EXACT RESULTS FOR THE TRANSMISSION PROBABILITIES IN LINEAR ARRAY OF FLUCTUATING BARRIERS

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The diffusion of a particle in a linear array of N fluctuating barriers was investigated. The barriers are characterized by two parameters: α_0 - the probability to be closed, and λ - frequency of fluctuations between closed and open state. The rigorous analytical results for limit cases $\lambda = 0$, $\alpha_0 = 0$ and $\lambda = 0$, $\alpha_0 = 1$ were obtained. The phenomenon of stochastic resonance in the case of a particle moving with velocity $\pm v$ and the process of switching between opposite velocities being a random telegraph process was investigated by numerical simulations.

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1. Introduction

Diffusion in disordered media has been the subject of many works (see, *e.g.*, the reviews [1, 2]). In general, the disorder of the medium in which a particle is moving is supposed to be quenched, and so, is completely static. This is a very good approximation in normal physical situations, in particular in electronic conduction (from which the point model, Lorentz model, is issued) and in any case where the time scale of the motion of the particle is much faster than the time scale of the fluctuation of the external disorder. The opposite case, namely the case where the time scale of the fluctuation of the external disorder is much faster than the time scale of the motion of the particle, leads to the representation of diffusion by Markov processes (like Brownian motion) and has been extensively studied. On the other hand, there are also many situations where the time scales are of the same order of magnitude and the conditions of both approximations break down. This is the case, in particular, for diffusional approach of two nearby reactants in dense solvents. In this case, the potential created by the solvent is fluctuating in time. In [3, 4] we introduced a model potential fluctuating in time under the form of barriers either open or closed and in [5, 6] we proved stochastic resonance phenomena in the case of two barriers. Stochastic resonance has also been studied by [7, 8] for more realistic fluctuating potentials using a standard diffusion dynamics, but our results do not depend on the details of the dynamics.

In this work, we extend our methods and results to the case of the diffusion of a particle in a linear array of N fluctuating barriers. The barrier is characterized by two numbers: the probability α_0 to find it closed and the frequency λ of fluctuations between the closed state and the open state. In [3] we already studied the limit case of $\lambda = +\infty$ and found the correction to the markovian approximation. Here, we obtain rigorous analytical results for the following limit cases: $\lambda = 0, \alpha_0 = 0$ and $\alpha_0 = 1$. In each of these cases, we give exact formulas which have the structure of the law of addition of inverses, although the hypotheses to obtain this law are absolutely not fulfilled.

Detailed proofs are rather complicated and will be given elsewhere.

2. Diffusion in a linear array of fluctuating barriers

We consider an interval of length N (N is an integer). In each interval, $[j, j+1]$, one has a certain stochastic process which is characterized by the following quantities:

1. $s_j(t)dt$ is the probability that the particle entering the interval $[j, j+1]$ at point j and at time 0, leaves the interval through point $j+1$ for the first time between t and $t+dt$
2. $r_j(t)dt$ is the probability that the particle entering the interval $[j, j+1]$ at point j at time 0 leaves the interval through j for the first time between t and $t+dt$.

We assume that the stochastic process is symmetric with respect to the exchange of j and $j+1$.

Moreover, at each point j we place a barrier which can be in state $\varepsilon_j = 0$ (open barrier) or 1 (closed barrier). The state of the barrier fluctuates in time according to a dichotomous Markov process, so that the conditional probability for finding the barrier in state ε at time t, knowing that it is in state ε' at time 0 is given by

$$\varphi_{\varepsilon,\varepsilon'}(t) = \alpha_\varepsilon + (\delta_{\varepsilon,\varepsilon'} - \alpha_\varepsilon)e^{-\lambda t}\,,$$

α_0 (resp. α_1) are the stationary probabilities to find the barrier in state $\varepsilon = 0$ (resp. in state $\varepsilon = 1$) (Fig. 1).

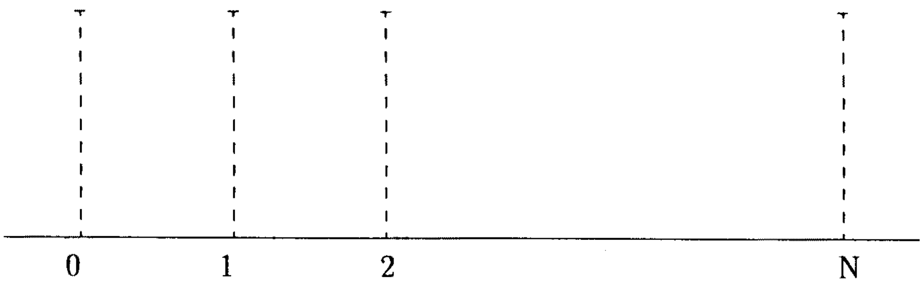

Fig. 1. Linear array of fluctuating barriers.

Finally, each barrier fluctuates independently.

A particle moves in the array in the following way: in the interval $[j, j+1]$ it follows the corresponding stochastic motion. If the particle reaches an extremity of the interval, for instance j, and if at that time the barrier at j is open ($\varepsilon_j = 0$), the particle enters $[j-1, j]$ through j and begins an independent stochastic motion in $[j-1, j]$ starting from j. If the particle finds the barrier at j closed ($\varepsilon_j = 1$), it stays in the interval $[j, j+1]$ and starts again a motion in $[j, j+1]$ at point j.

The fluctuations of the barriers are independent of the stochastic motion of the particle in each interval.

We are interested in the probability $S_{[0,N]}$ that the particle, entering the interval $[0, N]$ at point 0 at time 0 leaves the interval at point N. We cannot, in general, obtain exact expressions for this quantity, but we shall study its asymptotic for large N and various limiting situations $\lambda = 0$ or $+\infty$, $\alpha_0 = 0$ or 1.

3. The two-barrier case

First of all we consider the case $N = 1$ where we can obtain exact analytical results. In this section we denote $S(t; a, \{\varepsilon\} \mid a', \{\varepsilon'\})dt$ the conditional probability that the particle leaves the interval [0,1] at point a for the first time between t and $t + dt$, the states of the two barriers at that time being $\{\varepsilon\}$, knowing that it starts at time 0 from point a', the states of the barriers at time 0 being $\{\varepsilon'\}$ (here a and a' can be 0 or 1). Note that $\varepsilon_a = 0$ necessarily, because the barriers at the point a must be open to let the particle out. We introduce the Laplace transform

$$\hat{S}(\theta; a, \{\varepsilon\} \mid a', \{\varepsilon'\}) = \int_0^\infty e^{-\theta t} S(t; a, \{\varepsilon\} \mid a', \{\varepsilon'\}) dt \,,$$

and note $S(a, \{\varepsilon\} \mid a', \{\varepsilon'\})$ the value at $\theta = 0$. We also note

$$\hat{S}(\theta; a \mid a', \{\varepsilon'\}) = \sum_{\{\varepsilon\}} \hat{S}(\theta; a, \{\varepsilon\} \mid a', \{\varepsilon'\}) \,.$$

We have already studied this case in [5, 6] and pointed out that a resonance phenomenon can occur for appropriate values of parameters. We shall denote

$$\hat{r}(\theta) = \int_0^\infty e^{-\theta t} r(t) dt \,,$$

$$\hat{s}(\theta) = \int_0^\infty e^{-\theta t} s(t) dt \,,$$

$$R = \hat{r}(0) \qquad S = \hat{s}(0) \qquad R + S = 1 \,.$$

Here we shall mainly give asymptotic results

1. Asymptotic results for α_0 tending to 0

1.1. $\theta > 0$

In this case

$$\hat{S}(\theta; a \mid 0, \{\varepsilon'\}) = 0 \quad \text{if} \quad \varepsilon'_a = 1$$

thus the probability of leaving $[0, 1]$ by a if at time 0 the barrier at a is closed, is 0 at any finite time scale, which is quite natural since this barrier has 0 probability to open in a finite time if $\alpha_0 \to 0$.

On the other hand the other $\hat{S}(\theta; a \mid 0, \{\varepsilon'\})$ are not 0 in general: when $\alpha_0 \to 0$ we obtain for instance

$$\hat{S}(\theta; 1 \mid 0; \varepsilon'_0 = 0, \varepsilon'_1 = 1) = \hat{r}(\lambda + \theta) + \frac{\hat{s}(\lambda + \theta)^2}{1 - \hat{r}(\lambda + \theta)} \,,$$

$$\hat{S}(\theta; 1 \mid 0; \varepsilon'_0 = 0, \varepsilon'_1 = 0) = \hat{s}(\lambda + \theta) + \frac{(\hat{r}(\lambda + \theta) - \hat{r}(2\lambda + \theta))\hat{s}(\lambda + \theta)}{1 - \hat{r}(\lambda + \theta)} \,.$$

1.2. $\theta = 0$

In this case we obtain

$$S(0 \mid 0; \varepsilon_0' = 1, \varepsilon_1' = 1) = S(1 \mid 0; \varepsilon_0' = 1, \varepsilon_1' = 1) = \tfrac{1}{2}$$

whereas the corresponding $\hat{S}$ vanish if $\theta > 0$ or if $\alpha_0 = 0$. This apparently surprising result means that in an infinite time interval the particle finds its way out of $[0, 1]$ with probability 1, provided that the probability α_0 to find always the barrier open is not exactly 0.

Furthermore, we have for instance

$$S(1 \mid 0; \varepsilon_0' = 1, \varepsilon_1' = 0) = \frac{1}{2} + \frac{1}{2}\frac{\hat{s}(\lambda)}{1 - \hat{r}(\lambda)},$$

$$S(1 \mid 0; \varepsilon_0' = 0, \varepsilon_1' = 1) = \frac{1}{2}\left[1 - \hat{r}(\lambda) - \frac{2\hat{s}(\lambda)^2}{1 - \hat{r}(\lambda)} + \frac{S\hat{s}(\lambda)}{1 - \hat{r}(\lambda)}\right].$$

2. Asymptotic results for λ tending to 0. In this limit, the barriers are frozen.

2.1. $\theta > 0$

Again $\hat{S}(\theta; a \mid a'; \{\varepsilon'\}) = 0$ if $\varepsilon_a' = 1$; furthermore

$$S(\theta; 1 \mid 0; \varepsilon_0' = 1, \varepsilon_1' = 0) = \frac{\hat{s}(\theta)}{1 - \hat{r}(\theta)}.$$

2.2. $\theta = 0$

We obtain

$$S(1 \mid 0; \varepsilon_0' = 1, \varepsilon_1' = 0) = 1,$$
$$S(1 \mid 1; \varepsilon_0' = 1, \varepsilon_1' = 1) = \tfrac{1}{2},$$
$$S(1 \mid 0; \varepsilon_0' = 0, \varepsilon_1' = 1) = 0,$$
$$S(1 \mid 0; \varepsilon_0' = 0, \varepsilon_1' = 0) = S.$$

All these results can be easily understood, since in this limit the barriers never change their state. However, the second result can be commented as in Section 1.2: if both barriers are closed initially, although they have a very low probability to change their states in a finite time, in an infinite time interval the particle finds its way out with probability 1 provided λ is not exactly 0.

4. Asymptotic results for α_0 tending to 0 and large N

We shall denote $S(j+1 \mid j; \varepsilon_j = 0, \varepsilon_{j+1} = 1)$ the probability in the two-barrier system on the interval $[j, j+1]$ to leave the interval through $j+1$, knowing that the particle enters the interval at point j at time 0, the states of the barriers being $\varepsilon_j = 0, \varepsilon_{j+1} = 1$. In the limit $\alpha_0 \to 0$ we have from the previous section

$$S(j+1 \mid j; \varepsilon_j = 0, \varepsilon_{j+1} = 1) = \frac{1}{2}\left[1 - \hat{r}_j(\lambda) - \frac{2\hat{s}_j(\lambda)^2}{1-\hat{r}_j(\lambda)} + \frac{S_j \hat{s}_j(\lambda)}{1-\hat{r}_j(\lambda)}\right].$$

Then we have the addition formula, still in the limit $\alpha_0 = 0$

$$\frac{1}{S_{[0,N]}} - 1 = \sum_{j=0}^{N-1}\left(\frac{1}{S(j+1 \mid j; \varepsilon_j = 0, \varepsilon_{j+1} = 1)} - 1\right)$$

Here $S_{[0,N]}$ is the total transmission probability for the particle to leave interval $[0, N]$ through N, knowing that it starts from 0 at time 0, the barrier being in state $\varepsilon'_0 = 0$, and all the other barriers at point $j \geq 1$ being in state $\varepsilon'_j = 1$ (namely they are in equilibrium in the limit $\alpha_0 = 0$).

At first sight, this result may seem surprising, because the system is highly non markovian and the inverse addition law holds essentially in markovian case. On the other hand, the motion of the particle can be viewed as follows. Suppose the particle enters the interval $[j, j+1]$ for the first time at j. This means that $\varepsilon_j = 0$ at that instant, due to some fluctuation (although most of the time barriers are closed, but if one waits a sufficiently long time they finally open). Then the particle is trapped between $[j-1, j+1]$, but the barrier at j will close before one of the barriers at $j-1$ or $j+1$ will open and so the particle is finally trapped either in $[j-1, j]$ (as it was before it entered $[j, j+1]$ or in $[j, j+1]$. So, in a sense, and at least for the quantity $S_{[0,n]}$, everything will be equivalent to a particle moving in a linear array, such that the effective transmission probability between j and $j+1$ is $S(j+1 \mid j; \varepsilon_j = 0, \varepsilon_{j+1} = 1)$. The rigorous proof will be given elsewhere.

We can, nevertheless, remark that one cannot use perturbation theory by running only on a finite number of paths. We have really to sum over the full set of paths and we can never truncate this set of paths. In fact, to any finite order perturbation theory, the transmission probability vanishes. The non vanishing result we obtain here is due to the fact that we resum an infinite number of trajectories. To see the mathematical phenomenon which appears here it is useful to consider the two-barriers case, together with the ballistic motion of the particle between the barriers (see Fig. 1).

In this case, the particle enters the interval $[0,1]$ at 0. If it finds the barrier open at 1, it gets out. But it can make also a finite number of ballistic motions between 0 and 1, finding each time the barriers closed, and finally finding the barrier at 1 open. The probability to make $2n+1$ such ballistic motions and finally leave $[0,1]$ at 1 is

$$P_n = \alpha_1 \varphi_{10}(2\tau)(\varphi_{11}(2\tau)^{n-1}\varphi_{01}(2\tau)\,,$$

where τ is the transition time between 0 and 1 in the ballistic motion and P_0 is just α_0.

So

$$\sum_{n=0}^{\infty} P_n = \alpha_0 + \alpha_1 \frac{\varphi_{10}(2\tau)\varphi_{01}(2\tau)}{1-\varphi_{01}(2\tau)}$$

$$= \alpha_0 + \alpha_1\varphi_{10}(2\tau) \sim 1 - \mathrm{e}^{-2\lambda\tau} \text{ for } \alpha_0 \sim 0\,.$$

But if we only take the first n terms of this perturbation expansion they are all 0 when α_0 is 0. The cancellation is due to the summation of the entire geometric series. Notice that in this case the average exit time by 1 will be infinite when α_0 tends to 0.

On the other hand, for α_0 near zero and λ tending to 0, the average time of exit will stay finite, but the mean square of this time will diverge.

5. Asymptotic results for λ tending to 0

In this case we denote $S(j+1 \mid j)$ the transmission probability in the process on $[j, j+1]$ without barriers

$$S(j+1 \mid j) = \int_0^{\infty} s_j(t)dt\,.$$

Then, if the barriers are at equilibrium, except the one at 0 which is open,

$$S_{[0,N]} = \alpha_0^N S_{[0,N]}(\{0\}_{k\geq 0})\,,$$

where $S_{[0,N]}(\{0\}_{k\geq 0})$ is the transmission probability knowing that all barriers are open at time 0. Moreover we have an addition formula

$$\frac{1}{S_{[0,N]}(\{0\}_{k\geq 0})} - 1 = \sum_{j=0}^{N-1}\left(\frac{1}{S(j+1 \mid j)} - 1\right)\,.$$

In this case also, the addition law holds, except for the factor α_0^N which is exponentially decreasing, although in the limit $\lambda = 0$ the system becomes completely non markovian.

Remark: in the limit $\lambda = \infty$ the system is really markovian, the particle seeing an independent environment at each time step.

6. Asymptotic results for $\alpha_0 = 1$ and resonance

In this case it is obvious that $S_{[0,N]}\,|_{\alpha_1=0}$ is the transmission probability from 0 to N in absence of any barrier and is given by a usual inverse addition law and there is nothing surprising about that. What is more interesting is that one can compute explicitly the first correction in α_1. We again denote $S_{[0,N]}$ the total transmission probability from o to N, the barrier at 0 being open, and all other barriers being at equilibrium. A detailed computation proves that

$$\left.\frac{\partial S_{[0,N]}}{\partial \alpha_1}\right|_{\alpha_1=0,\lambda=0} < 0$$

$$\left.\frac{\partial S_{[0,N]}}{\partial \alpha_1}\right|_{\alpha_1=0,\lambda=\infty} = S_{[0,N]}\Big|_{\alpha_1=0}\left(1 - (N+1)S_{[0,N]}\Big|_{\alpha_1=0}\right),$$

and in particular it is positive provided that

$$S_{[0,N]}\,|_{\alpha_1=0} < \frac{1}{N+1}\,.$$

In particular, in this case, there must be a certain value $\lambda^*(\alpha_1)$ of λ such that $S_{[0,N]}$ will be an increasing function of α_1 for α_1 sufficiently small and $\lambda > \lambda^*(\alpha_1)$. In other words, there will be a certain range Λ of λ such that when λ is in this range, $S_{[0,N]}$ has a maximum at a non trivial value of α_1.

This is a stochastic resonance phenomenon, whereby one finds a maximum of the transmission probability $S_{[0,N]}$ with respect to α_1, for a non zero value of α_1 (at least in certain frequency range).

We investigated the above phenomenon by numerical simulations. We took a particle moving with velocity $\pm v$, the process of switching between opposite velocities was a random telegraph process (RTP) with frequency σ. Such a process was already used by some of the present authors [9] in the study of absorption dynamics. If the particle is moving in the 1-dimensional array of independent barriers fluctuating with relaxation frequency λ, then for suitably chosen values of λ and σ a maximum in the dependence of S on α_1 is observed (Fig. 2).

This extends the case $N = 1$ (two barriers case) which was treated exactly in [5, 6].

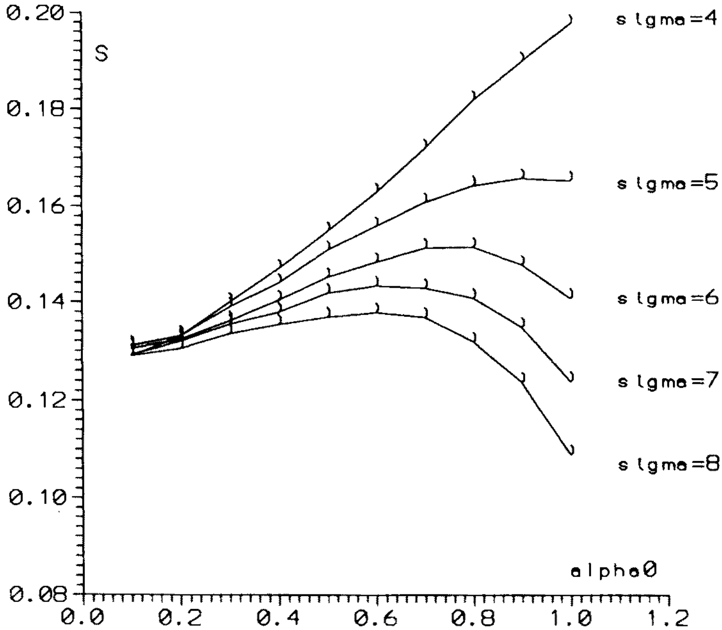

Fig. 2. The dependence of S on α_0 for different values of σ.

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