem

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Abstract

We present a one-dimensional model for diffusion in a fluctuating lattice; that is a lattice which can be in two or more states. Transitions between the lattice states are induced by a combination of two processes: one periodic deterministic and the other stochastic. We study the dynamics of a system of particles moving in that medium, and characterize the problem from different points of view: mean first passage time (MFPT), probability of return to a given site ($P_{s0}$), and the total length displacement or number of visited lattice sites ($\Lambda$). We observe a double resonant activation-like phenomenon when we plot the MFPT and $P_{s0}$ as functions of the intensity of the transition rate stochastic component.

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A. Introduction

The problem of diffusion in media submitted to global and/or local fluctuations has strongly attracted the attention of researchers. The main motivation was its interest in the study and analysis of a large variety of processes. To name just a few examples, we consider: random-walks in disordered systems \cite{1,2,3} (ionic conduction in polymeric solid electrolytes \cite{4}); transport of Brownian particles that can be in two or more states executing a diffusion process in each of them but with different diffusion constants \cite{5,6}; resonant activation over fluctuating barriers \cite{7} and escape from fluctuating systems \cite{8,9}; diffusion of ligand with stochastic gating \cite{10,11,12}; dynamical trapping problems \cite{13,14,15,16}. Examples of potential applications are charge transport in molecular scale systems \cite{17} and photochemical reactions \cite{18} among others.

The above indicated phenomena share the property that the switching between the different configurations or states of the medium is independent of the transport or diffusion processes of the walker. Usually, it is assumed that the states are independent of each other and that the particles are subject to a Markovian process inducing their motions within each state, described by Master or Fokker-Planck equations.

In previous studies we have considered on one hand the problem of diffusion in fluctuating media subject to Markovian and/or non Markovian switchings \cite{19}. On the other hand we have studied a stochastic resonance-like phenomenon in a gated trapping system \cite{16}. Motivated by those previous works, we study here the evolution of particles diffusing in a fluctuating medium when the switching mechanism that governs the transition between the states has two components: one deterministic and the other stochastic. The parameters were chosen in such a way that the effect of the deterministic mechanism alone is not enough to produce the switching. However, the simultaneous action of both signals can induce the jump over the potential barrier and produce the switching in the medium. Here, we consider a periodic signal for the deterministic process, while the stochastic component is characterized by a Gaussian white noise of zero mean and intensity $\xi_0$. In this way we expect to capture some basic aspects of the dynamics of more realistic diffusing systems and find situations where the tuning between the stochastic and the deterministic rates can induce some resonant phenomena as in \cite{16}.

In order to study this problem we have analyzed the Mean First Passage Time (MFPT)
in an infinite system. We have also analyzed the probability that the particle returns to the initial position \( P_{s_0} \), characterizing in this way the system’s capacity to restore its initial condition. We also study a measure of the total length displacement or number of distinct visited lattice sites. As it is well known, the MFPT is an extremely important quantity because it gives insight into the reaction processes (trapping, etc) and their dependence on the details of the underlying dynamics of the systems. The MFPT also provides a useful measure of the efficiency of the trapping and has been investigated in a broad range of problems from chemistry to biology [20, 21, 22, 23].

The main goal of this work is the observation of a double resonant activation-like phenomenon when we analyze the MFPT and the \( P_{s_0} \) as functions of the noise intensity of the stochastic component of the transition rate among lattice states.

The organization of the paper is as follows. In the next Section we describe the model in a formal way. After that, we present the results of numerical simulations. In the final Section we discuss the results and draw some conclusions.

**B. The Model**

In order to fix ideas we start considering the problem of a particle performing a random walk on a continuous or discrete fluctuating medium characterized by \( N \) states which are labelled by the index \( j \) (with \( j = 1, 2, \ldots N \)). Following van Kampen [24] we define the probability \( u_j(t) \) that the medium has stayed in the \( j \) state after a time \( t \) since its arrival at \( t = 0 \) as

\[
u_j(t) = \exp \left( - \int_0^t \sum_i \gamma_{ij}(t') dt' \right),
\]

where \( \gamma_{ij}(t) \) is the probability per unit time for the medium to jump from level \( j \) to level \( i \) and \( t \) is the time it has sojourned in \( j \).

The *switching statistics* of the medium \( v_{ij}(t) \); defined as the probability that the medium ends its sojourn in the state \( j \) after a time between \( t \) and \( t + dt \) since it arrived at state \( j \) at \( t = 0 \) by jumping to a given state \( i \); is

\[
v_{ij}(t)dt = u_j(t)\gamma_{ij}(t)dt.
\]

It is worth remarking here that Eq. (2) is completely general and no extra assumption has been made in writing it [24]. As is well known, if the \( v_{ij}(t) \) are exponential functions of time,
that is the \( \gamma_{ij}(t) \) are \( t \)-independent functions (see for instance \[20\]), we have a Markovian switching process between the states of the medium.

In order to simplify the problem, we assume that the system can fluctuate between only two states. The new aspect here is that we have used a combination of noisy and deterministic switching mechanisms to describe the transitions between those states. We assume that \( v_{ij}(t) \) is given by

\[
v_{ij}(t) = \theta[B \sin(\omega t) + \xi - \xi_c],
\]

where \( \theta(x) \) is the step function, and determines when the lattice is in one state or in the other. The dynamics of this mechanism is the following: if the signal, composed of a harmonic part plus the noise contribution \( \xi \), reaches a threshold \( \xi_c \) the lattice changes its state, otherwise it doesn’t. We are interested in the case where \( \xi_c > B \), that is, without noise the deterministic signal is not able to induce a change of the lattice’s state.

Finally, in order to complete the model, we must give the statistical properties of the noise \( \xi \). We assume that \( \xi \) is an uncorrelated Gaussian noise of width \( \xi_0 \), i.e.

\[
\langle \xi(t)\xi(u) \rangle = \delta_{t,u}\xi_0^2.
\]

Note that this is not a standard white noise \[21\] due to the Kronecker symbol (instead of Dirac’s delta \( \delta(t-u) \)). For each fixed state \( j \) of the medium the transport process is Markovian and we denote its corresponding “propagator” \[24\] by \( A_j \). These propagators are differential operators (matrices) in the case of a continuous (discrete) medium and its structure depends strongly on the character of the fluctuations.

In \[19\] we have been able to obtain some analytical results for the MFPT in the case of Markovian and non-Markovian processes that were satisfactorily compared with numerical simulations. However, and due to the complex dynamics of the present case, we were not able to solve this problem analytically and have resorted to MonteCarlo simulations.

The numerical simulations were performed on a one dimensional infinite lattice. The particles were initially located at the lattice site \( s_0 \) in a given state. We assumed that the propagators \( A_j \) were arrays \( W \) describing a discrete one dimensional random walk in each state of the lattice, and also assumed jumps only to first neighbors. The jumps within each state were characterized by two parameters: \( \lambda_j \), the temporal rate of jump and \( \eta_j \), the “bias” to make a jump in a given direction. For the case in which we studied the return to the
origin, the system started its motion at the origin. All simulations shown in the following figures correspond to averages over 100000 realizations.

In the next Section we present several figures where we show the results of our simulations. In the whole study we have used state 1 as the standard state, characterized by the following parameters: \( \lambda_1 = 1 \) and \( \eta_1 = 1 \) (we have chosen the bias to the left side of the lattice), while state 2 is the test state characterized by \( \lambda_2 = 1 \). We have chosen the same temporal rates because we want to focus on the effect of the bias and the noise intensity on the system response. Hence, \( \eta_2 \) together with \( \xi_0 \), are the parameters we varied. In addition, and for all figures, we have adopted the following parameters for the deterministic signal: frequency \( \omega = 1 \), and amplitude \( B = 1 \); while the activation threshold is \( \xi_c = 2 \).

C. MonteCarlo Results

In Fig. 1 we show the results for the MFPT to reach the origin \((s = 0)\) for a particle that started its motion at site \( s_0 = 4 \), as a function of the noise intensity \( \xi_0 \). From this figure, it is apparent that there is an optimal value \( \xi_0 \) for which the MFPT has a minimum (or vice versa, the “activation rate” has a maximum). This behavior, that is a manifestation of the so called resonant activation phenomenon \([7, 8, 9]\), is one of the main results of this work. When \( \xi_0 \) is small, the transition rate is low, and the particle is in an “unfavorable” state, it will remain there for a long time, contributing to a larger MFPT. When \( \xi_0 \) is large, the transition rate will be high, and the particle will not show a net motion, again yielding a large MFPT. But there is an optimal \( \xi_0 \) where the combination between transition rate and motion yields a minimum of the MFPT. It is worth remarking here that this situation occurs when the bias in each state is strong enough but they are in opposite directions, however the phenomenon disappears when the tendencies in both states are similar.

Figure 2 shows the dependence of the MFPT on \( \eta_2 \) for two values of \( \xi_0 \) corresponding to low and high noise intensities. In this figure we can recognize two main aspects. Firstly, the MFPT decreases as \( \eta_2 \) grows, which is a logical result because increasing \( \eta_2 \) means that we have an increasing bias to the origin. Secondly the figure shows an important difference in the MFPT for small \( \eta_2 \), where we see that the noise intensity plays an important role. For small \( \xi_0 \) the transition rate between the states is low and the particle can remain a long time moving to or away from the origin. For large \( \eta_2 \), the differences between the behavior
for different noise intensities disappear. Also, at intermediate $\eta_2$ values, the MFPT remains higher for a smaller noise intensity.

Figure 3 depicts $P_{s_0}$, the probability of return to the origin, as a function of $\eta_2$. The initial condition of the system was at site zero ($s_0 = 0$) in state one, and the simulation time was 10000. For comparison, the case of only one lattice is also shown in this figure. The latter presents a maximum for an intermediate value of $\eta_2$, that is when there is no privileged direction, otherwise the probability decreases as the particle is forced to move away from the origin. For the two state case, we can see that, for small noise intensities, the noise enhances the system response for a fixed (small) value of $\eta_2$. This is due to the possibility of changing from the unfavorable state to the one where the particle has a larger probability of moving.
FIG. 2: MFPT vs $\eta_2$, the bias in state 2. The circles corresponds to the MFPT values for $\xi_0 = 1.0$, and the squares for $\xi_0 = 10.0$.

towards the origin. If we increase the noise intensity, the response is enhanced, that is the return probability becomes larger. However, if we continue increasing the noise intensity finally the response for low $\eta_2$ is reduced and there appears a maximum in the probability indicating that there is an *optimal* value of $\eta_2$. For large $\eta_2$ values, the response becomes smaller for all noise intensities as expected. Here we have another important result of our study, a kind of *double resonant* behavior both in $\xi_0$ and $\eta_2$.

Figure 4 depicts $P_{s0}$ as a function of the noise intensity $\xi_0$, for different values of $\eta_2$. The increase of this probability with increasing $\xi_0$ is apparent, reaching a kind of plateau for $\xi_0 \geq 10$. However, for $\eta_2 = 0.3$, a maximum around $\xi_0 = 10$ is insinuated, resembling a
FIG. 3: \( P_{s_0} \) vs \( \eta_2 \). The circles represent the one-state case, the squares are the data for \( \xi_0 = 5.0 \), the crosses for \( \xi_0 = 10.0 \) and the triangles for \( \xi_0 = 20.0 \).

resonant like phenomenon. The fact that this probability decreases with increasing \( \eta_2 \) is again a logical result because larger \( \eta_2 \) implies an increasing bias to the origin.

Figure 5 shows the total length displacement or number of different lattice sites visited, that we indicate with \( \Lambda \), as a function of the noise intensity \( \xi_0 \), for different values of \( \eta_2 \). For small noise intensity there are no differences among different values of \( \eta_2 \), but for increasing \( \xi_0 \) the number of visited sites is strongly reduced for \( \eta_2 = 0.3, 0.5 \), but remains still high for \( \eta_2 = 0.9 \). This is again consistent with a larger bias to the origin with \( \eta_2 \) larger.

Figures 6, 7 and 8 show the total length displacement or number of visited lattice sites, indicated with \( \Lambda \), as a function of \( \eta_2 \) and for different values of \( \xi_0 \). In all three cases the
FIG. 4: $P_{s_0}$ vs $\xi_0$. The circles represents the data for $\eta_2 = 0.3$, the squares for $\eta_2 = 0.5$ and the crosses for $\eta_2 = 0.9$.

Simulation time was $t = 1000$, and the initial state of the system was the state 1. In Fig. 6 we compare different cases where the noise intensities differ by an order of magnitude. When $\xi_0 \simeq 1$ (more precisely $\xi_0 = 1.5$), the number of visited sites remains almost constant with $\eta_2$. For $\xi_0 = 10$, the curve starts at a small number of sites and increases monotonically, almost linearly, with $\eta_2$. For larger values of $\xi_0$ ($\xi_0 = 100$), the presence of a minimum is apparent. A remarkable fact is that before and after the minimum in $\Lambda$, $\Lambda$ behaves linearly with $\eta_2$. It seems that the high number of visited sites for small $\xi_0$ when $\eta_2$ is also small, reduces with increasing $\xi_0$ before rising again for still larger values of $\xi_0$. This argument was supported by complementary simulations, see for instance Fig. 7 where we have depicted
FIG. 5: $\Lambda_0$ vs $\xi_0$. The simulation time in this and the following figures was $t = 1000$. The circles represent the data for $\eta_2 = 0.3$, the squares for $\eta_2 = 0.5$ and the crosses for $\eta_2 = 0.9$.

the same situation but now for a lattice with only one state, as well as for the two-state lattice and in the range of large noise intensities ($\xi_0 = 20, 30, 100$). The indicated effect is apparent. For the one-state lattice, the minimum is located at $\eta = 0.5$. The reason is that $\eta = 0.5$ corresponds to the situation of unbiased particle motion, that is we have the same probability of moving to the left and to the right of the lattice. This is a point of symmetry in the sense that a larger or smaller $\eta$ implies a biased motion in one direction or the other (changing $\eta$ by $1 - \eta$ only changes the direction of motion but not the number of visited sites).

We can see how the noise changes the position of the minimum in the two-state lattice.
FIG. 6: $\Lambda$ vs $\eta_2$. The crosses represent the data for $\xi_0 = 1.5$, the squares for $\xi_0 = 10.0$ and the circles for $\xi_0 = 100.0$. The decrease in the value for small $\eta_2$ is also shown in Fig. 8 where we have depicted the same situation as before but now for $\xi_0 = 1.5, 3.$ and $5.$ The indicated decrease is clearly seen. From this figure we can see that the indicated minimum disappears for small noise intensities, and the “full” linear dependence of $\Lambda$ on $\eta_2$ in this range.
FIG. 7: $\Lambda$ vs $\eta_2$. The result for a one-state lattice is indicated by circles. The black-squares represents the data for $\xi_0 = 100.0$, the black-triangles for $\xi_0 = 30.0$ and the crosses for $\xi_0 = 20.0$.

D. Conclusions

We have studied here the evolution of particles diffusing in a fluctuating medium when the switching mechanism that governs the transition between the states has two components: one deterministic and the other stochastic. We have chosen a periodic signal for the deterministic part while the stochastic component is characterized by a Gaussian white noise of zero mean. The parameters were chosen in such a way that the effect of the deterministic mechanism alone is not enough to produce the switching, but the simultaneous action of the deterministic and the stochastic signals can induce the jump over the potential barrier and produce the
FIG. 8: Λ vs \( \eta_2 \). The circles represent the data for \( \xi_0 = 1.5 \), the squares for \( \xi_0 = 3.0 \) and the crosses for \( \xi_0 = 5.0 \).

switching. The problem was characterized studying the MFPT in an infinite system, and we have also analyzed the probability that the particle returns to the initial position, and the total length displacement or number of visited lattice sites.

The main goal of this work is the observation (see fig. 11) of a resonant activation-like phenomenon when considering the MFPT as a function of the noise intensity of the stochastic component of the transition rate. Another important result is the kind of double resonant behavior, both in \( \xi_0 \) and \( \eta_2 \), observed in fig. 8.

It is also worth remarking here the behavior of the number of visited lattice sites (\( \Lambda \)) as a function of \( \eta_2 \), with \( \xi_0 \) as a parameter. For the case of the one-state lattice, a minimum
in the number of visited lattice sites exists for $\eta = 0.5$. For the two-state lattice, that minimum changes with the noise intensity. For large values of $\xi_0$, it shifts but is still well marked. However, when $\xi_0$ is reduced the minimum is less marked and finally, for very small values of $\xi_0$, it disappears. This is another example of the “constructive” role that noise can play, in this case associated to diffusion on a lattice with several (here two) states. Another remarkable fact is the “piece-wise” linear dependence of $\Lambda$ on $\eta_2$

According to the discussion above on the motivations of the present work, a natural step in this research of diffusion in a fluctuating medium will be, as in Ref. [16], the inclusion of a gated trap mechanism at the origin. The aim will be to analyze the interplay between both deterministic-plus-stochastic mechanisms, the switching and the gating one, and the coherent or interference effects that could arise. This problem will be the subject of further work.

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[1] J.Sancho and M. San Miguel, J. Stat. Phys. 37, 151 (1984).
[2] M. Rodriguez, L. Pesquera, M. San Miguel and J. Sancho, J. Stat. Phys. 40, 669 (1985).
[3] A.K. Harrison and R. Zwanzig, Phys. Rev. A 32, 1072 (1985).
[4] A. Nitzan and M.A. Ratner, J. Phys. Chem. 98, 1765 (1994).
[5] H.L. Friedman and A. Ben-Naim, J. Chem. Phys. 48, 120 (1968).
[6] G.H. Weiss, J. Stat. Phys. 8, 221 (1973).
[7] C.R. Doering and J.C. Gadoua, Phys. Rev. Lett. 69, 2318 (1992).
[8] A. Bar-Haim and J. Klafter, Phys. Rev. E, 60, 2554 (1999).
[9] N. Eizenberg and J. Klafter, Physica A 249, 424 (1998).
[10] A. J.A. Mc Cammon and S.H. Northrup, Nature 293, 316 (1981).
[11] T. Novotny and P. Chvosta, Phys. Rev. E 63, 012102 (2000).
[12] A. Szabo, D. Shoup, S.H. Northrup and J.A. Mc Cammon, J. Phys. Chem. 77, 4484 (1982).
[13] J.L. Spouge, A. Szabo and G.H. Weis, Phys. Rev. E 54, 2248 (1996).
[14] M.A. Re, C.E. Budde and M.O. Caceres, Phys. Rev. E 54, 4427 (1996).
[15] Wen-Shyan Sheu; J. Chem. Phys. 110, 5469 (1999).
[16] A.D. Sánchez, J.A. Revelli and H.S. Wio, Physics Letters A 277, 304-309 (2000); H.S. Wio, J.A. Revelli and A.D. Sánchez, Physica D 168-169C, 167-172 (2002).
[17] J. Jortner and M. Ratner, Molecular Electronics (IUPAC, 1997).
[18] D. L. Jiang and T. Aida, Nature (London) 388, 454 (1997); D. M. Jounge and D. V. McGrath, Chem. Common. (Cambridge), 857 (1997).
[19] J.A Revelli, C.E. Budde and H.S Wio, Phys. Lett. A 306, 104-109 (2002).
[20] G. H. Weiss, Adv. Chem. Phys 13, 1 (1966); G.H. Weiss, in Aspects and Applications of the Random Walk, (North Holland, Amsterdam, 1994) and references therein.
[21] N.G. Van Kampen, Stochastic Processes in Physics and Chemistry (North Holland, Amsterdam, 1981).
[22] J. Procaccia, S. Mukamel, and J. Ross Chem Phys. 68, 3244 (1978).
[23] V. Seshadri, B. J. West and K. Lindenberg, J. Chem. Phys. 72, 1145 (1980).
[24] N.G. van Kampen,Physica A 96, 435 (1979).