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LETTER TO THE EDITOR

Non-Markov noise in barrier-fluctuation model

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Abstract. We investigate the thermally activated escape of a particle over a potential barrier whose height fluctuates between two values. The barrier-switching process is constructed as a semi-Markov alternating process: the times at which a change of the barrier state can occcur form a general renewal process and the probability of leaving a state depends on the time the barrier resides in the state before the jump. During the interjump interval, the barrier is fixed in one of the two states and the crossing dynamics is described by a general (not necessarily exponential) decay law. We give the general formulae describing the averaged escape dynamics, where the averaging runs over all possible histories of the switching process. Using the above device of the selective residence times, the recently discussed phenomenon of resonant activation (a minimal averaged lifetime of the particle in the potential well) emerges also within the framework of the conventional exponential escape dynamics.

1. Introduction

During the last decade the thermally activated escape of a particle from a potential well [1, 2] has been studied in systems in which other (independent) dynamical processes are present. One area of current interest is that of resonance activation [3–7].

Consider the problem of thermal escape out of a potential well, whose barrier height switches at random between two values: low and high barrier, designated in the following by the indexes '$\pm$'. The two basic ingredients of the combined dynamics are (i) the switching process and (ii) the escape dynamics with the barrier fixed in one of the two possible states. We assume the two ingredients are independent (thus, for example, the escape dynamics with the fixed barrrier do not depend on the previous history of the switching process).

As for the switching mechanism, one usually implements the standard dichotomous process: the residence times in the two individual states form a system of identical, mutually independent and exponentially distributed random variables. More formally, the barrier resides in the $\pm$ state for a random time, described by the probability density $\phi_\pm(t) = \gamma \exp(-\gamma t)$, where $1/\gamma$ is the mean interjump time. After a jump, the new residence period begins and its length is statistically independent of the previous one.

Turning our attention to the escape dynamics, suppose the barrier is fixed in one of the two possible states, say in the '$+$'-state. The particle is influenced by a potential force (depending on the detailed form of the potential well) and by an additive Langevin force (usually taken as the Gaussian white noise). Occasionally, the particle sustains a strong enough impulse, surmounts the barrier and leaves the well. Consequently, as a result of the complex diffusion dynamics, the particle's probability $g_+(t)$ of being found within the attractive basin of the potential minimum decays with time. The decay is usually

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approximated by an exponential [8], $g_+(t) = \exp(-\kappa_+ t)$, with the decay rate κ_+ being proportional to the Boltzmann factor, $\kappa_\pm \propto \exp[-E_+/(k_B T)]$, and E_+ denoting the height of the barrier. Formally, we can introduce the random variable T_+ representing 'the lifetime of the particle in the well'. Thereupon, all pertinent features of the complex diffusion problem are pictured either by the above decay law $g_+(t)$ or, equivalently, by the probability density for the variable T_+:

$$g_+(t) = \mathrm{Prob}\{\mathsf{T}_+ > t\} = 1 - \mathrm{Prob}\{\mathsf{T}_+ \leqslant t\} = 1 - \int_0^t \psi_+(t')\,\mathrm{d}t'. \qquad (1)$$

The above exponential decay law is compatible with the density $\psi_+(t) = \kappa_+ \exp(-\kappa_+ t)$. However, as indicated by the exact analysis of the diffusion process in the static potential well [9], the decay law $g_+(t)$ need not be necessarily exponential and our designation already anticipates the generalization.

After the separate presentation of the two ingredients, let us consider a *fixed* (non-random) sequence of n jump events, say at times $0 < s_1 < s_2 < \cdots < s_n < t$, preceding an arbitrary time t. We now invoke the following assumption: after an arbitrary jump, the dynamics start anew with the decay law $g_+(t)$ or $g_-(t)$ (corresponding to the new state of the barrier) and with the initial condition given by the final value of the previous evolution. Accordingly, the probability of remaining in the well at time t conditioned upon the above realization of the switching process reads $g_\pm(t - s_n) \ldots g_\mp(s_2 - s_1) g_\pm(s_1)$. It follows a continuous curve which in an alternating manner switches between the functions $g_\pm(t)$, matched together at the switching points $s_1, \ldots, s_n$. Averaging the area below the curve over all possible histories of the switching process, one arrives at the *mean lifetime* τ. In the following, we wish to focus on the calculation of this quantity.

As an example, consider the switching as being described by the standard Markov dichotomous process (see the definition above) and take the decay laws in the two states of the barrier to be exponential, $g_\pm(t) = \exp(-\kappa_\pm t)$. Then the resulting mean lifetime reads [5]

$$\tau(\gamma) = \frac{1}{2} \frac{\kappa_- + \kappa_+ + 4\gamma}{\kappa_- \kappa_+ + \gamma(\kappa_- + \kappa_+)}. \qquad (2)$$

It decreases in a monotonic way from its maximum value in the static limit, $\tau(0) = \bar{\tau}$, $\bar{\tau} = (1/\kappa_- + 1/\kappa_+)/2$, down to the minimum value in the fast-switching limit, $\tau(\infty) = 1/\bar{\kappa}$, $\bar{\kappa} = (\kappa_- + \kappa_+)/2$ (i.e. the resulting rate is the average of the two individual rates).

The Markovian switching between two *non-exponential* decay laws has been recently analysed in [5]. One observes an interplay between the typical residence time $1/\gamma$ of the barrier in its individual states and the most probable instant of the escape event (which does not exist in the case of the exponential escape dynamics). As a result, the function $\tau(\gamma)$ develops a *minimum* at an 'escape-optimized' rate γ_{res}; the phenomenon was characterized by Doering and Gadoua [3] as 'resonant activation'. We wish to investigate an even more general setting, where an arbitrary decay law combines with the semi-Markov switching mechanism.

2. Semi-Markov switching mechanism

Let us first concentrate on the construction of the barrier-switching process. Assume the barrier starts at time $s_0 = 0$ with probability $\xi_{j_0}^{(0)}$ in the state $j_0 (j_0 = \pm)$. It resides in this state for a random time, described by the probability density $\phi_{j_0}(t)$. At the end of this random interval, say at time s_1, the transition $j_0 \to j_1$ occurs with the *time-dependent* probability $p_{j_1,j_0}(s_1)$ (note that the barrier can also remain in its original state—the 'test' point s_1 may be but also need not be the point of an actual switching). Then the whole procedure starts anew. We now consider an arbitrary but fixed realization of the barrier-switching process. Namely, we take the n-point realization which runs through a fixed sequence of states $\{j_k\}_{k=0}^n$, switches between them at the fixed sequence of instants $\{s_k\}_{k=1}^n$ and occurs at time t still in the state j_n. Its probability density assumes the form

$$p(t, n; j_n, \dots, j_0; s_n, \dots, s_1) = f_{j_n}(t - s_n) \prod_{k=1}^{n} p_{j_k, j_{k-1}}(s_k - s_{k-1}) \phi_{j_{k-1}}(s_k - s_{k-1}). \tag{3}$$

Here $f_{j_n}(t - s_n) = 1 - \int_0^{t-s_n} \phi_{j_n}(t')\,\mathrm{d}t'$ gives the probability of there being no test point in the interval $\langle s_n, t\rangle$ while the barrier resides in the state j_n.

Let us designate as $\xi_\pm(t)$ the overall probability of finding the barrier at time t in the state '$\pm$'. In order to evaluate this quantity, one has to 'sum' the probabilities of all realizations which end at time t in the given state. The 'summation' actually means (i) the summation over any possible succession of the two states during the n test points, (ii) the integration over any possible occurrence times of the n test points and (iii) the summation over any possible number n of test points. The first part of the procedure is greatly facilitated if we introduce a suitable (2×2)-matrix. In the second step one benefits from the multiple-convolution structure of the underlying formulae and one invokes the Laplace transform. Finally, the summation over the number of test points emerges as a geometrical series. The details of the calculation will be given elsewhere [10]; we focus on the final formula for the Laplace transform of the occupation probabilities (here $p_\pm(t) = p_{\mp,\pm}(t)$):

$$\tilde{\xi}_\pm(z) = \frac{1}{z}\,\frac{\tilde{\pi}_\mp(z) + z\xi_\pm^{(0)}}{z + \tilde{\pi}_-(z) + \tilde{\pi}_+(z)} \qquad \tilde{\pi}_\pm(z) = \frac{z\tilde{\sigma}_\pm(z)}{1 - \tilde{\phi}_\pm(z)} \qquad \sigma_\pm(t) = p_\pm(t)\phi_\pm(t). \tag{4}$$

The preceding construction provides a large family of semi-Markov noises (we are preserving the limited-memory property characteristic for the Markov processes and we sacrifice the exponential form of the evolution operator for the occupation probabilities [11, 12]). Generally, they are non-stationary and they evolve to some stationary state (see the discussion). Their stationary two-time correlation function has a damped (generally non-exponential) form. Some special cases are the alternating process ($p_\pm(t) = 1$, i.e. the barrier necessarily changes its state at any test point) and the Markov asymmetric dichotomous noise ($p_\pm(t) = p_\pm \neq 1$, $\phi_\pm(t) = \gamma_\pm \exp(-\gamma_\pm t)$, the constant rates in the equations for the occupation probabilities are then $p_\pm\gamma_\pm$). In our model, the time-dependent probabilities $p_\pm(t)$ have been included to describe the varying tendency to realize a true jump event after some time has elapsed from the previous test point. For instance, if the lengths of the test intervals are exponentially distributed (the Poisson process) and if the functions $p_\pm(t)$ are decreasing, the importance of long residence times is reduced: it is then less probable that the test point at the end of a long interval will be selected to become the true switching point. In the following, we denote $p_\pm(t)$ as the *selection functions*.

3. Averaged decay law

Combining both the switching and the decay process, we wish to calculate the *averaged* decay law $u(t)$. Basically, the averaging procedure runs along the straightforward prescription

$$u(t) = \sum_{\text{all realizations}} \begin{pmatrix} \text{probability for a} \\ \text{fixed realization} \end{pmatrix} \times \begin{pmatrix} \text{decay law} \\ \text{for this realization} \end{pmatrix}. \tag{5}$$

The first factor is given in (3). The second, i.e. the corresponding conditioned decay law, reads

$$u(t,n;\,j_n,\ldots,j_0;s_n,\ldots,s_1) = g_{j_n}(t-s_n)\ldots g_{j_1}(s_2-s_1)g_{j_0}(s_1)\xi_{j_0}^{(0)}. \tag{6}$$

At this point, one remark seems to be quite important. Assume the decay law is identical in the both states of the barrier, say $g_\pm(t) = g(t)$. Then the composed decay law (6) yields $u(t,n;\,j_n,\ldots,j_0;s_n,\ldots,s_1) = g(t)\xi_{j_0}^{(0)}$ *if and only if* $g(t)$ *is an exponential*. The observation is a direct consequence of the postulate we have stated in the introduction: any test point breaks the coherence of the decay, even if it does not imply a change of the decay law. After a test point, the decay process 'loses memory' and starts anew with the initial condition dictated as the final value of the previous evolution.

Finally, 'summation' in (5) has been explained in the preceding section. The success of the summation procedure rests again on the multiple-convolution structure of the emerging formula. The final expression for the Laplace transform of the averaged evolution reads

$$\tilde{u}(z) = \frac{\tilde{f}_-^{(g)}[\tilde{\sigma}_+^{(g)} + (1-\tilde{\phi}_+^{(g)})\xi_-^{(0)}] + \tilde{f}_+^{(g)}[\tilde{\sigma}_-^{(g)} + (1-\tilde{\phi}_-^{(g)})\xi_+^{(0)}]}{(1-\tilde{\phi}_-^{(g)})\,(1-\tilde{\phi}_+^{(g)}) + \tilde{\sigma}_-^{(g)}(1-\tilde{\phi}_+^{(g)}) + \tilde{\sigma}_+^{(g)}(1-\tilde{\phi}_-^{(g)})} \tag{7}$$

with $\sigma_\pm^{(g)}(t) = p_\pm(t)\phi_\pm(t)g_\pm(t)$, $\phi_\pm^{(g)}(t) = \phi_\pm(t)g_\pm(t)$ and $f_\pm^{(g)}(t) = f_\pm(t)g_\pm(t)$.

The last formula constitutes our main general result. Frequently, one still introduces a random variable T representing 'the switching-averaged lifetime of the particle in the well', its density $\psi(t)$ and its first moment, i.e. the mean switching-averaged lifetime. However, the last quantity is directly related to the Laplace transform (7). In fact the probability that the averaged escape process has not been realized up to time t reads $u(t) = 1-\int_0^t \psi(t')\,\mathrm{d}t'$ and hence

$$\tau \stackrel{\mathrm{def}}{=} \langle \mathsf{T}\rangle = \int_0^\infty t\,\psi(t)\,\mathrm{d}t = \int_0^\infty u(t)\,\mathrm{d}t = \lim_{z\to 0^+}\tilde{u}(z). \tag{8}$$

4. Discussion

Formulae (4) immediately yield the asymptotic probabilities

$$\xi_\pm^{(\infty)} = \lim_{t\to\infty}\xi_\pm(t) = \lim_{z\to 0^+} z\tilde{\xi}_\pm(z) = \frac{\tilde{\pi}_\mp(0)}{\tilde{\pi}_-(0)+\tilde{\pi}_+(0)} \tag{9}$$

i.e. the quantities $1/\tilde{\pi}_\pm(0)$ are nothing but the mean residence times in the individual states of the barrier. Assuming that the selection functions $p_\pm(t)$ are not time independent, the mean time between the true jumps is always longer than the mean time between the test points. The lengthening factor is $[\int_0^\infty p_\pm(t)\phi_\pm(t)\,\mathrm{d}t]^{-1}$. Choosing the Poisson system of test points, i.e. taking $\phi_\pm(t) = \gamma\exp(-\gamma t)$, the asymptotic values (9) are entirely controlled by the selection functions: $\xi_\pm^{(\infty)} = \tilde{p}_\mp(\gamma)/[\tilde{p}_-(\gamma)+\tilde{p}_+(\gamma)]$, i.e. *they depend* on the intensity γ. Anticipating our calculation below, we exemplify the effect by the choice $p_-(t) = \Theta(t-\sigma_-)$ and $p_+(t) = 1-\Theta(t-\sigma_+)$ ($\Theta(x)$ is the unit-step function), giving

$$\xi_-^{(\infty)}(\gamma) = [1-\exp(-\gamma\sigma_+)]/[1-\exp(-\gamma\sigma_+)+\exp(-\gamma\sigma_-)].$$

Although the test points are generated at mean spacing $1/\gamma$, the function $p_-(t)$ 'selects' only the intervals longer than σ_- to be followed by the true transition '$-$'→'$+$'. Similarly, after an interval shorter than σ_+, the transition '$+$'→'$-$' will be definitely realized. Altogether, by increasing the intensity γ, i.e. decreasing the mean time between the test points, the state '$-$' acquires preference and the asymptotic value $\xi_-^{(\infty)}(\gamma)$ increases up to unity.

Focusing our attention on the barrier-fluctuation problem, the calculation in [5] assumes $p_\pm(t) = 1$, $\phi_\pm(t) = \gamma \exp(-\gamma t)$ and a general form of $\psi_\pm(t)$. Note the misprints in the central formula (3) in [5] which should read

$$\tilde{u}(z) = \frac{1}{2}\frac{z'[1-\tilde{\psi}_-(z')\tilde{\psi}_+(z')] + (z'+2\gamma)[1-\tilde{\psi}_-(z')][1-\tilde{\psi}_+(z')]}{z'^2 - \gamma^2[1-\tilde{\psi}_-(z')][1-\tilde{\psi}_+(z')]} \qquad (10)$$

with $z' = z + \gamma$. Note that even if the escape dynamics is the same in both states of the barrier, i.e. $g_\pm(t) = g(t)$, the averaged decay law *is not* given by the function $g(t)$. The conclusion is again a consequence of the above assumption concerning the composed decay.

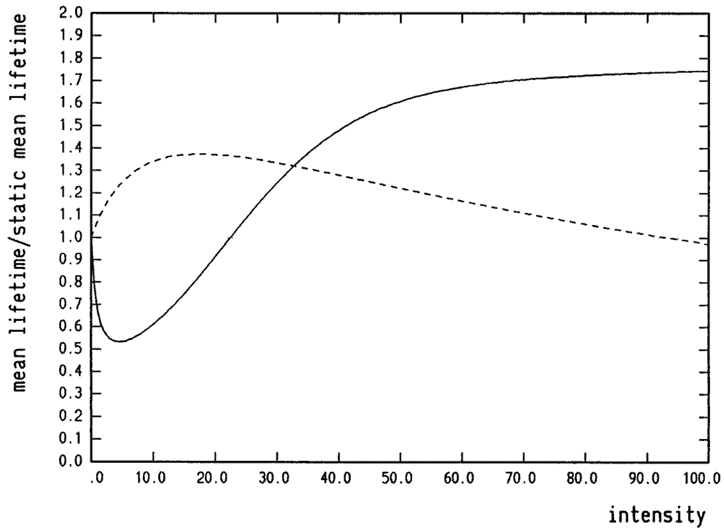

Figure 1. The mean lifetime $\tau(\gamma)$ reduced to its static value $\bar{\tau}$ against the intensity γ of the Poisson process. The escape dynamics is exponential with the parameters $\kappa_\pm$. The selection functions are $p_-(t) = \Theta(t-\sigma_-)$ and $p_+(t) = 1 - \Theta(t-\sigma_+)$, and the calculation is based on equation (12). The parameters used are: $\kappa_- = 1$, $\kappa_+ = 10$, $\sigma_- = 0.1$, $\sigma_+ = 0.1$ (full curve); and $\kappa_- = 10$, $\kappa_+ = 1$, $\sigma_- = 0.001$, $\sigma_+ = 0.001$ (broken curve).

In contrast to the setting in [5], we now consider the interplay between the exponential decay law and the semi-Markov switching mechanism. We assume $g_\pm(t) = \exp(-\kappa_\pm t)$, calculate the mean evolution (7) and carry out the limit in equation (8). The result reads

$$\tau = \frac{\kappa_-\xi_+^{(0)} + \kappa_+\xi_-^{(0)} + \tilde{\pi}_-(\kappa_-) + \tilde{\pi}_+(\kappa_+)}{\kappa_-\kappa_+ + \kappa_-\tilde{\pi}_+(\kappa_+) + \kappa_+\tilde{\pi}_-(\kappa_-)}. \qquad (11)$$

The mean lifetime depends on the initial conditions for the noise. The escape rates are combined with the switching mechanism through the effective rates $\tilde{\pi}_\pm(z)$. If, however, $\kappa_\pm = \kappa$, then of course $u(t) = \exp(-\kappa t)$ and $\tau = 1/\kappa$, whatever the switching mechanism. In order to particularize the effect of the selection functions, let us again implement the Poisson system of test points and the symmetric initial conditions $\xi_\pm^{(0)} = 1/2$. Equation (11) then implies

$$\tau(\gamma) = \frac{1}{2}\frac{\kappa_- + \kappa_+ + 2\gamma[(\gamma+\kappa_-)\tilde{p}_-(\gamma+\kappa_-) + (\gamma+\kappa_+)\tilde{p}_+(\gamma+\kappa_+)]}{\kappa_-\kappa_+ + \gamma[\kappa_+(\gamma+\kappa_-)\tilde{p}_-(\gamma+\kappa_-) + \kappa_-(\gamma+\kappa_+)\tilde{p}_+(\gamma+\kappa_+)]}. \qquad (12)$$

The static limit always gives $\tau(0) = (1/\kappa_- + 1/\kappa_+)/2$. However, in the high-intensity limit, the lifetime depends on the zero-time values of the selection functions: $\tau(\infty) =$

$[p_-(0)+p_+(0)]/[\kappa_+ p_-(0)+\kappa_- p_+(0)]$, i.e. it can be considerably different from the standard value $2/(\kappa_- + \kappa_+)$, valid for $p_\pm(t) = 1$. Moreover, for a specific form of the selection functions, the function $\tau(\gamma)$ can reveal both a minimum and a maximum. This feature is exemplified in figure 1 by choosing again the above unit-step selection functions. Having sufficiently high intensity, the '$-$'-state has preference. Increasing γ then causes either an increase (full curve) or decrease (broken curve) of the mean lifetime, depending on the mutual relation between the rates $\kappa_\pm$.

In order to give a physical meaning to the above construction, one has to consider a microscopic origin of the noise. Assume the test points are generated by a completely independent stationary source, whereas the selection mechanism is an intrinsic element of a system. For instance, the rate γ is defined by the tunnelling frequency of a host molecule which stimulates the jumps of the barrier height for a neighbouring impurity unit. The actual realization of the jump also depends on the coupling between the impurity and a phonon system. The selection mechanism can be attributed to the phonon-induced localization following every jump of the barrier. Having this picture in mind, a slow change of the temperature induces a slow modification of the tunnelling frequency of the host molecule and hence the spacing between the test point also changes. Our analysis then predicts a slow change of the mean lifetime describing the impurity unit.

In conclusion, coupling of the decay dynamics with the random switching of the barrier height produces a wide variety of behaviour. The new features of the switching process substantially influence the averaged decay.

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