STOCHASTIC MOTION OF A PARTICLE IN A MODEL FLUCTUATING MEDIUM*

M. Moreau[a], B. Gaveau[b], M. Frankowicz[c]

and A. Perera[a]

[a]Laboratoire de Physique Thórique des Liquides
Université P. et M. Curie, Boîte 121, 75252 Paris, France†

[b]U.F.R. de Mathématiques, Université P. et M. Curie, Paris, France

[c]Faculty of Chemistry, Jagellonian University
Ingardena 3, 30-060 Kraków, Poland

(Received February 22, 1993)

We present several models of time fluctuating media with finite memory, consisting in one and two-dimensional lattices, the nodes of which fluctuate between two internal states according to a Poisson process. A particle moves on the lattice, the diffusion by the nodes depending on their internal state. Such models can be used for the microscopic theory of reaction constants in a dense phase, or for the study of diffusion or reactivity in a complex medium. In a number of cases, the transmission probability of the medium is computed exactly; it is shown that stochastic resonances can occur, an optimal transmission being obtained for a convenient choice of parameters. In more general situations, approximate solutions are given in the case of short and moderate memory of the obstacles. The diffusion in an infinite two-dimensional lattice is studied, and the memory is shown to affect the distribution of the particles rather than the diffusion law.

PACS numbers: 02.50. Ey

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* Presented at the V Symposium on Statistical Physics, Zakopane, Poland, September 21–30, 1992.

† équipe associée au CNRS–URA 765

1. Introduction

The motion of a particle in a disordered medium has attracted considerable interest during the recent years [1–3], due to the importance of this problem in many fields of science such as the transport properties of porous media, membranes or biological materials, the transmission of energy or excitations in amorphous solids and imperfect crystals, or the transmission of a signal in a perturbed system. Similar questions also arise, for instance, in the theory of chemical reactivity, either for the macroscopic study of reaction kinetics in a complex medium [4–7] or for the microscopic calculation of rate constants in a dense phase [8, 9].

This problem is not only of great practical importance, but it is also very interesting from the theoretical point of view; it has been shown in a variety of cases that the fluctuations of the medium can play a predominant role and lead to anomalous kinetic laws, differing completely from the behaviour which can be expected from average properties or mean field theories [10]. However, if much work has been done on frozen disorder, where only space correlations are taken into account, time fluctuations have not been as well studied, although they obviously occur in many circumstances [11–14]. This is for instance the case in the calculation of rate constants in a liquid phase: the environment is always changing and the effective reaction potential, implying the interactions of all neighbouring molecules with the reacting complex, is strongly time-dependent; thus the time-averaged potential does not represent the effect of the instantaneous potential correctly, excepted in particular circumstances.

Our purpose is to model a time-dependent medium where the fluctuations of the medium are spatially uncorrelated but have a finite correlation time, so that it is needed to keep the past trajectories of a particle in memory in order to describe its motion. The medium will be represented by one- and two-dimensional lattices with time-dependent nodes, which permits to obtain a number of analytical results; on the other hand the models allow numerical simulations of the problem with a reasonable computer time, in spite of the finite memory of the medium.

We will first present one-dimensional models, which can be useful in the theory of reaction rates or in signal theory; in particular, it will be shown that the coupling of the fluctuations of the medium with an arbitrary random process can lead to examples of stochastic resonance.

Two-dimensional models will then be studied, mainly as models of diffusion of a particle in a fluctuating environment. It will be shown that the normal diffusion laws are modified by the memory of the medium, although less strongly than observed for a spatially correlated medium.

2. One-dimensional model: succession of fluctuating barriers

2.1. Introduction

In this section we study the evolution of a one-dimensional system, or 'particle', evolving according to a given stochastic process perturbed by fluctuating obstacles. The unperturbed stochastic process can be rather general and even non-Markovian, in a sense that will be precised later, but its laws are supposed to be completely known; on the contrary the obstacles are modelled in the simplest way by dichotonous barriers that, nevertheless, have a finite memory, the problem being to compute the overall laws of evolution of the particle. It is first necessary to give some definitions concerning the underlying stochastic process, which we call 'reactive process', since it can be used to describe the kinetics of a chemical reaction or, more generally, of many rate processes.

2.2. Model reactive process

We consider the stochastic motion of a particle, modeling for instance a chemical reaction leading from a stable chemical species A (the reactant) to another stable chemical species B (the product). The position of the particle is determined by the coordinate x. We assume that the laws of motion are known. In particular, if the particle moves between two points a, b we can calculate the conditional probability of leaving the interval $[a, b]$ for the first time by the extremity b (resp. a) between times t and $t + dt$ knowing that the particle starts at time 0 with velocity v from $x \in [a, b]$. We will denote these probabilities as $p(B, t|x, v)dt$ (resp. $p(A, t|x, v)dt$).

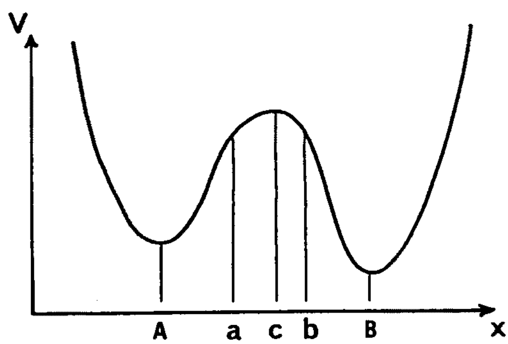

Fig. 1. Model bistable potential $V(x)$: **A**, **B**: bounded states; (a,b): potential barrier; c: top of the barrier.

Such probabilities [15] are especially useful in the theory of chemical reaction rates. If x is the reaction coordinate, the bound states A_0 and B_0 of the stable chemical species correspond to two minima of the interaction potential $V(x)$, whereas (a,b) denotes the top of the potential barrier (see Fig. 1). The reactant region $A = \{x : x < a\}$ and the product region $B = \{x : x > b\}$ are the regions where the chemical species A and B can be identified. According to the definitions based on correlation functions, used for instance by Chandler [16] and Hynes *et al.* [17], the rate constant k_{AB} of the reaction A $\longrightarrow$ B can be written [9]

$$k_{\mathrm{AB}} = \frac{1}{q_{\mathrm{A}}} \int_0^\infty dt \int dv p(B,t|x,v) v p(x,v)\,, \tag{1}$$

where $p(x,v)$ is the equilibrium probability density at (x,v) and q_{A} is the equilibrium probability of the reactant region A. $J(x,v) \equiv vp(x,v)$ is the equilibrium probability current at (x,v). x is an arbitrary point belonging to (a,b) (k_{AB} is independent of x [9]). More general definitions of J and k_{AB} can be given [18], but for the sake of simplicity we will not apply them here.

Let us assume that there are only two possible velocities $\pm v$; this assumption still leads to qualitatively reasonable models [9]. Then we get

$$k_{\mathrm{AB}} = \frac{vp(a,v)}{q_{\mathrm{A}}} \int_0^\infty dt p(B,t \mid a,v) \tag{2}$$

$$= \frac{vp(a,v)}{q_{\mathrm{A}}} \int_0^\infty dt[p(B,t \mid x,v) - p(B,t \mid x,-v)]\,. \tag{2'}$$

Here $J_x = |v|p(x,v) = |v|p(x)/2$ is the one-way equilibrium current at x.

2.3. *Fluctuating barriers*

We now assume that dichotomous fluctuating barriers of zero width are inserted at different points $x_1, x_2, \ldots, x_n$ of the interval $[a,b]$. All barriers are independent and obey the same law. Each barrier can be in two states: 0 (open) and 1 (closed). The waiting time in state i ($i = 0$ or 1) is exponential

$$P(t_i > t) = e^{-\lambda_i t}\,, \tag{3}$$

λ_0 and λ_1 are positive numbers [13].

The probability to find a barrier in state i knowing that it was in state j at time t is

$$\varphi_{ji}(t) = \alpha_j + (\delta_{ji} - \alpha_i)e^{-\lambda t}, \tag{4}$$

where δ_{ji} is the Kronecker symbol and

$$\lambda = \lambda_0 + \lambda_1, \tag{5}$$

$$\alpha_0 = \lambda_1/\lambda, \quad \alpha_1 = \lambda_0/\lambda, \tag{6}$$

$\{\alpha_i\}$ is the stationary probability distribution of the states of the barrier.

If the particle reaches the barrier when it is open (state 0), it crosses the barrier instantaneously without changing its velocity; if the barrier is closed (state 1), the particle is instantaneously reflected and its velocity is reversed.

In order to compute the effect of the barriers on the overall process, we assume that as soon as the particle crosses a barrier or is reflected, *loses all memory of past events*, and that its future motion does not depend on the previous value of velocity. The last condition is satisfied if, for instance, the velocity is randomized each time the particle touches the barrier, or if the particle can have only two velocities ($\pm v$); we will adopt the last hypothesis in the following sections.

2.4. Effect of one fluctuating barrier

We assume that a fluctuating barrier of the previous kind is inserted in some point c of the potential barrier $[a, b]$ separating the potential wells A and B corresponding to the stable chemical species. This barrier can crudely model the influence of a solvent molecule hindering the reaction; in the case of signal transmission, it can represent a fluctuating inhomogeneity or defect reflecting the signal [13]. The characteristic frequency of the passage from A to B is given by the rate constant k_{AB} (2) or (2').

In order to calculate k_{AB} for the overall process we introduce the following auxiliary conditional probability densities, defined supposing that c *is an absorbing point* (which of course can be reached only when the barrier is *open*

$\underline{s}_i(B, t \mid c, +)$ is the probability density to be absorbed in B at time t, starting at $t = 0$ just on the right of c with velocity $+v$ and the barrier in state i;

$\underline{r}_{0i}(c, +, t \mid c, -)$ is defined in the same way for the particle starting just on the left of c with velocity $-v$.

These auxiliary densities can be expressed in terms of quantities s and r defined analogously but *in the absence of the fluctuating barrier*; s and r depend only on the *unperturbed stochastic process* on the intervals $[a, c]$ and $[c, b]$ and are supposed to be known.

We assume that at $t = 0$ the stationary probability to find the barrier in the state i has the value α_i given by (6). Using definition (4) of the transition probabilities $\varphi_{ji}(t)$ of the barrier one can write

$$\underline{s}_i(B,t \mid c,+) = s(B,t \mid c,+) + \int_0^t dt' \underline{s}_1(c,t-t' \mid c,-)\varphi_{1i}(t) r(c,-,t \mid c,+), \tag{7a}$$

$$\underline{r}_{0i}(c,-\varepsilon,t \mid c,\varepsilon) = \varphi_{0i}(t) r(c,-\varepsilon,t \mid c,\varepsilon) + \int_0^t dt' \underline{r}_{01}(c,-\varepsilon,t-t' \mid c,\varepsilon)\varphi_{1i}(t) r(c,-\varepsilon,t \mid c,+\varepsilon), \tag{7b}$$

where $\varepsilon = \pm$; $-\varepsilon$ is the sign opposite to ε.

Introducing the Laplace transform of a function f(t)

$$\hat{f}(u) = \int_0^\infty dt e^{-ut} f(t)$$

and defining

$$\hat{r}_{ji}(c,-\varepsilon,u \mid c,\varepsilon) = \int_0^\infty \varphi_{ji}(t) r(c,-\varepsilon,t \mid c,\varepsilon) = \alpha_j \hat{r}(u) + (\delta_{ji} - \alpha_j)\hat{r}(u+\lambda), \tag{8}$$

we get from (7)

$$\hat{\underline{s}}_1(B,u \mid c,+) = \frac{\hat{s}(B,u \mid c,+)}{1 - \hat{r}_{11}(c,-,u \mid c,+)}, \tag{9a}$$

$$\hat{\underline{s}}_0(B,u \mid c,+) = \hat{s}(B,u \mid c,+) + \hat{\underline{s}}_1(B,u \mid c,+)\hat{r}_{10}(c,-,u \mid c,+), \tag{9b}$$

$$\hat{\underline{r}}_{01}(c,\varepsilon,u \mid c,-\varepsilon) = \frac{\hat{r}_{01}(c,\varepsilon,u \mid c,-\varepsilon)}{1 - \hat{r}_{11}(c,\varepsilon,u \mid c,-\varepsilon)}, \tag{9c}$$

$$\hat{\underline{r}}_{00}(c,\varepsilon,u \mid c,-\varepsilon) = \hat{r}_{00}(c,\varepsilon,u \mid c,-\varepsilon) + \hat{\underline{r}}_{01}(c,\varepsilon,u \mid c,-\varepsilon)\hat{r}_{10}(c,\varepsilon,u \mid c,-\varepsilon). \tag{9d}$$

If $u \to 0$, we get from (9)

$$\underline{S}_i \equiv \hat{\underline{s}}_i(0) = \int_0^\infty dt \underline{s}_i(t), \quad \underline{R}_{ji} \equiv \hat{r}_{ji}(0), \tag{10}$$

in terms of $S = \hat{s}(0)$ and $R_{ji} = \hat{r}_{ji}(0)$. In particular,

$$\underline{S}_1 = \frac{S}{\alpha_0(1-\hat{r}(\lambda)) + \alpha_1 S},$$
$$\underline{S}_0 = \frac{S(1-\hat{r}(\lambda))}{\alpha_0(1-\hat{r}(\lambda)) + \alpha_1 S}. \tag{11}$$

Using densities $\underline{s}$ and $\underline{r}$ we can calculate the conditional probability densities of absorption in B at time t starting at $t = 0$ from c with velocity εv and the barrier being in state 0, $p_0(B, t \mid c, \varepsilon)$. We have

$$p_0(B,t \mid c,+) = \underline{s}_0(B,t \mid c,+) + \int_0^t dt' p_0(B,t-t' \mid c,-)\underline{r}_{00}(c,-,t' \mid c,+), \tag{12a}$$

$$p_0(B,t \mid c,-) = \int_0^t dt' p_0(B,t-t' \mid c,+)\underline{r}_{00}(c,+,t' \mid c,-). \tag{12b}$$

These equations can be solved by Laplace transforms. We get the total probability to be absorbed in B starting from c with velocity $\pm v$

$$P_0(B \mid c,+) = \int_0^\infty dt p_0(B,t \mid c,+) = \frac{\underline{S}_0(B \mid c,+)}{1-\underline{R}_{00}(c,+ \mid c,-)\underline{R}_{00}(c,- \mid c,+)}, \tag{13a}$$
$$P_0(B \mid c,-) = \int_0^\infty dt p_0(B,t \mid c,-) = \frac{\underline{S}_0(B \mid c,+)\underline{R}_{00}(c,+ \mid c,-}{1-\underline{R}_{00}(c,+ \mid c,-)\underline{R}_{00}(c,- \mid c,+)}. \tag{13b}$$

Introducing

$$\underline{\psi} = P_0(B \mid c,+) - P_0(B \mid c,-) \tag{14}$$

and noticing that

$$\underline{S}_0(B \mid c,+) = 1 - \underline{R}_{00}(c,- \mid c,+),$$
$$\underline{S}_0(A \mid c,-) = 1 - \underline{R}_{00}(c,+ \mid c,-),$$

we obtain

$$\frac{1}{\underline{\psi}} = \frac{1}{\underline{S}_0(B \mid c,+)} + \frac{1}{\underline{S}_0(A \mid c,-)} - 1\,. \tag{15}$$

The above relation can be deduced directly from the properties of "chain-like" systems [9]. Using (11) we obtain [13]

$$\frac{1}{\underline{\psi}} = \frac{\alpha_0}{\psi} + \alpha_1 \left(\frac{1}{1-\hat{r}^{ac}(\lambda)} + \frac{1}{1-\hat{r}^{bc}(\lambda)} - 1 \right), \tag{15'}$$

where ψ is defined similarly to $\underline{\psi}$, but in the absence of the fluctuating barrier and we have introduced the condensed notation

$$\hat{r}^{bc}(\lambda) = \hat{r}(c,-,\lambda \mid c,+)\,,$$
$$\hat{r}^{ac}(\lambda) = \hat{r}(c,+,\lambda \mid c,-)\,.$$

If J_c is the one-way equilibrium current at c in the absence of the fluctuating barrier, the corresponding current in the presence of the barrier is $\alpha_0 J_c$; the overall reaction rate $\underline{k}_{\mathrm{AB}}$ is thus given by (2')

$$\underline{k}_{\mathrm{AB}} = \frac{\alpha_0 J_c \underline{\psi}}{q_{\mathrm{A}}} \tag{16}$$

and is related to the rate without barrier, $k_{\mathrm{AB}} = J_c \psi / q_{\mathrm{A}}$ by

$$\frac{k_{\mathrm{AB}}^{TST}}{\underline{k}_{\mathrm{AB}}} = \frac{k_{\mathrm{AB}}^{TST}}{k_{\mathrm{AB}}} + \frac{\alpha_1}{\alpha_0} \left(\frac{1}{1-\hat{r}^{ac}(\lambda)} + \frac{1}{1-\hat{r}^{bc}(\lambda)} - 1 \right), \tag{17}$$

if J_c/q_{A} is identified with the rate k_{AB}^{TST} of the Transition State Theory (which stipulates that the reaction is completes as soon as the particle reaches c).

It is clear from (17) that when λ increases from 0 to ∞, $\underline{k}_{\mathrm{AB}}$ *increases from* $\alpha_0 k_{\mathrm{AB}}$ *to* $\underline{k}_{\mathrm{AB}}^{\infty}$, given by

$$\frac{k_{\mathrm{AB}}^{TST}}{\underline{k}_{\mathrm{AB}}^{\infty}} = \frac{k_{\mathrm{AB}}^{TST}}{k_{\mathrm{AB}}^{\infty}} + \frac{\alpha_1}{\alpha_0} = \frac{1}{S^{ac}} + \frac{1}{S^{bc}} - 1 + \frac{1}{\alpha_0} - 1 \tag{18}$$

(which value can be found directly using the inverse addition law for chain-like systems[9]). It should be pointed out that the effective time-averaged barrier would simply be a barrier reflecting the particle with probability α_1 without the memory effects which corresponds to the limit $\underline{k}_{AB}^{\infty}$ which confirms that the fluctuating barrier cannot be correctly represented by a static one. On the other hand, $\underline{k}_{AB}$ *is always smaller than* k_{AB}, which, although reasonable, is not completely obvious *a priori*. More precisely,

$\underline{k}_{AB}$ increases from 0 to k_{AB} when the probability α_0 increases from 0 to 1. We can summarize these remarks by noticing that

$$\alpha_0 k_{AB} < \underline{k}_{AB} < k_{AB}^{\infty} < k_{AB} , \tag{19}$$

so that *the memory effects always decrease the reaction rate.* This conclusion is one of the main results of this paper. It holds not only for the particular cases studied here: it will be extended to a similar process including two fluctuating barriers and the approximation developed in Section 2.6 indicates that the same conclusion should hold for any number of barriers. It would be interesting to generalize it to other processes.

We will now see that the presence of several fluctuating barriers leads to other interesting behaviours due to the possible trapping of the particle between two barriers and to the corresponding memory effects.

2.5. Two fluctuating barriers and stochastic resonance

Let us now consider the particle moving according to a given stochastic process on the interval $[a, b]$. In this interval, just beyond the points a and b there are fluctuating barriers F_A and F_B. If one of these barriers is open at the moment the particle reaches it, the particle is absorbed at the corresponding extremity; if it is closed, the particle is reflected and loses the memory of all past events (see Fig. 2). F_A and F_B are independent and obey the laws given in 2.3.

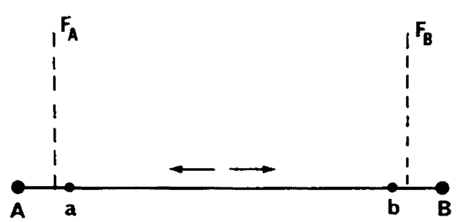

Fig. 2. Stochastic motion with two fluctuating barriers: **A**, **B**: absorbing states; $\mathbf{F_A}, \mathbf{F_B}$: fluctuating barriers; between a and b.

We first define the conditional probabilities corresponding to the stochastic process *without barriers* in the way similar to (2.4):

$s(B, t \mid a, +)$ is the probability density to be absorbed in B at time t, starting from a with velocity $+v$;

$r(A, t \mid a, +)$ is the probability density to be absorbed in A with the same conditions as above, *etc.*

We want to compute the overall probabilities for the system with fluctuating barriers, such as

$P(B \mid a,+;i,j)$ — the total probability to be absorbed in B starting from a with velocity $+v$ and barriers F_A and F_B in states i,j respectively.

The method is the same as in 2.4. However, the presence of two barriers makes it more intricate. To simplify the problem, let us assume that the process is symmetric, *i.e.*

$$s(B,t \mid a,+) = s(A,t \mid b,-) \equiv s(t)\,, \tag{20a}$$

$$r(A,t \mid a,+) = r(B,t \mid b,-) \equiv r(t)\,. \tag{20b}$$

Then we have

$$P(B \mid a,+;i,j) = P(A \mid b,-;j,i) \equiv \underline{S}_{ij}\,, \tag{21a}$$
$$P(A \mid a,+;i,j) = P(B \mid b,-;j,i) \equiv \underline{R}_{ij}\,. \tag{21b}$$

It is particularly important to compute

$$\underline{S}_0 = \sum_j \underline{S}_{0j}\alpha_j = \sum_j P(B \mid a,+;0,j)\alpha_j \tag{22}$$

which is the average transmission probability for the particle starting from a with velocity $+v$ with F_A open and F_B in its stationary distribution. It can be shown [19] that

$$\underline{S}_0 = S + \alpha_1 X \underline{S}_1 \tag{23}$$

with

$$S = \int_0^\infty s(t)dt = \hat{s}(0)\,; \quad R = 1 - S = \int_0^\infty r(t)dt = \hat{r}(0)$$

and

$$X = R - S - \hat{r}(\lambda) - \alpha_1 \hat{s}(\lambda) Y^{-1}\,,$$
$$Y = 1 - \alpha_1 \hat{r}(\lambda) - \alpha_0 \hat{r}(2\lambda) + \alpha_0 \hat{s}(2\lambda)\,,$$
$$\underline{S}_1 \equiv \sum_j \underline{S}_{1j}\alpha_j = [2S + \alpha_0 X]^{-1} S\,. \tag{24}$$

The above expressions, in spite of their complexity, can be investigated analytically [19]. The main conclusions are that *for any stochastic process between a and b* satisfying the conditions given in 2.3:

(i) **when λ increases from 0 to ∞** and α_0 is kept constant, $\underline{S}_0$ always increases from $\alpha_0 S$ to $S/(\alpha_0 + 2\alpha_1 S)$; since the relaxation time of the barriers is $1/\lambda$, we can conclude that *the transmission probability of the system decreases as the memory increases*, in analogy with the conclusions of section 2, concerning one barrier.

(ii) **when α_0 is varied** and λ is kept constant, we have two cases depending on the value of S (transmission probability in the absence of barriers):
- **if $S \geq 1/2$,** $\underline{S}_0$ increases up to S as α_0 increases from 0 to 1;
- **if $S < 1/2$,** there are two values λ^* and λ^{**} ($\lambda^* < \lambda^{**}$) defined by

$$1 - \hat{r}(\lambda^*) - 2S = 0\,,$$

$$[1 - \hat{r}(\lambda^{**}) - 2S][1 - \hat{r}(\lambda^{**})] - \hat{s}^2(\lambda^{**}) = 0\,,$$

such that
for $\lambda < \lambda^*$, $\underline{S}_0$ *increases* up to S as α_0 increases from 0 to 1;
for $\lambda^* < \lambda < \lambda^{**}$, $\underline{S}_0$ has a *maximum* for some $\bar{\alpha}_0 \in (0,1)$. $\underline{S}_0(\bar{\alpha}_0) > S$;
for $\lambda > \lambda^{**}$, $\underline{S}_0 \geq S$. Depending on the value of λ, $\underline{S}_0$ is monotonously *decreasing* with α_0 (large λ) or is *nonmonotonous*, with one or several maxima.

Thus if $S < 1/2$ *it is possible to improve and optimize the transmission probability by a convenient choice of* α_0 (*i.e.* a convenient choice of the relaxation frequencies of states 0 and 1 of the barrier): this effect can be considered as a *stochastic resonance* between the underlying stochastic process in $[a,b]$ and the fluctuations of the barriers.

2.6. Succession of n barriers

The calculations presented above become too complicated if the number of barriers increases. We will now present a simple approximation for the case of the ballistic motion between the barriers [13]; the time $\tau = d/v$ of crossing the distance between two successive barriers is constant. We assume that all barriers are independent, the parameter λ is the same for all barriers, but the values of α_i^k may be different for different barriers.

If $\tau \gg \lambda^{-1}$, we can approximately neglect the memory of the barriers and consider that the k-th barrier is in its stationary distribution $\{\alpha_i^k\}$ when the particle reaches it. One can see from (4) that the probability of any trajectory of the particle can be expanded in powers of $e^{-\lambda\tau}$. The zero order term corresponds to barriers without memory; the transmission probability is then given by the inverse addition law of chain systems [9]. If we introduce $S^{BA} = P(B \mid a, +) =$ probability to be eventually absorbed in B, starting from a with velocity v, when all n barriers have *no memory*, we get

$$\frac{1}{S^{BA}} = \sum_{k=1}^{n} \frac{\alpha_1^k}{\alpha_0^k} + 1\,, \tag{25}$$

or if all barriers are identical ($\alpha_i^k = \alpha_i$)

$$\frac{1}{S^{BA}} = n\frac{\alpha_1}{\alpha_0} + 1\,. \tag{25'}$$

The second term of the expansion is of order $e^{-2\lambda\tau}$ and can be obtained in the following way: we take an arbitrary trajectory from A to B, the probability of which is calculated *without memory* (*i.e.* with the zero order term of $\varphi_{ji}(t)$), and we add to this trajectory an excursion from barrier k ($k \in [1, n]$) to one of the accessible next neighbours $k \pm 1$ and return to k: the contribution of this excursion is calculated by using in $\varphi_{ji}(t)$ only the term with $e^{-2\lambda\tau}$. Summing up all these contributions it is found that the first correction to (25) is

$$\delta^{\bar{2}}\left(\frac{1}{S^{BA}}\right) = -\frac{\delta^{\bar{2}} S^{BA}}{\left(S^{BA}\right)^2} = \sum_{k=1}^{n-1} \alpha_1^k \alpha_1^{k+1} \left(\frac{1}{\alpha_0^k} + \frac{1}{\alpha_0^{k+1}}\right) e^{-2\lambda\tau}, \tag{26}$$

or for identical barriers

$$\delta^{\bar{2}}\left(\frac{1}{S^{BA}}\right) = 2(n-1)\frac{(\alpha_1)^2}{\alpha_0} e^{-2\lambda\tau}. \tag{27}$$

Thus, in agreement with our previous conclusions, *the overall transmission probability always decreases because of the barrier memory* in this approximation, and the effect increases with the probability α_1.

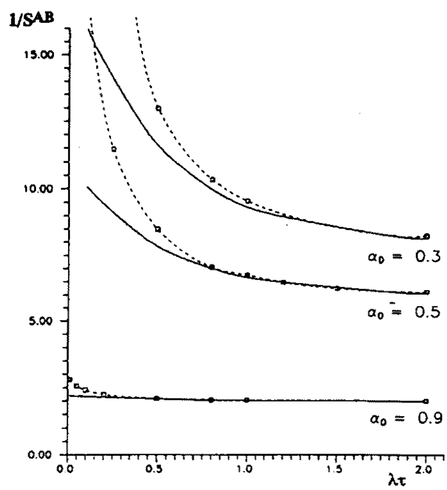

Fig. 3. Transition probability of a succession of 10 fluctuating barriers: S_{AB}: transmission probability; λ: relaxation frequency of barriers; τ: time for ballistic motion between two barriers; α_0: a priory probability of presence of a barrier. Solid lines: approximation (27); squares: numerical simulations.

Numerical simulations (Fig. 3) show that the present approximation is satisfactory if $\lambda\tau \geq 1$ and if $\alpha_1 \leq 0.7$. It is possible to compute higher terms of the expansion, of successive orders $e^{-4\lambda\tau}$, $e^{-6\lambda\tau}, \ldots$; the calculations become quite complicate, but they significantly improve the agreement with the results of simulations. Nevertheless if $\lambda\tau \ll 1$ the particle can be trapped for a long time between two barriers; so another kind of approximation has to be found.

It can be noticed that in the present case of n identical barriers with very short memory both the reaction time $\tau^{BA} \propto 1/S^{BA}$ and its first correction $\delta^{\bar{2}}\tau^{BA}$ are of order of n when $n \gg 1$, so the flux S^{BA} and $\delta^{\bar{2}}\tau^{BA}$ are of order $1/n$. An interesting case occurs when the barriers have equal λ, but different randomly distributed $\{\alpha_1^k\}$. Formulas (25)–(26) apply for each realization of $\{\alpha_1^k\}$ and it can be shown [14] that $\tau^{B,A}, \delta^{\bar{2}}\tau^{BA}$ and $S^{B,A}, \delta^{\bar{2}}S^{BA}$ are still of the respective orders n and $1/n$. This is due to the persistency of the particle motion, the displacement of the particle from a barrier being (partially) determined in function of the initial velocity.

If the condition of persistency is dropped, we obtain a model equivalent to the well known Sinai model [20]; it has been shown that in this case of diffusion in a random medium the flux $S^{B,A}$ has the anomalous dependence $1/\sqrt{n}$ [21].

3. Two-dimensional case: motion in a fluctuating lattice

3.1. The model

We consider a square lattice with each node switching randomly between two states 0 and 1. The mean waiting time in each state follows the exponential law (3); the transition probability $\varphi_{ji}(t)$ is given by (4). All nodes are fluctuating independently.

A particle is moving on the lattice and travels between two neighbouring nodes in time τ with constant velocity. At each node the direction of its velocity may change depending on the current state i of the node; it may follow the same direction with probability p_i, go backward with probability q_i or turn to the left or right with probability r^+ or r^-. For the sake of simplicity we will take

$$p_0 = 1, \quad p_1 = p, \quad q_1 = q, \quad r^+ = r^- = r, \quad (p + q + 2r = 1)$$

This model [14] extrapolates between two limiting cases. For $\lambda = 0$ the model corresponds to a Lorentz gas (the movement of a particle in a static medium). For $\lambda = \infty$ we have a persistent random walk [22]; at each node, the velocity may remain unchanged with probability $\alpha_0 + \alpha_1 p$, be reversed with probability $\alpha_1 q$ or be rotated by $\pm\pi/2$ with probability $\alpha_1 r$.

3.2. Transmission in a stratified medium

We consider a succession of n infinite horizontal layers (Fig. 4), supposing that they are uniform in the horizontal direction (Ox), *i.e.* all nodes of a k-th layer have the same α_i^k ($i = 0, 1$). The probabilities p, q, r are the same for all nodes of the lattice.

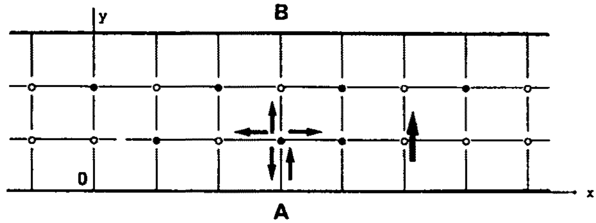

Fig. 4. Model stratified medium: black circles: diffusive nodes (state 1); white circles: open nodes (state 0).

For $\lambda = \infty$ (no memory) the vertical motion (in (Oy) direction) is equivalent to the one-dimensional motion considered in 2.6. The particle may cross the k-th layer with probability

$$P_k = \alpha_0^k + \alpha_1^k(p + r), \tag{28}$$

or be reflected with probability

$$Q_k = \alpha_1^k(q + r). \tag{28'}$$

The overall probability of crossing n layers (from region A ($y \leq 0$) to region B ($y \geq n$)) is

$$\frac{1}{S^{BA}} = \sum_{k=1}^{n} \frac{Q^k}{P^k} + 1. \tag{29}$$

For nodes with short memory ($\lambda\tau \gg 1$) we can generalize the approximation scheme described in 2.6 based on the expansion of the transmission probability in powers of $e^{-2\lambda\tau}$. The first correction is due to excursion from one node to a next neighbour and return, where the term in $e^{-2\lambda\tau}$ is taken into account in $\varphi_{ji}(2\tau)$. Summing up all these contributions gives [14, 22]

$$\delta^{\bar{2}}\left(\frac{1}{S^{BA}}\right) = \sum_{k=1}^{n-1} \alpha_1^k \alpha_1^{k+1} \left(\frac{\alpha_0^k}{(P^k)^2} + \frac{\alpha_0^{k+1}}{(P^{k+1})^2}\right). \tag{30}$$

Again it is seen that *the memory effects make the transmission probability to decrease.*

In fact, numerical simulations show that the approximation (30) is satisfactory in most circumstances, unless $\lambda\tau \ll 1$ and $\alpha_0 \ll 1$.

3.3. Diffusion in an infinite medium

It is interesting to consider the displacement $\mathbf{r}(t)$ of the particle during time t in an infinite fluctuating lattice with identical nodes. Numerical simulations show [14] that for any λ the diffusive regime is established very rapidly:

$$\frac{< \mathbf{r}^2(t) >}{4t} \to D\,,$$

if $t \to \infty$.

Naturally, the diffusion coefficient D increases with α_0 (without any particular behaviour at the percolation threshold $\alpha_0 \simeq 0.41$ [24]; D also increases, but not very strongly, with the relaxation frequency λ up to the value for a persistent random walk ($\lambda = \infty$), given by

$$D = \frac{1}{4}\frac{1+\gamma}{1-\gamma} \tag{31}$$

with

$$\gamma = \alpha_0 + \alpha_1(p-q)\,.$$

In order to study the possible Gaussian character of the distribution of $\mathbf{r}(t)$, one can consider the kurtosis[14, 25]

$$\chi = \langle r^4(t)\rangle - 2\langle r^2(t)\rangle^2 \tag{32}$$

which vanishes for a two-dimensional Gaussian distribution.

Computer simulations show that χ/t^2 varies quite differently from $\langle r^2\rangle/t$, and on a very different time scale; it eventually drops to a very small (although generally not 0, in times we could reach) plateau value, but only long time after the diffusive regime has been established (Fig. 5). It can be remarked that for $\lambda = \infty$, corresponding to a persistent random walk,

$$\chi/t^2 = -2\gamma/(1-\gamma)\,. \tag{33}$$

In the general case it is seen that the behaviour of χ strongly depends on the relaxation frequency λ of the nodes; for $\lambda < 0.1$, after a short transitory time, χ remains positive; for $\lambda > 0.1$ it remains negative, finally for $\lambda \simeq 0.1$ χ vanishes after a time of the same order as the time for setting up the diffusive regime. The positive kurtosis observed for very small values of λ corresponds to a distribution which is sharper around 0 than the Gaussian with the same variance; this can be interpreted by remarking that the particle after

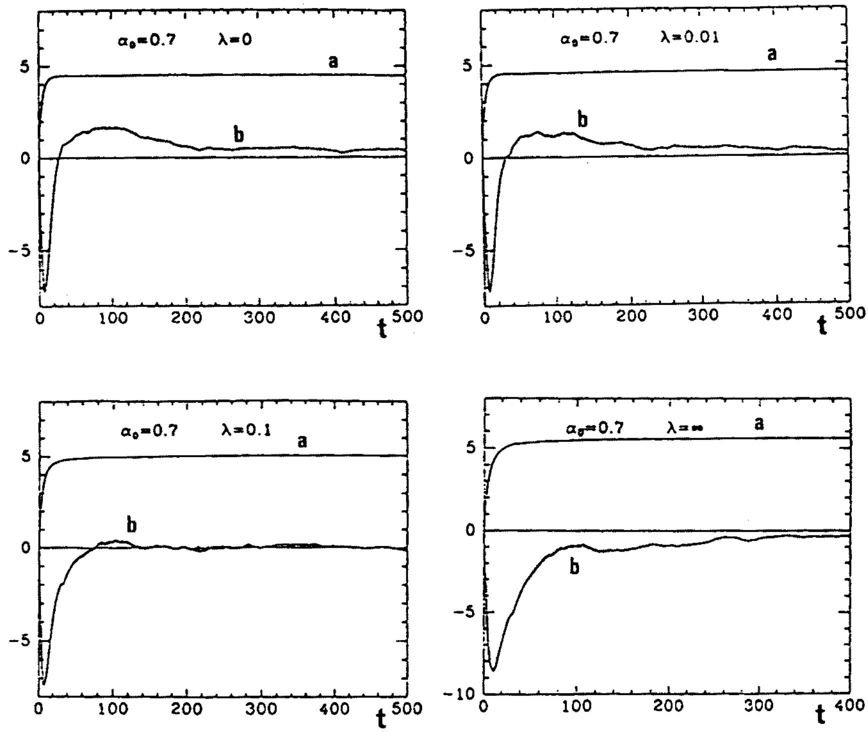

Fig. 5. Diffusion coefficient and kurtosis in a fluctuating square lattice for different values of α_0 (a priory probability of a state 0) and of λ (relaxation frequency of barriers): curves a: $\langle r^2 \rangle / t$; curves b: χ / t^2.

escaping from the neighbourhood of the origin, does not return to 0 easily, because it can be retained far away by local traps.

4. Conclusions

It has been shown that the motion of a particle in fluctuating media depends significantly on the memory of the medium. In several cases exact solutions were found; they show that the effective average potential does not represent correctly the motion of the particle in the case of a finite memory time λ^{-1}. They lead to the conclusion that the memory effects decrease the overall transmission probability of the system. They also permit to exhibit stochastic resonances, which can improve the overall transmission rate by a convenient choice of the parameters of the obstacles. In the case of the large number of fluctuating barriers or obstacles, approximations have been proposed. These approximation give good results for small and moderate correlation times of the barriers.

The diffusion of a particle is also modified by the memory of a fluctuating lattice. The effect concerns mainly the shape of the particle distribution, whereas a diffusive regime is rapidly established for all values of the memory time. In any case, the influence of fluctuations in time is not so strong as the influence of fluctuations in space, which can lead to anomalous kinetic laws [10, 21, 25].

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