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Mean escape time over a fluctuating barrier

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An approximate method for studying activation over a fluctuating barrier of potential is proposed. It involves considering separately the slow and fast components of barrier fluctuations, and it applies for any value of their correlation time τ. It gives exact results for the limiting values $\tau\to 0$ and $\tau\to\infty$, and the agreement with numerics in between is also excellent, both for dichotomic and Gaussian barrier perturbations.

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Ever since Kramers' seminal paper [1] the fluctuational escape over a potential barrier has been a paradigm for a thermal activation process. Recently, activation in the presence of time-varying fields has become a subject of great interest due to the discovery of many counterintuitive noise-assisted effects, such as stochastic resonance [2] or transport in Brownian motors [3]. The nonequilibrium character of these problems hinders, however, the direct application of many ideas and methods developed for investigation of the static Kramers problem [4] (e.g., detailed balance or rate concept). On the other hand, as the time scale of variation of the driving signal is independent of the internal dynamics of the system, standard adiabatic methods are restricted to certain ranges of parameters only. Hence, an approach which overcomes these difficulties and applies for the whole range of time variability of the perturbation is of great importance.

In this Brief Report, we address this problem for an activation over a randomly fluctuating barrier. The subject is interesting not only due to its ubiquity in many branches of physics, e.g., in relation to ligand binding to heme proteins [5], transport processes in glasses [6], or dye laser with a fluctuating pump parameter [7], but especially because of the phenomenon of *resonant activation* [8]—the appearance of a minimum of the mean activation time $\mathcal{T}$ as a function of the correlation time τ of barrier fluctuations. The dependence $\mathcal{T}(\tau)$ can be calculated exactly merely for simple models [8–10], for more general cases the approaches [11–15] proposed till now apply to some ranges of τ only. Irrespective of the technical differences, they are all based on the rate concept, which assumes a quasistationary equilibrium before the activation happens and applies for $\tau\ll\mathcal{T}$, and/or kinetic description for $\tau\gg\ln(1/q)$ (q states for the thermal noise intensity) when the escape events are uncorrelated with the potential variations. Although for small enough q in an extended region $\ln(1/q)\ll\tau\ll\mathcal{T}$ both approximations coexist and give similar results [11], nevertheless the proper smooth connection between them remains the main theoretical challenge. Below we present an approach which is valid for any τ. It gives exact values of $\mathcal{T}(\tau)$ in the limits $\tau\to 0$ and $\tau\to\infty$, and a very good approximation in between.

We study an overdamped Brownian particle driven by a (thermal) Gaussian white noise $\xi(t)$ of zero mean, which moves in a stochastically varying potential. Its static part $U(x)$ has a monostable or bistable form and the random part $V(x)z(t)$ is generated by a stationary Markovian noise $z(t)$ of zero mean and correlation $C(t)=Q/\tau\exp(-|t|/\tau)$. Following Refs. [16,17] we assume a general form for its intensity $Q(\tau)=Q_0\tau^\alpha$ $(0\leqslant Q_0=\text{const},\ 0\leqslant\alpha\leqslant 1)$, which gives the mostly studied cases with τ-independent intensity ($\alpha=0$) or variance ($\alpha=1$) as special cases. Two types of $z(t)$ are considered: an Ornstein-Uhlenbeck noise (OUN) which is Gaussian with variance $D=Q/\tau$ and a dichotomic noise (DN) which flips between two values $\pm\sqrt{D}$ with the rate $\gamma=1/(2\tau)$. Although they essentially differ—the former is continuous, the latter discrete—nevertheless, they influence the activation process very similarly [18] and the main steps of the presented description are the same. The dynamics of the system is given by the non-Markovian Langevin equation

$$\frac{dx}{dt}=-U'(x)-V'(x)z(t)+\xi(t). \tag{1}$$

Introducing the two-dimensional Markovian stochastic process $\{x(t),z(t)\}$ one can formulate the evolution equation for the joint probability distribution $P(x,z,t)$:

$$\frac{\partial}{\partial t}P(x,z,t)=[\mathcal{L}(x,z)+\Lambda(z)]P(x,z,t), \tag{2}$$

where $\mathcal{L}(x,z)=(\partial/\partial x)[U'(x)+V'(x)z]+q(\partial^2/\partial x^2)$ is the Fokker-Planck (FP) operator. The free evolution of the barrier noise is governed by the operator $\Lambda(z)=1/\tau[(\partial/\partial z)z+Q\partial^2/\partial z^2]$ for OUN or by the matrix $\Lambda=(-\gamma,\gamma;\gamma,-\gamma)$ for DN. Initially the particle is located at the bottom x_b of the well and the quantity of interest is the mean first passage time (MFPT) through a given threshold x_{thr} located either at the top x_t or far from it on the other side of the barrier.

A typical scenario of an escape event consists of two stages. For a long time t_b, the particle fluctuates in the vicinity of the bottom of the well, being subjected to small random impacts of $\xi(t)$. If a large enough outburst of $\xi(t)$ occurs, the particle will eventually surmount the barrier almost immediately during a short time t_t. The time variation of the potential exerts only a negligible effect on the first stage, but it can essentially modify the dynamics during the second one when the particle interacts with the whole slope of the barrier. Any realization of $\xi(t)$, which has been supposed to bring the particle over the top of a static barrier, may turn out to be insufficient if the barrier rises during the

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climbing stage. On the contrary, if the barrier decreases the particle does cross to the other side, but some smaller outbursts of $\xi(t)$ would also result in a successful escape. Because the rate of variation of the barrier shape depends on the correlation time of $z(t)$, the relationship between t_t and τ appears to be crucial in the analysis [17].

This discussion leads us to the central idea of the present approach—splitting the barrier noise into two independent components:

$$z(t)=z_s(t)+z_f(t). \tag{3}$$

The slow one z_s is defined as the mean value of z over the time interval of climbing $(t,t+t_t)$ and over its possible realizations (marked by $\langle \cdots \rangle$)

$$z_s(t)=\left\langle \frac{1}{t_t}\int_t^{t+t_t} ds\, z(s) \right\rangle=\frac{1}{\Delta}(1-e^{-\Delta})z(t), \tag{4}$$

where $\Delta=t_t/\tau$. It is supposed to be constant during the climbing stage, while its random character arises from the randomness of $z(t)$. Hence z_s is governed by the same statistics as z but with the variance

$$D_s=\langle z_s^2\rangle=\frac{Q}{t_t}\frac{1}{\Delta}(1-e^{-\Delta})^2. \tag{5}$$

Next, assuming that the fast part $z_f(t)$, which gives rapid fluctuations around $z_s(t)$, can be treated as uncorrelated, one calculates its intensity Q_f:

$$Q_f=Q\left[1-\frac{1}{\Delta}(1-e^{-\Delta})-\frac{1}{2}\frac{1}{\Delta}(1-e^{-\Delta})^2\right]. \tag{6}$$

If $z(t)$ is Gaussian it can always be written as the sum of two independent Gaussian components (3). So, in the OUN case both $z_s(t)$ and $z_f(t)$ are OUN's with correlation time τ and they differ only in the form of their intensities (variances) $D_i=Q_i/\tau$ $(i=f,s)$. If $\tau\to 0$ one has $Q_f=Q$, while the leading-order term of Q_s reads Q/Δ^2 so for any α it vanishes at least linearly with τ. Thus one is left with only the fast part of $z(t)$. In the opposite limit $\tau\to\infty$, the leading term of Q_f becomes $Q\Delta^2/3$, so D_f vanishes at least linearly with $1/\tau$, while $D_s=D$. Only the slow part of $z(t)$ survives. One can check that, ignoring the dependence of Q on τ, the intensities Q_f and Q_s are monotonic functions of τ. While for $\tau=0$ one has the white-noise limit of $z(t)$ with rapid fluctuations $z_f(t)$, an increase of τ increases the role of z_s at the expense of decrease of the intensity of z_f, eliminating it completely as $\tau\to\infty$. Thus the fundamental difference between $z_s(t)$ and $z_f(t)$ consists in the different regimes of values of τ in which they exist: $z_s(t)$ occurs for $\tau\gtrsim t_t$ and hence fluctuates slowly, while $z_f(t)$ persists for $\tau\lesssim t_t$ and varies rapidly. Only for $\tau\sim t_t$ do they coexist.

A similar summation property to that for Gaussian noise does not apply to the dichotomic noise — one cannot display a given dichotomic noise as the sum of two independent dichotomic noises. However, the great similarity between the statistical properties of OUN and DN suggests treating the DN case in the same way. The definitions (3) and (4) involve the asymmetric character of two-state noise $z_f(t)$ and its dependence on $z_s(t)$, but for simplicity we assume that both $z_s(t)$ and $z_f(t)$ are symmetric, independent dichotomic noises of zero mean. Since OUN and DN have the same correlation function, the formulas (4)–(6) apply to the DN case as well.

We should also determine the value of integration interval t_t. For an unperturbed potential, it equals the relaxation time t_r from the top to the bottom of the well, but fluctuations of the potential lead to far-from-equilibrium conditions, so that this equality does not hold [19]. However, we do not intend here to consider the relationship between the processes of climbing up and relaxing down the fluctuating barrier. Rather, we need a tool for calculating the order of the duration of the second stage of the escape event. It is enough to take for it the value of t_r for a static barrier, which may be calculated as the MFPT from the top x_t to the bottom x_b of the well. It is shown in Fig. 1 that our results depend almost unnoticeably on the variation of t_t within the range of tens of percent. A more careful analysis would require us to take into account, not only the mean value, but also the statistical distribution of relaxation times [15].

Using the decomposition (3), the escape problem may be considered as a three-dimensional Markovian process. Its joint probability distribution $P(x,z_f,z_s,t)$ evolves accordingly to the FP equation similar to Eq. (2) but with two Λ's operators for z_f and z_s (with Q_f or Q_s instead of Q, respectively), and $z=z_f+z_s$ in $\mathcal{L}(x,z)$. Such a formulation allows for a clear separation of different time scales of the system dynamics. Since, by definition, z_s remains constant while the particle climbs the barrier, its dynamics may be analyzed by the kinetic approach. On the contrary, z_f vanishes for τ slightly greater than t_r, but still for $\tau\ll\mathcal{T}$, so rate theory applies. Thus we seek the probability distribution in the form $P(x,z_f,z_s,t)=p(x,z_f,t;z_s)\rho(z_s,t)$ [20].

The fast equilibration process is described by the evolution of $p(x,z_f,t;z_s)$, which is governed by the equation

$$\frac{\partial}{\partial t}p(x,z_f,t;z_s)=[\mathcal{L}(x,z_f;z_s)+\Lambda(z_f)]p(x,z_f,t;z_s), \tag{7}$$

where $\mathcal{L}(x,z_f;z_s)=(\partial/\partial x)[\mathcal{U}'(x;z_s)+V'(x)z_f]+q(\partial^2/\partial x^2)$ and the slow component of barrier fluctuations gives rise to different forms of potential configurations $\mathcal{U}(x;z_s)=U(x)+V(x)z_s$. Following a standard method, one looks for the quasipotential Φ being the dominant exponential term of the reduced (quasi)stationary probability distribution $\langle p(x,z_f;z_s)\rangle_{z_f}=p(x;z_s)\sim\exp[-\Phi(x;z_s)/q]$ of Eq. (7). For the DN case, we obtain an equation

$$\Phi'(x;z_s)[\mathcal{U}'(x;z_s)-\Phi'(x;z_s)]^2 =\frac{q}{\tau}[G(x)\Phi'(x;z_s)-\mathcal{U}'(x;z_s)], \tag{8}$$

whose middle (of the three always real) solution gives the quasipotential. This equation is formally similar to the result of Reimann and Elston [12], who consider the case $\tau\ll\mathcal{T}$,

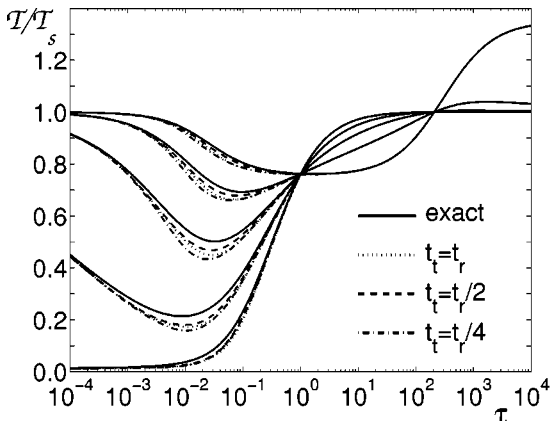

FIG. 1. Relative mean escape time $\mathcal{T}/\mathcal{T}_s$ versus τ for DN case with a triangle barrier $U(x)=10(1-|x|)$ and $V(x)=1-|x|$ confined to the interval $(-1,1)$ for $Q_0=1$, $q=1$, $x_{thr}=0$, $t_r=0.09$, and $\alpha=0$, 0.25, 0.50, 0.75, and 1.0 from the bottom to the top on the left-hand side, respectively. Solid lines show the exact results and the others the approximation (13) for few values of t_t.

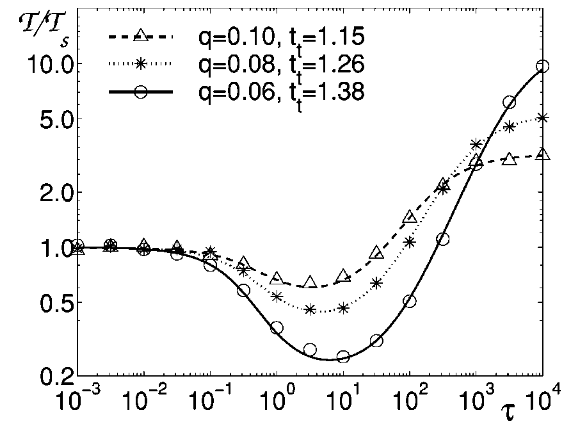

FIG. 2. Relative mean escape time $\mathcal{T}/\mathcal{T}_s$ versus τ for OUN case and the system with $U(x)=x^4/4-x^2/2$, $V(x)=U(x)+1/4$ for $|x|\leqslant 1$, and $V(x)=0$ elsewhere, for $q=0.08$, $Q_0=0.8$, $t_t=t_r/2=1.26$, and three values of α. The lines present our approximation and markers are from the numerical simulation of Eq. (1).

however. The only difference is the form of diffusion function $G(x)=1+(Q_f/q)V'(x)^2$. In Ref. [12] the total noise intensity Q is used, which gives an improper limiting value of Φ' for $\tau\to\infty$ for $\alpha=1$. Here $G(x)$ depends on Q_f, which vanishes for any α as $\tau\to\infty$, so one obtains the exact expression $\Phi'(x;z_s)\to\mathcal{U}'(x;z_s)$. In the opposite limit of $\tau\to 0$, the solution of Eq. (8) converges to the exact form $U'(x)/G(x)$. This suggests to deal not with the quasipotential but rather with an effective one

$$\mathcal{U}'_{eff}(x;z_s)=\Phi'(x;z_s)G(x). \tag{9}$$

Finally, exploiting the well-known form of the exact FP equation in the white-noise limit [21], one can write the effective FP operator

$$\mathcal{L}_{eff}(x;z_s)\equiv\frac{\partial}{\partial x}\mathcal{U}'_{eff}(x;z_s)+q\frac{\partial}{\partial x}\sqrt{G(x)}\frac{\partial}{\partial x}\sqrt{G(x)}, \tag{10}$$

which governs the fast part of the evolution.

A convenient way of finding the quasipotential in the OUN case formulates the problem by means of path integral or Hamiltonian techniques [22]. In general, the problem cannot be elaborated analytically, but asymptotic expressions for small and large τ, are available [11,13]. To attempt an interpolation between the two limits of τ we construct a 2-2 Padé approximant [23]:

$$\Phi'(x;z_s)=\frac{\mathcal{U}'(x;z_s)}{G(x)}\times\frac{1+\tau 2Q_fV'(x)^2\mathcal{W}(x;z_s)/G(x)+\tau^2\mathcal{W}(x;z_s)^2}{1+\tau^2\mathcal{W}(x;z_s)^2/G(x)}, \tag{11}$$

with $\mathcal{W}(x;z_s)=[G(x)/V'(x)][\mathcal{U}'(x;z_s)V'(x)/G(x)]'$. One can note that as a function of τ expression (11) has no singularities and it monotonically increases with τ, which is an anticipated property of quasipotential [13,22]. As for DN, we may also introduce an effective potential (9). Using Eq. (10), calculation of the MFPT $\mathcal{T}(z_s)$ for both types of barrier noise is straightforward.

In the slow time scale, the evolution of the system is governed by the Smoluchowski equation with a sink term,

$$\frac{\partial}{\partial t}\rho(z_s,t)=[\Lambda(z_s)-k(z_s)]\rho(z_s,t). \tag{12}$$

It describes stochastic switchings between the potential configurations of different z_s and an escape process from each of them $[k(z_s)=\mu/\mathcal{T}(z_s)$ with $\mu=1/2$ for $x_{thr}=x_t$, or $\mu=1$ for x_{thr} far from it]. One gets the mean escape time integrating $\rho(z_s,t)$ over $t\in(0,\infty)$, and summing/integrating over z_s for DN/OUN. For the dichotomic switching, the result is immediate:

$$\mathcal{T}=\frac{2\mathcal{T}_+\mathcal{T}_-+\mu\tau(\mathcal{T}_++\mathcal{T}_-)}{\mathcal{T}_++\mathcal{T}_-+2\mu\tau}, \tag{13}$$

where $\mathcal{T}_\pm$ are the MFPT's for $\mathcal{U}_\pm(x)=U(x)\pm\sqrt{D_s}V(x)$, respectively. Although Eq. (13) resembles the well-known solution [9,24] of a very simple set of equations (12), which constitutes the long-τ approximation of the problem [12], the dependence of $\mathcal{T}_+$ and $\mathcal{T}_-$ on $Q_f(\tau)$ involves also the fast part of the dynamics in formula (13).

The problem is much more complicated in the OUN case. To the best of the author's knowledge, there is no universal approximation of Eq. (12) valid for any τ [25]. One may calculate asymptotic expressions for small and large τ [11,26] and construct a Padé approximant to interpolate in between; however, the complicated exponential dependence of expansion terms on the amplitude of fluctuations yields a very bad approximation [27]. Hence, in what follows, we solve Eq. (12) numerically.

To test the method, we take the triangular barrier model [8] with DN. In Fig. 1, we plot $\mathcal{T}(\tau)/\mathcal{T}_s$ ($\mathcal{T}_s$ is the MFPT for a static barrier) for the exact analytical results and for the present method, in each case for few values of α. The relaxation time calculated from the exact formula [15] for the MFPT from $x_t=0$ to $x_b=1$ equals $t_r=0.09$. We show three sets of curves with $t_t=t_r$, $t_t=t_r/2$, and $t_t=t_r/4$, respectively. The agreement with the exact plot is very good, but in the interval $10^{-3}<\tau<10^{-1}$ our method gives slightly lower values. We have found the smallest deviation for $t_t=t_r/2$, but even when t_t is twice as large or small the difference is still not very significant. This validates the way we estimate the interval of integration t_t in Eq. (4). For simplicity in the next example we use $t_t=t_r/2$, but to be more precise, for each system a careful analysis of its best value should be done [27]. In Fig. 2, we display $\mathcal{T}(\tau)/\mathcal{T}_s$ for OUN case and three values of α. The agreement between the theory and numerical simulation of Eq. (1) is very good, but also with some underestimation in the region of the resonant activation minima. The results for other systems and other values of parameters are also excellent [27].

To conclude, we have presented a method of investigation of thermal activation in the presence of barrier fluctuations for arbitrary duration of their correlation. Dividing the barrier noise into two components—the slow and fast ones—we can separate two time scales of the evolution of the system for any value of τ and use both rate and kinetic approaches in the analysis without any sewing procedure. The noise division is done through an averaging over a finite interval of time t_t (4), hence we call the approach *a partial noise-averaging method* (PNAM). For a dichotomic perturbation, formula (13) together with the MFPT obtained for the FP operator (10) provides the analytical expression for the dependence $\mathcal{T}(\tau)$ for any $\tau\in[0,\infty)$, for arbitrary potentials $U(x)$ and $V(x)$, and a large class of noises. For the OUN we had to use a computer at the final step, but the accordance of the present result with the full-numerical ones confirms the power of PNAM. Although the method is presented in terms of MFPT, it can be expressed by means of any of the standard approaches [4] to the activation process. We hope also that the presented idea of splitting the noise could be useful in other problems where different time scales coexist, making the proposed approach valuable for many applications.

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