Nondecay probability of a metastable state: almost exact analytical description in wide range of noise intensity

Svetlana P. Nikitenkova
Nizhny Novgorod State Technical University, Applied Mathematics Dpt.,
24 Minin str., Nizhny Novgorod, 603155, Russia. E-mail: spn@waise.mntu.sci-nnov.ru

Andrey L. Pankratov
Institute for Physics of Microstructures of RAS, GSP 105,
Nizhny Novgorod, 603600, RUSSIA. E-mail: alp@ipm.sci-nnov.ru

This paper presents a complete description of noise-induced decay of a metastable state in a wide range of noise intensity. Recurrent formulas of exact moments of decay time valid for arbitrary noise intensity have been obtained. The nondecay probability of a metastable state was found to be really close to the exponent even for the case when the potential barrier height is comparable or smaller than the noise intensity.

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I. INTRODUCTION

Overdamped Brownian motion in a field of force (Markov process) is a model widely used for description of noise-induced transitions in different polystable systems. In many practical tasks (e.g. tasks of Josephson electronics, kinetics of chemical reactions and so on) it is enough to know the probability of transition or even only a time scale of transition. When the transition occurs over a potential barrier high enough in comparison with noise intensity, the probability of transition is a simple exponent \( \sim \exp(-t/\tau) \), where \( \tau \) is the mean transition time. In this case the mean transition time gives complete information about the probability evolution. The boundaries of validity of exponential approximation of the probability were previously studied in [2], [3]. In [2] authors extended the Mean First Passage Time to the case of "radiation" boundary condition and for two barrierless examples demonstrated good coincidence between exponential approximation and numerically obtained probability. In a more general case the exponential behavior of observables was demonstrated in [3] for relaxation processes in systems having steady states. Using the approach of "generalized moment approximation" the authors of [3] obtained the exact mean relaxation time to steady state and for particular example of a rectangular potential well demonstrated good coincidence of exponential approximation with numerically obtained observables. The considered in [3] example of the rectangular well does not have a potential barrier, and the authors of that paper supposed that their approach (and the corresponding formulas) should also give good approximation in tasks with diffusive barrier crossing for a wide range of noise intensity.

In the frame of this paper we consider a different case than in [2], [3]: we present investigation of nondecay probability of a metastable state. We treat the decay as a transition of Markov process trajectory outside the region of a metastable state. We consider namely the probability to find a realization of Markov process in a given interval, but not the probability to pass the boundary for the first time (First Passage Time formalism), since usually in experiment we can measure only the first one. In most of applied tasks no absorbing boundaries can be introduced and the precision of the used equipment allows to register the only fact of leaving the considered domain, but the boundary may be crossed many times during the transition (infinite number of times for Markov process, since this process is not differentiable).

Using the approach proposed by Malakhov [1], [2], that requires only knowledge of the behavior of a potential at \( \pm \infty \), we have decomposed the nondecay probability into a set of moments (cumulants), obtained recurrent formulas for these moments and approximately summarized them into the required probability. The obtained nondecay probability demonstrates exponential behavior with a good precision even in the case of a small potential barrier in comparison with noise intensity.

II. MAIN EQUATIONS AND SET UP OF THE PROBLEM

Consider a process of Brownian diffusion in a potential profile \( \Phi(x) \). Let a coordinate \( x(t) \) of the Brownian particle described by the probability density \( W(x, t) \) at initial instant of time has a fixed value \( x(0) = x_0 \) within the interval \( (c, d) \), i.e. the initial probability density is the delta function: \( W(x, 0) = \delta(x - x_0) \), \( x_0 \in (c, d) \).
In this case the one-dimensional probability density \( W(x,t) \) is the transition probability density from the point \( x_0 \) to the point \( x \): \( W(x,t) = W(x,t;x_0,0) \). It is known that the probability density \( W(x,t) \) of the Brownian particle in the overdamped limit satisfies to the Fokker–Planck equation (FPE):

\[
\frac{\partial W(x,t)}{\partial t} = -\frac{\partial G(x,t)}{\partial x} = \frac{1}{B} \left\{ \frac{\partial}{\partial x} \left[ \frac{d\varphi(x)}{dx} W(x,t) \right] + \frac{\partial^2 W(x,t)}{\partial x^2} \right\}.
\]

with the delta-shaped initial distribution. Here \( B = h/kT \), \( G(x,t) \) is the probability current, \( h \) is the viscosity (in computer simulations we put \( h = 1 \)), \( T \) is the temperature, \( k \) is the Boltzmann constant and \( \varphi(x) = \Phi(x)/kT \) is the dimensionless potential profile. In this paper we restrict ourselves by the case of metastable potentials, i.e. we consider an overdamped Brownian motion in a potential field \( \varphi(x) \) in systems, having metastable states, such that \( \varphi(-\infty) = +\infty \) and \( \varphi(+\infty) = -\infty \). This leads to the following boundary conditions: \( G(-\infty,t) = W(+\infty,t) = 0 \).

Note, that the results obtained may be generalized for potentials of arbitrary types, e.g. for such that \( \varphi(\pm\infty) = \infty \).

It is necessary to find the probability \( P(x_0,t) \) of a Brownian particle, located at the point \( x_0 \) \((t = 0)\) within the interval \((c,d)\) to be at the time \( t > 0 \) inside the considered interval: \( P(x_0,t) = \int_c^d W(x,t)dx \). Further we for simplicity will call the probability \( P(x_0,t) \) as nondecay probability. We suppose, that \( c \) and \( d \) are arbitrary chosen points of an arbitrary potential profile \( \varphi(x) \) and boundary conditions at these points may be arbitrary: \( W(c,t) \geq 0, W(d,t) \geq 0 \). In this case there is the possibility for a Brownian particle to come back in the interval \((c,d)\) after crossing boundary points.

### III. MOMENTS OF DECAY TIME

Consider the nondecay probability \( P(x_0,t) \). We can decompose this probability to the set of moments. On the other hand, if we know all moments, we can in some cases construct a probability as the set of moments. Thus, analogically to moments of the First Passage Time \([6]–[8]\) we can introduce moments of decay time (2), generally, moments of transition time, see \([9]\), where it was performed for the probability \( P(x,0,\infty) \) of a Brownian particle, located at the point \( x \) \((t = 0)\) within the interval \((c,d)\) to be at the time \( t > 0 \) inside the considered interval: \( P(x_0,t) = \int_c^d W(x,t)dx \). Further we for simplicity will call the probability \( P(x_0,t) \) as nondecay probability. We suppose, that \( c \) and \( d \) are arbitrary chosen points of an arbitrary potential profile \( \varphi(x) \) and boundary conditions at these points may be arbitrary: \( W(c,t) \geq 0, W(d,t) \geq 0 \). In this case there is the possibility for a Brownian particle to come back in the interval \((c,d)\) after crossing boundary points.

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\[
\tau_n(c,x_0,d) = < t^n > = \frac{\int_0^\infty t^n \frac{\partial P(x_0,t)}{\partial t} dt}{P(x_0,\infty) - P(x_0,0)}.
\]

Here we can formally denote the derivative of the probability divided by the normalization factor as \( w(x_0,t) \) and thus introduce the probability density of decay time \( w(x_0,t) \) in the following way:

\[
w(x_0,t) = \frac{\partial P(x_0,t)}{\partial t} \frac{1}{[P(x_0,\infty) - P(x_0,0)]}.
\]

It is important to mention that the moments of decay (transition) time \([2]\) is a generalization of the well-known moments of the First Passage Time for the case of arbitrary boundary conditions (see discussion in \([3]\)). For example, in the considered case of the potential \( \varphi(x) \) (such that \( \varphi(-\infty) = +\infty \) and \( \varphi(+\infty) = -\infty \)) the moments of decay time coincide with the corresponding moments of the First Passage Time, if a reflecting boundary at the point \( c \) and an absorbing boundary at the point \( d \) are introduced. On the other hand, if we consider the decay of metastable state as transition over a barrier top, and compare mean decay time obtained via approach discussed in the present paper (case of a smooth potential without absorbing boundary) and the mean First Passage Time (MFPT) of the absorbing boundary located at the barrier top, we get two times difference between these time characteristics even in the case of a high potential barrier in comparison with the noise intensity. This is due to the fact, that the MFPT does not take into account the backward probability current and therefore is sensitive to the location of an absorbing boundary. For the considered situation, if we will move the boundary point down from the barrier top, the MFPT will increase up to two times and tend to reach value of the corresponding mean decay time, which is less sensitive to the location of the boundary point over a barrier top. Such weak dependence of the mean decay time from the location of the boundary point at the barrier top or further is intuitively obvious: much more time should be spent to reach the barrier top (activated escape) than to move down from the barrier top (dynamic motion).

The required moments of decay time may be obtained via the approach proposed by Malakhov \([3, 4]\). This approach is based on the Laplace transformation method of the FPE \([4]\). Following this approach, one can introduce the function \( H(x,s) \equiv s\tilde{G}(x,s) \), where \( \tilde{G}(x,s) = \int_0^\infty G(x,t)e^{-st}dt \) is the Laplace transformation of the probability current, and expand it in the power series in \( s \):

\[
H(x,s) = \sum_{n=0}^{\infty} \frac{\partial^n \tilde{G}(x,s)}{\partial s^n} \bigg|_{s=0} x^n.
\]
\[ H(x, s) \equiv s\hat{G}(x, s) = H_0(x) + sH_1(x) + s^2H_2(x) + \ldots \] \hspace{1cm} (4)

It is possible to find the differential equations for \( H_n(x) \) (see [4], [5]; \( dH_0(x)/dx = 0 \)):

\[
\begin{align*}
\frac{dH_1(x)}{dx} &= \delta(x - x_0), \\
\frac{d^2H_n(x)}{dx^2} + \frac{d\varphi(x)}{dx} \frac{dH_n(x)}{dx} &= BH_{n-1}(x), \quad n = 2, 3, 4, \ldots 
\end{align*}
\]

Using the boundary conditions \( W(+\infty, t) = 0 \) and \( G(-\infty, t) = 0 \), one can obtain from (5) \( H_1(x) = 1(x - x_0) \) and

\[
\begin{align*}
H_2(x) &= -B \int_{-\infty}^{x} e^{-\varphi(v)} \int_{v}^{\infty} \varphi(y) 1(y - x_0) dy dv, \\
H_n(x) &= -B \int_{-\infty}^{x} e^{-\varphi(v)} \int_{v}^{\infty} \varphi(y) H_{n-1}(y) dy dv, \quad n = 3, 4, 5, \ldots
\end{align*}
\]

Why did we calculate this recurrent formula for the functions \( H_n(x) \)? The matter is, that from formula (2) (taking the integral by parts and Laplace transforming it using the property \( P(x_0, 0) - s\hat{P}(x_0, s) = \hat{G}(d, s) - \hat{G}(c, s) \) together with the expansion (3)) one can get the following expressions for moments of decay time:

\[
\begin{align*}
\tau_1(c, x_0, d) &= -H_2(d) - H_2(c), \\
\tau_2(c, x_0, d) &= 2H_3(d) - H_3(c), \\
\tau_3(c, x_0, d) &= -2 \cdot 3H_4(d) - H_4(c), \ldots \\
\tau_n(c, x_0, d) &= (-1)^n n! (H_{n+1}(d) - H_{n+1}(c)).
\end{align*}
\]

One can represent the \( n \)-th moment in the following form:

\[ \tau_n(c, x_0, d) = n!\tau_1^n(c, x_0, d) + r_n(c, x_0, d). \] \hspace{1cm} (8)

This is a natural representation of \( \tau_n(c, x_0, d) \) due to the structure of recurrent formulas (3), which is seen from the particular form of the first and the second moments for the case \( c = -\infty \) \( (c < x_0 < d) \). From the recurrent formulas (3), (4) one can obtain:

\[
\begin{align*}
\tau_1(-\infty, x_0, d) &= B \left\{ \int_{-\infty}^{d} e^{-\varphi(x)} dx \cdot \int_{0}^{\infty} \varphi(v) dv - \int_{0}^{x_0} e^{-\varphi(x)} \int_{0}^{\infty} \varphi(v) dv dx \right\}, \\
\tau_2(-\infty, x_0, d) &= 2B^2 \left\{ [\tau_1(-\infty, x_0, d)]^2 + \\
&\quad + \int_{-\infty}^{d} e^{-\varphi(x)} dx \cdot \int_{0}^{\infty} \varphi(v) \int_{d}^{\infty} e^{-\varphi(u)} \int_{0}^{\infty} e^{v(z)} dz du dv - \\
&\quad - \int_{0}^{x_0} e^{-\varphi(x)} \int_{0}^{\infty} \varphi(v) \int_{d}^{\infty} e^{-\varphi(u)} \int_{0}^{\infty} e^{v(z)} dz du dv dx \right\}.
\end{align*}
\]

Using the approach, applied in the paper by Shenoy and Agarwal [11] for analysis of moments of the First Passage Time, it can be demonstrated, that in the limit of a high barrier \( \Delta \varphi \gg 1 \) \( (\Delta \varphi = \Delta \Phi/kT \) is the dimensionless barrier height) the remainders \( r_n(c, x_0, d) \) in formula (3) may be neglected. For \( \Delta \varphi \approx 1 \), however, a rigorous analysis should be performed for estimation of \( r_n(c, x_0, d) \). Let us suppose, that the remainders \( r_n(c, x_0, d) \) may be neglected in wide range of parameters and further we will check numerically when our assumption is valid.

The cumulants of decay time \( \gamma_n \) [3], [8] are much more useful for our purpose to construct the probability \( P(x_0, t) \), that is the integral transformation of the introduced probability density of decay time \( w(x_0, t) \) [3]. Unlike the representation via moments, the Fourier transformation of the probability density (3) - the characteristic function - decomposed into the set of cumulants may be inversely transformed into the probability density.

Analogically to representation for moments (3), similar representation can be obtained for cumulants \( \gamma_n \):

\[ \gamma_n(c, x_0, d) = (n - 1)!\gamma_1^n(c, x_0, d) + R_n(c, x_0, d). \] \hspace{1cm} (11)
It is known that the characteristic function $\Theta(x_0, \omega) = \int_0^\infty w(x_0, t) e^{j\omega t} dt$ ($j = \sqrt{-1}$) can be represented as the set of cumulants ($w(x_0, t) = 0$ for $t < 0$):

$$\Theta(x_0, \omega) = \exp \left[ \sum_{n=1}^{\infty} \frac{c_n(x_0, d)}{n!} (j\omega)^n \right].$$ (12)

In the case, when the remainders $R_n(c, x_0, d)$ in (14) (or $r_n(c, x_0, d)$ in (8)) may be neglected, the set (12) may be summarized and inverse Fourier transformed:

$$w(x_0, t) = \frac{e^{-t/\tau}}{\tau},$$ (13)

where $\tau$ is the mean decay time [4], [3] ($\tau(c, x_0, d) \equiv \tau_1 = \omega_1$):

$$\tau(c, x_0, d) = B \left\{ \int_x^d e^{\varphi(x)} \int_c^d e^{-\varphi(v)} dv dx + \int_x^d e^{\varphi(x)} dx \int_c^d e^{-\varphi(v)} dv \right\}.$$ (14)

This expression is a direct transformation of formula (8), where $c$ is arbitrary, such that $c < x_0 < d$.

Probably, similar procedure was previously used (see [7], [4], [2], [13]) for summation of the set of moments of the First Passage Time, when exponential distribution of the First Passage Time probability density was demonstrated for the case of a high potential barrier in comparison with noise intensity.

IV. NONDECAY PROBABILITY EVOLUTION

Integrating probability density (14), taking into account definition (3), we get the following expression for the nondecay probability $P(x_0, t)$ ($P(x_0, 0) = 1$, $P(x_0, \infty) = 0$):

$$P(x_0, t) = \exp(-t/\tau),$$ (15)

where mean decay time $\tau$ is expressed by (14). Probability (15) represents a well-known exponential decay of a metastable state with a high potential barrier [1]. Where is the boundary of validity of formula (15) and when can we neglect by reminders $r_n$ and $R_n$ in formulas (8),(11)? To answer this question we have considered three examples of potentials having metastable states and compared numerically obtained nondecay probability $P(x_0, t) = \int W(x, t) dx$ with its exponential approximation (15). We used the usual explicit difference scheme to solve the FPE (2), supposing the reflecting boundary condition $G(c_6, t) = 0$ ($c_6 < c$) far above the potential minimum and the absorbing one $W(d_6, t) = 0$ ($d_6 > d$) far below the potential maximum, instead of boundary conditions at $\pm \infty$, such that the influence of phantom boundaries at $c_6$ and $d_6$ on the process of diffusion was negligible.

The first considered system is described by the potential $\Phi(x) = ax^2 - bx^3$. We have taken the following particular parameters: $a = 2$, $b = 1$ that leads to the barrier height $\Delta \Phi \approx 1.2$, $c = -2$, $d = 2a/3b$, and $kT = 0.5; 1; 3$. The corresponding curves of the numerically simulated probability and its exponential approximation are presented in Fig.1. In the worse case when $kT = 1$ the maximal difference between the corresponding curves is 3.2%. For comparison, there is also presented a curve of exponential approximation with the mean First Passage Time (MFPT) of the point $d$ for $kT = 1$ (dashed line). One can see, that in the latter case the error is significantly larger.

The second considered system is described by the potential $\Phi(x) = ax^4 - bx^5$. We have taken the following particular parameters: $a = 1$, $b = 0.5$ that leads to the barrier height $\Delta \Phi \approx 1.3$, $c = -1.5$, $d = 4a/5b$, and $kT = 0.5; 1; 3$. The corresponding curves of the numerically simulated probability and its exponential approximation are presented in Fig.2. In the worse case ($kT = 1$) the maximal difference between the corresponding curves is 3.4%.

The third considered system is described by the potential $\Phi(x) = 1 - \cos(x) - ax$. This potential is multistable. We have considered it in the interval $[-10, 10]$, taking into account three neighboring minima. We have taken $a = 0.85$ that leads to the barrier height $\Delta \Phi \approx 0.1$, $c = -\pi - \arcsin(a)$, $d = \pi - \arcsin(a)$, $x_0 = \arcsin(a)$, and $kT = 0.1; 0.3; 1$. The corresponding curves of the numerically simulated probability and its exponential approximation are presented in Fig.3. In difference with two previous examples, this potential was considered in essentially longer interval and with smaller barrier. The difference between curves of the numerically simulated probability and its exponential approximation is larger. Nevertheless, the qualitative coincidence is good enough.
Finally, we have considered an example of metastable state without potential barrier: $\Phi(x) = -bx^3$, where $b = 1$, $x_0 = -1$, $d = 0$, $c = -3$ and $kT = 0.1; 1; 5$. By dashed curve an exponential approximation with the MFPT of the point $d$ for $kT = 1$ is presented. It is seen, that even for such example the exponential approximation (with the mean decay time (14)) gives an adequate description of the probability evolution and that this approximation works better for larger noise intensity.

V. CONCLUSION

In the present paper the decay of metastable states, described by the model of Markov process, has been considered. Recurrent formulas of exact moments of decay time, valid for arbitrary noise intensity, have been obtained. Some concrete examples of metastable states have been analysed numerically, and the time evolution of the nondecay probability of a metastable state is found to be really close to the exponent even for the case when the potential barrier height is comparable or smaller than the noise intensity if the exact mean decay time (14) is substituted into the factor of exponent.

For all investigated examples, the exponential approximation gives an adequate behavior of the probability. This approximation may be used in a wide range of parameters, enough for solution of many practical tasks, but it is necessary to remark, that the exponential approximation may lead to a significant error in the case of extremely large noise intensity, and in the case when the noise intensity is small, the potential is tilted, and the barrier is absent (purely dynamical motion slightly modulated by noise perturbations).

VI. ACKNOWLEDGMENTS

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FIG. 1. Evolution of the nondecay probability for the potential $\Phi(x) = ax^2 - bx^3$ for different values of noise intensity; the dashed curve denoted as MFPT (mean First Passage Time) represents exponential approximation with MFPT substituted into the factor of exponent.
FIG. 2. Evolution of the nondecay probability for the potential \( \Phi(x) = ax^4 - bx^5 \) for different values of noise intensity.
FIG. 3. Evolution of the nondecay probability for the potential $\Phi(x) = 1 - \cos(x) - ax$ for different values of noise intensity.
FIG. 4. Evolution of the nondecay probability for the potential $\Phi(x) = -bx^3$ for different values of noise intensity; the dashed curve denoted as MFPT (mean First Passage Time) represents exponential approximation with MFPT substituted into the factor of exponent.