

## Non-Markovian fission rate within the Kramers model

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We investigate possible non-Markovian effects in fission dynamics of highly excited nuclei by using the generalized Langevin approach for a single nuclear shape parameter. We estimate the effective friction and stiffness coefficients of the non-Markovian dynamics for different values of the correlation time of the random force in the Langevin equation of motion. We discuss the found nonmonotonic dependence of the fission rate on the correlation time. We also show how to extend the Kramers theory of fission rate in the case of non-Markovian thermal diffusion over barrier.

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### I. INTRODUCTION

Starting from the pioneering work by Kramers [1], the induced fission of highly excited nuclei is considered as a diffusion process in the space of nuclear shape variables. The Kramers approach is a classical one and it does not take into consideration the Fermi statistic of nucleons, which is a significant ingredient of nuclear dynamics. The Fermi motion of nucleons creates the specific phenomenon of the Fermi surface distortion, which produces the dissipation processes and the non-Markovian (memory) effect on the nuclear dynamics; see Ref. [2]. One of well-known manifestations of such effects is a shift of the energy of the nuclear giant multipole resonances to the high-energy region with respect to the prediction of nuclear liquid drop model [3].

An advantage of the Kramers theory is that it connects fission characteristics to both the nuclear viscosity and the dissipation. On the other hand, the dissipation is related to the fluctuations of the corresponding collective variables because of the fluctuation-dissipation theorem. This fact allows one to apply Langevin approaches to study nuclear fission dynamics [4–6]. Both the dissipation and the fluctuations can be described by the introduction of friction and random forces, related to each other by the fluctuation-dissipation theorem. In general, the basic equations of motion for the nuclear shape parameters describing fission have a non-Markovian structure [7], which is caused by the energy flow between the macroscopic collective and intrinsic nucleonic modes. In an attempt to describe the rate characteristics of a nuclear fission process, the functional integral approach has been widely used [8]. The quantum decay rate of the nuclear compound state has been also derived within the local harmonic approximation [9], where non-Markovian effects were considered. In spite of such wide literature on the subject, the problem of classical activated (escape) rate over a nuclear fission barrier in the presence of non-Markovian effects has been left without appropriate attention. We are going to renew this deficiency by measuring a general quantitative impact of memory effects on the nuclear fission dynamics. In this respect, it is worth mentioning a series of works by Boilley [10], where some quantitative features of non-Markovian diffusion over a schematic parabolic barrier are discussed in terms of over-passing probability and saddle-to-scission time. Our main goal here is to investigate the non-Markovian effect on

the classical escape rate characteristics of the nuclear fission dynamics and to try to derive analytical expression for the escape rate. With this, we are aimed to extend the Kramers theory of escape rate to non-Markovian systems.

The plan of the paper is as follows. In Sec. II, we set in the generalized Langevin approach for a single nuclear shape parameter and discuss small and large correlation time limits of the fission dynamics. In Sec. III, we study the non-Markovian diffusive motion over a simple parabolic barrier in terms of some effective friction and stiffness coefficients, estimated for the motion near both the potential minimum position and barrier top. We compare the numerically found value of the fission rate with the analytical expression derived from our non-Markovian extension of the Kramers theory in Sec. IV. Summary and conclusions are given in Sec. V.

### II. FISSION DYNAMICS WITHIN THE NON-MARKOVIAN LANGEVIN APPROACH

To describe a process of symmetric fission of atomic nuclei, we use a phenomenological Langevin equation of motion for a single time-dependent variable  $q(t)$ , defining the shape of a nucleus:

$$B\ddot{q}(t) = -\frac{\partial E_{\text{pot}}}{\partial q} - \kappa_0 \int_0^t \exp\left(-\frac{|t-t'|}{\tau}\right) \dot{q}(t') dt' + \xi(t). \quad (1)$$

The generalized Langevin equation of the type (1) for collective modes of motion in Fermi systems has been first derived in Ref. [11] and rederived in many subsequent works; see, for example, Refs. [7,12–14].

In Eq. (1),  $B$  stands for a nuclear mass parameter,  $E_{\text{pot}}$  is the potential energy,  $\xi(t)$  is the random force, and the correlation time  $\tau$  measures the time spreading of the memory integral. For  $E_{\text{pot}}$ , we use a simple parabolic barrier, smoothly joined at  $q = q^*$  with a harmonic oscillator potential (Kramers potential, see Fig. 1),

$$E_{\text{pot}} = \begin{cases} (C_A/2)(q - q_A)^2, & q \leq q^*, \\ E_b + (C_B/2)(q - q_B)^2, & q > q^*, \end{cases} \quad (2)$$

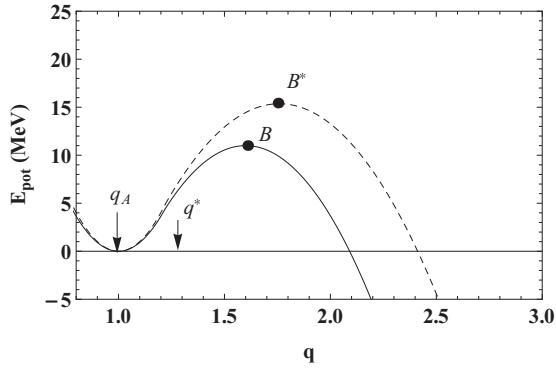


FIG. 1. The memory-induced renormalization (18) of the potential energy of the non-Markovian system (1)–(5), calculated at  $\kappa_0/|C_B| = 0.15$ , is shown by the dashed line. The Kramers potential  $E_{\text{pot}}$  (2) is given by the solid line.

where  $E_b$  is a height of the barrier and  $C_A, C_B$  are the values of a stiffness of the system,

$$C \equiv \frac{\partial^2 E_{\text{pot}}(q)}{\partial q^2} = \begin{cases} C_A, & q \leq q^*, \\ C_B, & q > q^*, \end{cases} \quad (3)$$

in the vicinity of the potential minimum position  $q_A$  and near barrier top at  $q_B$ , respectively.

Dissipative and fluctuating properties of the nuclear shape variable  $q(t)$  are determined by the random force  $\xi(t)$  Eq. (1) through the fluctuation-dissipation theorem:

$$\langle \xi(t)\xi(t') \rangle = \kappa_0 \exp\left(-\frac{|t-t'|}{\tau}\right), \quad (4)$$

where angular brackets mean the ensemble averaging. The correlation time  $\tau$  defines the characteristic interval within which the values of the random force  $\xi$  at different moments of time  $t$  and  $t'$  correlate significantly. The random force term  $\xi(t)$  in Eq. (1) corresponds to the Ornstein-Uhlenbeck process [15] defined as

$$\dot{\xi}(t) = -\frac{\xi(t)}{\tau} + \sqrt{\frac{\kappa_0 T}{\tau}} \zeta(t), \quad (5)$$

where  $\zeta(t)$  is a Gaussian white noise with

$$\langle \zeta(t) \rangle = 0, \quad \langle \zeta(t)\zeta(t') \rangle = 2\delta(t-t'). \quad (6)$$

The nuclear mass parameter  $B$  in Eq. (1) is taken as (see Ref. [7])

$$B = \frac{1}{5} Am R_0^2 \left(1 + \frac{1}{2q^3}\right), \quad (7)$$

where the shape parameter  $q$  of the deformed nucleus is measured in terms of a radius  $R_0$  of the equal volume spherical nucleus,  $A$  is a mass number of the nucleus, and  $m$  is the nucleon mass. In the sequel, we ignore the  $q$  dependence of the mass parameter  $B$  by putting  $q = q_B$  in Eq. (7). The stiffness coefficients  $C_A$  and  $C_B$ , characterizing the Kramers potential (2), are taken from Ref. [16]:

$$C_A = 182.4 \text{ MeV}, \quad C_B = -91.3 \text{ MeV}. \quad (8)$$

Numerical calculations were performed for a symmetric fission of the nucleus  $^{236}\text{U}$  at temperature  $T = 2 \text{ MeV}$  and with

$$q_A = 1, \quad q_B = 1.6, \quad q^* = 1.22, \quad E_b = 11 \text{ MeV}. \quad (9)$$

The parameter  $\kappa_0$ , measuring the strength of the dissipative and fluctuating properties (5) of the nuclear fission dynamics (1), is taken from the nuclear Fermi liquid-drop model [2,7]

$$\kappa_0 = \frac{6}{5} A \epsilon_F \frac{1}{q^2}, \quad (10)$$

where  $\epsilon_F$  is the Fermi energy and it is assumed that  $q = q_B$ . At last, the correlation time  $\tau$  in Eq. (1) is considered as a free parameter of the model varying in the range

$$\tau \in (0 \div 10) \times 10^{-23} \text{ s}. \quad (11)$$

Such a characteristic interval for the correlation time's variations appears in the calculations of the total kinetic energy and the variance of kinetic energy of fission fragments within the non-Markovian model (1)–(5) of nuclear fission dynamics; see Ref. [4]. Note that the range of the correlation time's variations (11) is in order smaller than the estimations of the corresponding time parameters used in the random matrix approach [17] or the linear response theory [18].

#### A. Small-correlation-time limit of non-Markovian dynamics

In order to clarify the role of non-Markovian effects in the Langevin fission dynamics (1)–(5), we shall consider qualitatively different regimes of the dynamics depending on the correlation time  $\tau$ .

At quite small correlation times  $\tau$ , one can use the following expansion for the time-retarded force in Eq. (1):

$$\begin{aligned} & -\kappa_0 \int_0^t \exp\left(-\frac{|t-t'|}{\tau}\right) \dot{q}(t') dt' \\ & = -\kappa_0 \tau \dot{q}(t) + O[(\sqrt{|C|/B}\tau)^2], \quad \sqrt{|C|/B}\tau \ll 1, \end{aligned} \quad (12)$$

In the same limit, we have for the random force  $\xi(t)$  (5)

$$\xi(t) = \sqrt{\kappa_0 \tau T} \zeta(t) + O[(\sqrt{|C|/B}\tau)^{3/2}], \quad \sqrt{|C|/B}\tau \ll 1. \quad (13)$$

Therefore, at sufficiently small correlation times  $\tau$  we obtain the Markovian Langevin limit of the fission dynamics (1)–(5),

$$\begin{aligned} B\ddot{q}(t) & = -C(q(t) - q_{A,B}) - \kappa_0 \tau \dot{q}(t) + \sqrt{\kappa_0 \tau T} \zeta(t) \\ & + O[(\sqrt{|C|/B}\tau)^2], \quad \sqrt{|C|/B}\tau \ll 1, \end{aligned} \quad (14)$$

described by a linear in  $\tau$  friction coefficient  $\kappa_0 \tau$ . Note that the memory-induced correction to the stiffness coefficient  $C$  appears in Eq. (14) from  $\tau^2$ -order terms only.

#### B. Large-correlation-time limit of non-Markovian dynamics

At fairly large correlation times  $\tau$ , one can show that

$$\begin{aligned} & -\kappa_0 \int_0^t \exp\left(-\frac{|t-t'|}{\tau}\right) \dot{q}(t') dt' \\ & = -\kappa_0 (q(t) - q[t=0]) + O\left(\frac{1}{\sqrt{|C|/B}\tau}\right), \quad \sqrt{|C|/B}\tau \gg 1, \end{aligned} \quad (15)$$

and

$$\xi(t) = \sqrt{\frac{\kappa_0 T}{\tau}} \int_0^t \zeta(t') dt' + O\left(\frac{1}{(\sqrt{|C|/B\tau})^{3/2}}\right),$$

$$\sqrt{|C|/B\tau} \gg 1. \quad (16)$$

As in the case of quite small correlation times  $\tau$  [see Eq. (14)], we get the Markovian equation of motion for the nuclear shape variable  $q(t)$ :

$$B\ddot{q}(t) = -\frac{\partial \tilde{E}_{\text{pot}}}{\partial q} + \sqrt{\frac{\kappa_0 T}{\tau}} \int_0^t \zeta(t') dt', \quad (17)$$

where

$$\tilde{E}_{\text{pot}}(q) = E_{\text{pot}}(q) + (1/2)\kappa_0(q - q[t = 0])^2 \quad (18)$$

is a renormalized potential energy.

To demonstrate the memory-induced renormalization (18) of the potential energy of the non-Markovian system (1)–(5) we plotted in Fig. 1 the value of  $\tilde{E}_{\text{pot}}$  by dashed curve, calculated at  $\kappa_0/|C_B| = 0.15$ . Such a quite small value for the ratio  $\kappa_0/|C_B|$  is used here just to demonstrate how the memory effects' renormalization of the system's potential energy (18) shows up. In all the subsequent calculations, it is used the value  $\kappa_0/|C_B| = 42$  [2,7]. The Kramers potential  $E_{\text{pot}}$  (2) is plotted in Fig. 1 by the solid line.

We see that at fairly large correlation times  $\tau$  the non-Markovian effects in the fission dynamics significantly enhance the system's stiffness (3),  $\tilde{C} = C + \kappa_0$ . Also one can claim that the memory-induced correction to the potential energy  $E_{\text{pot}}(q)$  greatly suppresses the escape over the fission barrier.

### III. FRICTION AND STIFFNESS COEFFICIENTS OF NON-MARKOVIAN DYNAMICS

In the general case, one can assume that the time-retarded force in the Langevin equation of motion (1) contains some time-irreversible (friction) part,  $-\gamma(t)\dot{q}(t)$ , and time-reversible (conservative) part,  $-C'(t)[q(t) - q(t = 0)]$ ,

$$-\kappa_0 \int_0^t \exp\left(-\frac{|t-t'|}{\tau}\right) \dot{q}(t') dt'$$

$$= -\gamma(t)\dot{q}(t) - C'(t)[q(t) - q(t = 0)]. \quad (19)$$

Such a friction-conservative splitting of the time-retarded force (19) at any value of the correlation time  $\tau$  is a natural generalization of the short-correlation time limit (12) (when the time-retarded force is reduced to Markovian friction force) and long-correlation time limit (15) (when the time-retarded force gives rise to the appearing of conservative force). As we will see below, this splitting is exact as far as the linearized motion of Eq. (1) is considered. We also point out that formally one can represent the time integral in Eq. (1) as a sum,

$$-\kappa_0 \int_0^t \exp\left(-\frac{|t-t'|}{\tau}\right) \dot{q}(t') dt' = -\kappa_0 \sum_{n=1}^{\infty} I_n(t) q^{(n)}(t), \quad (20)$$

where

$$I_n(t) = \int_0^t \exp\left(-\frac{t-t'}{\tau}\right) \frac{(t')^n}{n!} dt' \quad (21)$$

and  $q^{(n)}(t)$  stands for the  $n$ th-order time derivative of  $q(t)$ . In Eq. (20), the odd-order derivatives of the coordinate  $q(t)$  contribute to the time-irreversible friction part while the even-order derivatives give rise to the time-reversible conservative part of the retarded force. But higher-order (higher than the second one) derivatives  $q^{(n)}(t)$  can be expressed in terms of  $q(t)$ ,  $\dot{q}(t)$ , and  $\ddot{q}(t)$  by subsequent time differentiation of the Langevin equation of motion (1). This makes the splitting (19) reasonable.

For the motion near the potential minimum or barrier top (where the integrodifferential equation (1) may be linearized), the functions  $\gamma(t)$  and  $C'(t)$  in Eq. (19) can be found explicitly as

$$\gamma(t) = (-B) \frac{\ddot{A}(t)\mathcal{B}(t) - A(t)\ddot{\mathcal{B}}(t)}{\dot{A}(t)\mathcal{B}(t) - A(t)\dot{\mathcal{B}}(t)}, \quad (22)$$

$$C'(t) = C + B \frac{\ddot{A}(t)\dot{\mathcal{B}}(t) - \dot{A}(t)\ddot{\mathcal{B}}(t)}{\dot{A}(t)\mathcal{B}(t) - A(t)\dot{\mathcal{B}}(t)},$$

where  $\mathcal{A}(t)$  and  $\mathcal{B}(t)$  determine a general solution,

$$q(t) - q_{A,B} = \mathcal{A}(t)q(t = 0) + \mathcal{B}(t)v(t = 0)$$

$$+ \int_0^t \mathcal{B}(t-t')\xi(t') dt', \quad (23)$$

of the linear integrodifferential equation of motion (1). The result, Eq. (22), is obtained by plugging Eqs. (19) and (23) into Eq. (1) and equating coefficients in front of the initial position  $q(t = 0)$  and initial velocity  $v(t = 0) \equiv \dot{q}(t = 0)$ . Moreover,

$$\mathcal{A}(t) = 1 - \frac{C}{B} \int_0^t \mathcal{B}(t') dt',$$

$$\mathcal{B}(t) = D_1 e^{s_1 t} + D_2 e^{s_2 t} + D_3 e^{s_3 t}, \quad (24)$$

where  $s_1, s_2$ , and  $s_3$  are roots of the secular equation

$$s^3 + \frac{1}{\tau} s^2 + \frac{C + \kappa_0}{B} s + \frac{C}{\tau} = 0 \quad (25)$$

and the coefficients  $D_1, D_2$ , and  $D_3$  are equal to

$$D_1 = \frac{(s_1 + 1/\tau)}{(s_1 - s_2)(s_1 - s_3)}, \quad D_2 = \frac{-(s_2 + 1/\tau)}{(s_1 - s_2)(s_2 - s_3)},$$

$$D_3 = \frac{(s_3 + 1/\tau)}{(s_1 - s_3)(s_2 - s_3)}. \quad (26)$$

Different solutions of the cubic secular equation (25) are defined by a sign of the discriminant,

$$\Delta(\tau) = \frac{18C(C + \kappa_0)}{B\tau^2} - \frac{4C}{\tau^4} + \frac{(C + \kappa_0)^2}{B^2\tau^2}$$

$$- \frac{4(C + \kappa_0)^3}{B^3} - \frac{27C^2}{\tau^2}. \quad (27)$$

If  $\Delta > 0$ , then the cubic equation has three distinct real roots. If  $\Delta < 0$ , then one root (let us call it  $s_1$ ) is real, while the other two roots,  $s_2$  and  $s_2$ , are complex conjugated. In this respect, it is relevant to introduce into consideration a threshold value,

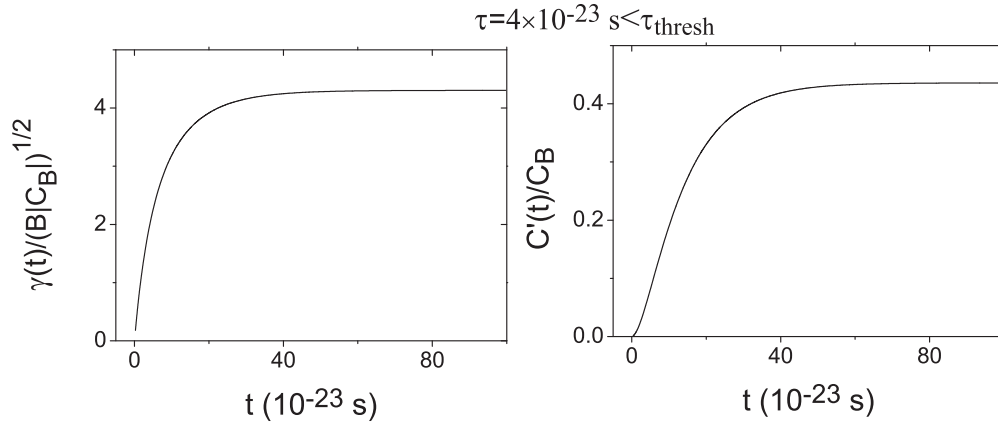


FIG. 2. Time dependences of the functions  $\gamma(t)$ ,  $C'(t)$  (22), defining the general friction-conservative splitting (19) of the time-retarded force in the Langevin equation of motion (1), for the motion near the barrier top and at correlation times  $\tau < \tau_{\text{thres}}$ .

$\tau_{\text{thres}}$ , of the correlation time  $\tau$  at which the discriminant (27) of the cubic equation (25) changes its sign,

$$\Delta(\tau = \tau_{\text{thres}}) = 0. \quad (28)$$

For the present choice of the model parameters (7)–(10) the threshold value of the correlation time  $\tau_{\text{thres}}$  is about  $4 \times 10^{-23}$  s.

### A. Motion near the barrier top

In the case of motion near the barrier top at  $q = q_B$  [when  $C \equiv C_B < 0$  in Eq. (25)], the first root  $s_1$  of the cubic secular equation (25) is positive at any value of the correlation time  $\tau$ . This root sets in an exponentially unstable mode of motion in Eq. (24), describing a subsequent drift from the barrier top.

The other two roots  $s_2$  and  $s_3$  of the cubic equation (25) are both real and negative at  $\tau < \tau_{\text{thres}}$  [see Eqs. (27) and (28)]. Modes of motion, associated with them, are exponentially decaying in time and of minor importance in comparing to the  $e^{s_1 t}$  mode. This fact can be illustrated in terms of the functions  $\gamma(t)$ ,  $C'(t)$  (22), defining the friction-conservative splitting (19) of the time-retarded force in the non-Markovian Langevin equation of motion (1), which are shown in Fig. 2.

We see that both functions  $\gamma(t)$ ,  $C'(t)$  subsequently saturate with time and approach the values [see Eqs. (22) and (24)]

$$\begin{aligned} \gamma_{0,B} &= (-2B)[s_1 + \min(s_2, s_3)], \\ C'_{0,B} &= (-B)[s_1 - \min(s_2, s_3)]^2, \quad \tau < \tau_{\text{thres}}, \end{aligned} \quad (29)$$

which can be treated as some effective friction,  $\gamma_{0,B}$ , and stiffness correction,  $C'_{0,B}$ , coefficients. In other words, at  $\tau < \tau_{\text{thres}}$  in the long time limit the non-Markovian dynamics (1)–(5) can be reduced to the corresponding Markovian one, in the presence of usual friction  $-\gamma_{0,B}\dot{q}(t)$  and conservative  $-C_B(q - q_B)$  forces.

The situation is principally different at the correlation times  $\tau$ , which are larger than the threshold value  $\tau_{\text{thres}}$ . Now, if the first root  $s_1$  of the secular equation (25) remains positively defined, the second  $s_2$  and third  $s_3$  roots become complex conjugated numbers. This means that the system (23) and (24) are initially trapped in the memory-induced dynamical barrier  $\tilde{E}_{\text{pot}}(q)$  (18) (see also Fig. 1), where it undergoes damped oscillations with a frequency  $(s_2 - s_3)/[2i]$  and damping rate  $-(s_2 + s_3)/2$ . Due to oscillatory character of motion at large correlation times  $\tau$ , the functions  $\gamma(t)$  and  $C'(t)$  have complex time behavior and do not have well-defined long time limits. In spite of that, we associate the effective friction coefficient  $\gamma_0$  to the damping rate  $-(s_2 + s_3)/2$  of the characteristic coordinate

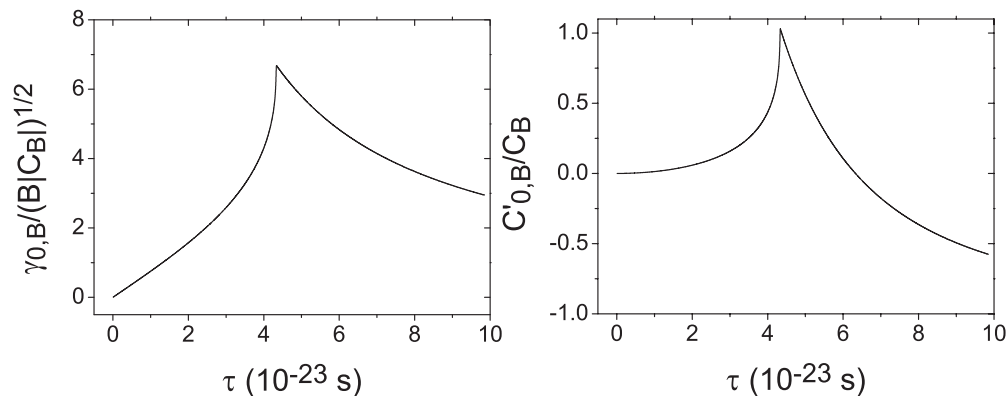


FIG. 3. The correlation-time dependence of the effective friction coefficient  $\gamma_{0,B}$  and the memory-induced correction  $C'_{0,B}$  to the stiffness (29) and (31) of the non-Markovian Langevin system (1)–(5) for the motion near the barrier top.

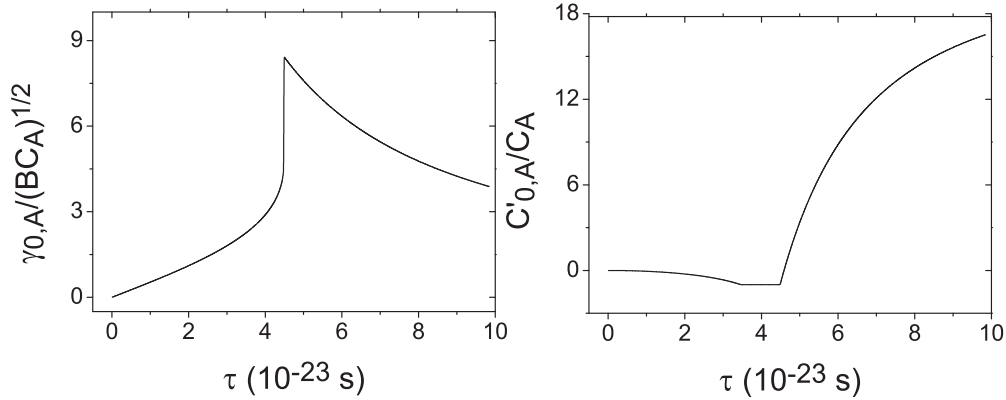


FIG. 4. The correlation-time dependence of the effective friction coefficient  $\gamma_{0,A}$  and the memory-induced correction  $C'_{0,A}$  to the stiffness (32) of the non-Markovian Langevin system (1)–(5) for the motion near the potential minimum.

oscillations, while the effective correction  $C'_0$  to the stiffness of the system can be estimated from the condition that

$$\sqrt{\left(\frac{\gamma(t)}{2B}\right)^2 - \frac{(C_B + C'(t))}{B}} - \frac{\gamma(t)}{2B} \rightarrow s_1, \quad \sqrt{|C_B|/Bt} \gg 1. \quad (30)$$

Thus,

$$\begin{aligned} \gamma_{0,B} &= (-B/2)(s_2 + s_3), \\ C'_{0,B} &= -C_B - B(4s_1^2 + 4s_1\gamma_{0,B}/B), \quad \tau > \tau_{\text{thresh}}. \end{aligned} \quad (31)$$

In Fig. 3, we reproduced the whole dependence of the effective friction coefficient  $\gamma_{0,B}$  and the memory-induced correction  $C'_{0,B}$  to the system's stiffness (3) on the correlation time  $\tau$ , given by the expressions (29) and (31).

We see that at sufficiently small correlation times  $\tau$  the friction coefficient  $\gamma_{0,B}$  grows linearly with  $\tau$  in accordance with the analytical result (14) and drops out at large values of  $\tau$  [see Eq. (17)]. On the other hand, the system's stiffness (3) gets a negative quadratic in  $\tau$  correction  $C'_0$  at small correlation times  $\tau$  while at fairly large correlation times ( $\tau > \tau_{\text{thresh}}$ ) the system's stiffness increases due to the positive additive  $C'_{0,B}$ .

### B. Motion near the potential minimum

Taking into account of the memory effects in the fission dynamics does not violate the oscillatory character of motion of the system (1)–(5) near the potential minimum at  $q_A$  [when  $C \equiv C_A > 0$  in Eq. (25)]. Thus, the time oscillations of the system's coordinate  $q(t)$  (23) are still defined by the complex conjugated roots  $s_2$  and  $s_3$  of the secular equation (25) and the root  $s_1$  is of minor importance as far as it is negative and the corresponding mode of motion  $e^{s_1 t}$ , associated with this root, drops out much faster than the periodic modes  $e^{s_2 t}$  and  $e^{s_3 t}$ . In view of this circumstance, we associate the effective friction coefficient  $\gamma_{0,A}$  of the non-Markovian fission dynamics (1)–(5) with damping rate of the system's oscillations and define the correction factor  $C'_0$  to the system's stiffness (3) through the difference between the memory-renormalized frequency of the oscillations and unperturbed value  $\omega_A$  (2),

$$\gamma_{0,A} = (-B/2)(s_2 + s_3), \quad C'_{0,A} = (B/4)(s_2 - s_3)^2 - C_A. \quad (32)$$

The parameters  $\gamma_{0,A}$  and  $C'_{0,A}$  as functions of the correlation time  $\tau$  are plotted in Fig. 4.

As in the case of motion near the barrier top (see Fig. 3), the friction coefficient  $\gamma_0$  behaves nonmonotonically with the correlation time  $\tau$ , increasing linearly [according to the result (14)] with  $\tau$  at quite small correlation times and dropping out [in agreement with the result (17)] at fairly large correlation times. Notice that at  $\tau < \tau_{\text{thresh}}$ , the memory effects diminish the system's stiffness (3) and significantly enhance it at  $\tau \geq \tau_{\text{thresh}}$ ; see Eq. (18).

## IV. FISSION RATE

It is of interest to look at how the previously described time features of the non-Markovian Langevin dynamics (1)–(5) manifest themselves in observable characteristics like fission rate. With this purpose, we introduce a rate,  $R(t)$ , of probability over the barrier as

$$R(t) = -\frac{1}{\mathcal{P}(q[t] \leq q_B)} \frac{d[\mathcal{P}(q[t] \leq q_B)]}{dt}, \quad (33)$$

where  $\mathcal{P}(q[t] \leq q_B)$  is a probability of finding the system  $q(t)$  on the left from the barrier top  $q_B$  up to time  $t$ . In Fig. 5, we present the time-dependent probability rate  $R(t)$  (33) of

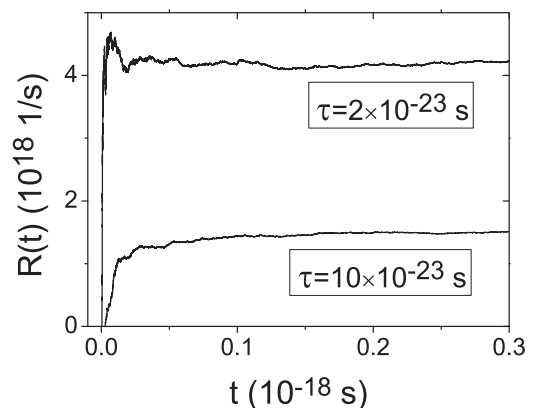


FIG. 5. Time dependence of the probability rate  $R(t)$  (33) at the correlation times  $\tau = 2 \times 10^{-23}$  s and  $\tau = 10 \times 10^{-23}$  s.



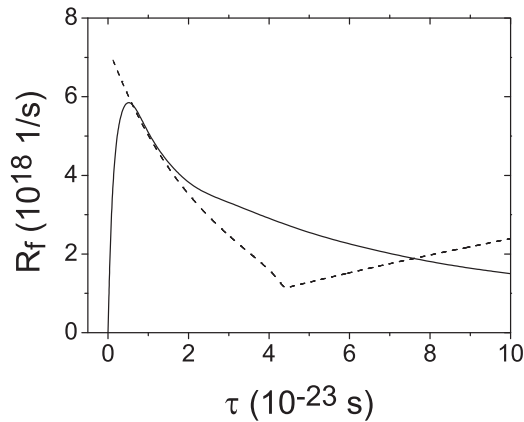


FIG. 6. The fission rate  $R_f$  as an asymptotic value of the probability rate (33) (solid line) as a function of the correlation time  $\tau$ . The standard Kramers formula (34) for the fission rate with the  $\tau$ -dependent friction coefficient  $\gamma_{0,B}$  of Eqs. (29) and (31) is given by the dashed line.

the non-Markovian dynamics (1)–(5) at  $\tau = 2 \times 10^{-23}$  s and  $\tau = 10 \times 10^{-23}$  s.

Importantly that the rate  $R(t)$  of the probability flow across the barrier subsequently saturates with time and approaches some constant value  $R_f$  both at sufficiently small correlation times  $\tau = 2 \times 10^{-23}$  s (when the memory effects in the fission dynamics are relatively weak) and at quite large correlation time  $\tau = 10 \times 10^{-23}$  s (when the memory effects are strong enough). The constancy of the probability rate  $R(t)$  at large times  $t$  implies the stationary regime of thermal nuclear diffusion (1)–(5) over the fission barrier, which is characterized by the fission rate  $R_f$ . The fission rate  $R_f$  (33) as a function of the correlation time  $\tau$  is displayed in Fig. 6 by a solid line. For comparison, we showed in Fig. 6 by a dashed line the fission rate calculated within the standard Kramers formula [1], which in our notation reads as

$$R_{\text{Kr}} = \frac{1}{2\pi} \sqrt{\frac{C_A}{B}} \left( \sqrt{\left( \frac{\gamma_{0,B}}{2\sqrt{B|C_B|}} \right)^2 + 1} - \frac{\gamma_{0,B}}{2\sqrt{B|C_B|}} \right) \times \exp\left(-\frac{E_b}{T}\right), \quad (34)$$

where the  $\tau$ -dependent friction coefficient  $\gamma_{0,B}$  is given by the expressions (29) and (31).

The fission rate increases from zero up to some value at  $\tau \approx 0.5 \times 10^{-23}$  s. We believe that for our choice  $\kappa_0 \exp(-|t - t'|/\tau)$  for the memory kernel in the non-Markovian Langevin equation of motion (1) the initial growth of the fission rate at small correlation times  $\tau$  has a threshold character. It follows

from Eq. (14) that the thermal diffusion across the barrier is absent at  $\tau = 0$  and rises linearly with the correlation time  $\tau$ . The relative role of the friction force  $|\gamma_0 \dot{q}(t)|$  in the fission dynamics also grows linearly with  $\tau$  [according to Eq. (14)] but it remains much smaller than the effect of the conservative force  $|C(q - q_{A,B})|$  on the dynamics  $\gamma_0/\sqrt{B|C|} \ll 1$  at  $\tau < 0.5 \times 10^{-23}$  s (see Figs. 3 and 4). Only at the correlation time  $\approx 0.5 \times 10^{-23}$  s are the contributions from the friction and conservative forces comparable and the thermal diffusion across the barrier stops rising. From  $0.5 \times 10^{-23}$  s to the threshold value  $4.5 \times 10^{-23}$  s (when the memory effect on the fission dynamics is still relatively weak), the friction part of the time-retarded force in Eq. (1) dominates over the conservative part  $|C'_0(q - q_{A,B})|$  and we observe the corresponding decrease of the fission rate with the correlation time  $\tau$ . When the non-Markovian effects in the fission dynamics (1)–(5) are relatively strong (as at  $\tau \geq \tau_{\text{thresh}}$ ), the decrease of the rate  $R_f$  of thermal diffusion over the barrier is caused by the growing role of the conservative part  $|C'_0(q - q_{A,B})|$  of the time-retarded force in Eq. (1), when the system's stiffness is enlarged by amount  $C'_0 > 0$ ; see Figs. 3 and 4.

We see that taking into account of only the friction part  $|\gamma_0 \dot{q}(t)|$  of the time-retarded force in Eq. (1) leads to the increase of the fission rate with the correlation time at  $\tau \geq \tau_{\text{thresh}}$ . The same quantitative conclusion on the non-Markovian impact on the fission dynamics can be met in Ref. [10], where it is made by evaluating the overpassing probability over a schematic parabolic barrier. There, because of a different choice,  $(1/\tau)\exp(-|t - t'|/\tau)$ , of the memory kernel in the generalized Langevin equation of the type (1), the relative role of the time-retarded force  $\int_0^t (1/\tau)\exp(-|t - t'|/\tau)\dot{q}(t')dt'$  diminishes with the correlation time  $\tau$ . This, in turn, leads to the non-Markovian acceleration of thermal diffusion over the barrier. In our case of the memory kernel  $\exp(-|t - t'|/\tau)$  of the Langevin equation of motion (1), the friction part  $|\gamma_0 \dot{q}(t)|$  of the time-retarded force drops out at the long correlation time limit while the conservative part  $C_0(q(t) - q_0)$  survives and significantly enhances the system's stiffness; see Eq. (15). Therefore, the system's stiffness near the barrier top  $C_B$  in the Kramers formula (34) should be appropriately renormalized in order to correctly reproduce the decrease of the fission escape rate at large values of the correlation time  $\tau$ . With this purpose, we are going to extend the Kramers theory [1] on non-Markovian diffusion over the barrier, Eqs. (1)–(5).

#### A. Non-Markovian extension of the Kramers theory

The non-Markovian dynamics (1)–(5) may be considered as a two-dimensional Gaussian random process  $(q(t), q_0; v(t), v_0; t)$ , defined by the probability distribution function [15],

$$W(q, q_0; v, v_0; t) = \frac{1}{2\pi \sigma_q(t) \sigma_v(t) \sqrt{1 - r_{qv}(t)}} \times \exp a \left( -\frac{1}{2[1 - r_{qv}^2(t)]} \left\{ \frac{[q - \langle q(t) \rangle]^2}{\sigma_q^2(t)} + \frac{[v - \langle v(t) \rangle]^2}{\sigma_v^2(t)} - \frac{2r_{qv}(t)[q - \langle q(t) \rangle][v - \langle v(t) \rangle]}{\sigma_q(t) \sigma_v(t)} \right\} \right),$$

where, as it follows from Eq. (23),

$$\langle q(t) \rangle = A(t)q_0 + B(t)v_0, \quad \langle v(t) \rangle = \dot{A}(t)q_0 + \dot{B}(t)v_0, \quad (35)$$

and

$$\begin{aligned} \sigma_q^2(t) &\equiv \langle q^2(t) \rangle - \langle q(t) \rangle^2 = \kappa_0 T \int_0^t dt_1 \int_0^t dt_2 B(t-t_1)B(t-t_2) \exp\left(-\frac{|t_1-t_2|}{\tau}\right), \\ r_{qv}(t) &\equiv \langle q(t)v(t) \rangle = \kappa_0 T \int_0^t dt_1 \int_0^t dt_2 B(t-t_1)\dot{B}(t-t_2) \exp\left(-\frac{|t_1-t_2|}{\tau}\right), \\ \sigma_v^2(t) &\equiv \langle v^2(t) \rangle - \langle v(t) \rangle^2 = \kappa_0 T \int_0^t dt_1 \int_0^t dt_2 \dot{B}(t-t_1)\dot{B}(t-t_2) \exp\left(-\frac{|t_1-t_2|}{\tau}\right). \end{aligned} \quad (36)$$

Knowing the probability distribution function  $\mathcal{W}(q, q_0; v, v_0; t)$ , one can obtain the corresponding Fokker-Planck equation of the non-Markovian fission dynamics (1)–(5). By using the result of Ref. [19], we write the Fokker-Planck equation as

$$\frac{\partial W}{\partial t} + v \frac{\partial W}{\partial q} + \frac{[C + C'(t)]}{B} q \frac{\partial W}{\partial v} = \frac{\gamma(t)}{B} \frac{\partial}{\partial v} [vW] + \frac{T\gamma(t)}{B} \frac{\partial^2 W}{\partial v^2} + \frac{C'(t)}{C} T \frac{\partial^2 W}{\partial v \partial q}, \quad (37)$$

where the functions  $\gamma(t)$ ,  $C'(t)$  are given by Eq. (22) and the system's stiffness  $C$  is defined by Eq. (3). The non-Markovian character of the fission dynamics shows up in the Fokker-Planck equation (37) through the time dependencies of the functions  $\gamma(t)$ ,  $C'(t)$  and in the presence of a cross-term,  $\sim \partial^2 W / \partial v \partial q$ .

We would like to find a stationary solution,  $W_{\text{stat}}$ , to the Fokker-Planck equation (37). In the vicinity of the potential minimum  $q_A$ , the stationary solution is given by modified a Maxwell-Boltzmann distribution,

$$W_{\text{stat},A}(q \equiv q - q_A; v) = \text{const} \cdot \exp\left(-\frac{(B/2)v^2}{T} - \frac{(C_A/2)q^2}{T(1 + C'_{0,A}/C_A)}\right), \quad (38)$$

while near the barrier top  $q_B$ , it can be seen in the following form:

$$W_{\text{stat},B}(q \equiv q - q_B; v) = \text{const} \cdot F(q, v) \cdot \exp\left(-\frac{(B/2)v^2}{T} - \frac{[E_b + (C_B/2)q^2]}{T(1 + C'_{0,B}/C_B)}\right). \quad (39)$$

In Eqs. (38) and (39) it is assumed that in the long time limit the functions  $\gamma(t)$ ,  $C'(t)$  (22) may be associated with the effective friction coefficient  $\gamma_0$  and the memory-induced correction  $C'_0$  to the system's stiffness at any value of the correlation time  $\tau$ ; see our remarks on the validity of this assumption before Eqs. (31) and (32).

By substituting the solution (39) into Eq. (37), we obtain an equation for unknown function  $F(q, v)$ :

$$\left(1 + \frac{C'_{0,B}}{C_B}\right) v \frac{\partial F}{\partial q} + \left(-\frac{C_B}{B(1 + C'_{0,B}/C_B)} q + \frac{\gamma_{0,B}}{B} v\right) \frac{\partial F}{\partial v} = \frac{T\gamma_{0,B}}{B} \frac{\partial^2 F}{\partial v^2} + \left(1 + \frac{C'_{0,B}}{C_B}\right) \frac{T}{B} \frac{\partial^2 F}{\partial v \partial q}. \quad (40)$$

Let us make the ansatz for the function  $F$ :

$$F \equiv F(v - aq) \equiv F(\chi), \quad (41)$$

where a constant  $a$  is defined by the boundary conditions:

$$F \rightarrow 1, \quad \chi \rightarrow -\infty; \quad F \rightarrow 0, \quad \chi \rightarrow +\infty. \quad (42)$$

Here, we assumed that the relative locations  $q \equiv q - q_B$  of the potential minimum and the barrier top are far from each other so that initially almost all the particles concentrate near the potential minimum ( $F \rightarrow 1$ ,  $\chi \rightarrow -\infty$ ), while there is no particles on the right from the barrier top ( $F \rightarrow 0$ ,  $\chi \rightarrow +\infty$ ).

One can show that

$$F(\chi) = F_0 \int_{-\infty}^{\chi} \exp\left[-\frac{[(1 + C'_{0,B}/C_B)a - \gamma_{0,B}/B]}{(2T/B)[\gamma_{0,B}/B - (C'_{0,B}/C_B)a]} \chi'^2\right] d\chi', \quad (43)$$

with

$$F_0 = \sqrt{\frac{[(1 + C'_{0,B}/C_B)a - \gamma_{0,B}/B]}{(2\pi T/B)[\gamma_{0,B}/B + (C'_{0,B}/C_B)a]}} \quad (44)$$

and

$$a = \frac{1}{(1 + C'_{0,B}/C_B)} \sqrt{\frac{|C_B|}{B}} \left[ \sqrt{\left(\frac{\gamma_{0,B}}{2\sqrt{B}|C_B|}\right)^2 + (1 + C'_{0,B}/C_B)} + \frac{\gamma_{0,B}}{2\sqrt{B}|C_B|} \right]. \quad (45)$$

Following Kramers [1], we calculate a number of particles,  $\nu_A$ , in the vicinity of the potential minimum as [see Eq. (38)]

$$\nu_A = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} W_{\text{stat},A}(q; v) dq dv \quad (46)$$

and a particle's current,  $j_B$ , across the barrier top as [see Eq. (39)]

$$j_B = \int_{-\infty}^{+\infty} W_{\text{stat},B}(q = q_B; v) v dv. \quad (47)$$

In Eq. (46), the integration limits over  $q \equiv q - q_A$  were extended from  $-\infty$  to  $+\infty$  as far as the main contribution to the integral arises from a small region near  $q = 0$ . We define a stationary rate of escape of particles over the barrier as a ratio

$$R_{\text{Kr-nonMark}} = \frac{j_B}{\nu_A}. \quad (48)$$

The result reads

$$R_{\text{Kr-nonMark}} = \frac{1}{2\pi} \sqrt{\frac{C_A}{B}} \left( \sqrt{\left(\frac{\gamma_{0,B}}{2\sqrt{B}|C_B|}\right)^2 + (1 + C'_{0,B}/C_B)} - \frac{\gamma_{0,B}}{2\sqrt{B}|C_B|} \right) \exp\left(-\frac{E_b}{T}\right). \quad (49)$$

In fact, the non-Markovian character of the thermal diffusion across the barrier (1)–(5) reveals itself in the renormalization of the system's stiffness coefficient near the barrier top,  $C_B \rightarrow C_B + C'_{0,B}$ . We point out that our result (49) for the non-Markovian Kramers rate coincides with the result of transition-state theory, developed by Grote and Hynes in Ref. [20]:

$$R_{\text{Kr}}^{TST} = \frac{1}{2\pi} \sqrt{\frac{C_A}{|C_B|}} s_1 \exp\left(-\frac{E_b}{T}\right), \quad (50)$$

where  $s_1$  is the largest positive root of the secular equation (25) and where Eq. (30) was used.

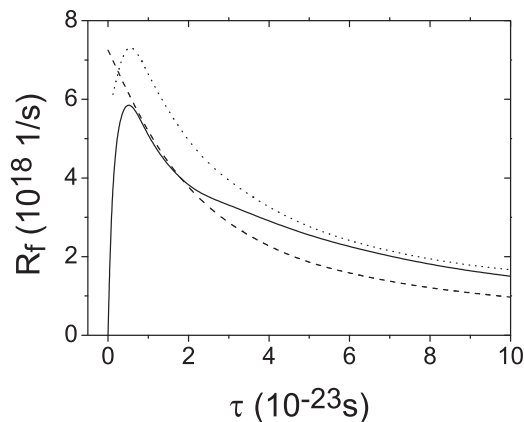


FIG. 7. The fission rate  $R_f$  as an asymptotic value of the probability rate (33) (solid line) vs the correlation time  $\tau$ . The non-Markovian extension of the Kramers theory (49) for the fission rate is shown by the dashed line. The dotted line represents the fission rate  $R_f$  calculated as inverse first-passage time (51).

In Fig. 7, we compared the fission rate  $R_f$  (33), numerically calculated from the non-Markovian Langevin dynamics (1)–(5) and which is shown by solid line, with our analytical estimation (49) of the fission rate, represented in the figure by the dashed line. Also, in the figure we present (by dotted line) the value of the fission rate  $R_f$  calculated as

$$R_f = \frac{1}{\langle t_{AB} \rangle}, \quad (51)$$

where  $\langle t_{AB} \rangle$  is the mean time of motion from the potential minimum position (point A in Fig. 1) to the barrier top (point B in Fig. 1).

We see that the memory-modified Kramers formula (49) correctly reproduces the decrease of the fission rate  $R_0$  at moderate and fairly large values of  $\tau$ . Notice that the difference between the result (49) and numerically calculated value of the fission rate grows with the correlation time  $\tau$ , due to the possibly inaccurate estimation (31) of the memory-induced correction  $C'_{0,B}$  to the system's stiffness near the barrier top.

It is interesting that the inverse mean first-passage time estimation (51) for the fission rate perfectly describes the  $R_f$  at large correlation times  $\tau$ . As the correlation time  $\tau$  increases, the expression (51) better fits the numerically calculated value of the fission rate. The reason for that is probably the over-damped character of motion at large values of the correlation times, when the memory effects are relatively strong but the effective friction coefficient  $\gamma_{0,B}$  is much larger than the renormalized stiffness coefficient  $|C_B + C'_{0,B}|$ ; see Fig. 3.

## V. SUMMARY

In attempt to understand the influence of non-Markovian character of collective motion on the rate of symmetric fission of highly excited atomic nuclei, we have applied the



generalized Langevin approach (1)–(5) for a single nuclear shape variable  $q(t)$ . The potential energy of the deformation of a nucleus  $E_{\text{pot}}$  (2) has been taken in a simple form of a smooth joining of the harmonic oscillator potential with the inverted parabolic potential [see Eq. (2)]. The strength of the non-Markovian effects in the nuclear fission dynamics (1)–(5) has been measured by the correlation time  $\tau$ , defining different regimes of the motion. We have demonstrated that the non-Markovian effects disappear either (i) at quite small correlation times, when the motion undergoes in the presence of usual friction and  $\delta$ -correlated random forces (14), or (ii) at fairly large correlation times, when the stiffness of the system (3) is significantly enhanced; see Eq. (18) and the dashed lines in Fig. 1.

At moderate values of the correlation time  $\tau$ , we have assumed general friction-conservative splitting (19) of the time-retarded force in the Langevin equation of motion (1). The time-dependent functions  $\gamma(t), C'(t)$ , determining such a splitting, have been found analytically (22) through the solution to the secular equation (25), and those roots define different modes of motion of the system. We have shown that in the case of weak memory effects (when all roots of the secular equation are real) the functions  $\gamma(t), C'(t)$  go with time to finite limiting values, which may be naturally associated with some effective friction coefficient  $\gamma_0$  and memory-induced correction  $C'_0$  to the system's stiffness  $C$  (3); see Figs. 3 and 4. The proposed analytical expressions for the coefficients  $\gamma_0, C'_0$  [Eqs. (31) and (32)] in the opposite case of quite strong memory effects (when two roots of the secular equation (25) are complex conjugated and the motion of the system becomes oscillating) show the decrease of friction with the size  $\tau$  of the memory effects and the enhancement of the system's stiffness  $C + C'_0$  with the growth of  $\tau$ .

To calculate the rate characteristics of symmetric fission of heavy nuclei, we have solved numerically the Langevin equation of motion (1) for the probability flow  $R(t)$  (33) across the parabolic barrier and have defined the fission rate  $R_f$  as a corresponding long time limit of  $R(t)$ ; see Fig. 5. Nonmonotonic dependence of the fission rate on the size  $\tau$  of the non-Markovian effects in the Langevin dynamics (1), when the rate of symmetric fission grows initially at small values of  $\tau$  and decreases at large correlation times  $\tau$ , has been observed (see Fig. 6). We have attributed the initial growth of the fission rate to the action of the usual conservative force  $-\partial E_{\text{pot}}/\partial q$ , which is slightly enhanced by the non-Markovian effects (see Figs. 3 and 4) and which remains sufficiently larger than the friction force  $-\gamma_0 \dot{q}(t)$ . The subsequent decrease of the fission rate in Fig. 6 at moderate correlation times  $\tau$  has been explained by the growing role of the friction, when the motion of the system becomes overdamped. At large correlation times  $\tau$ , the fission rate drops out due to the blocking of the system, appearing as a result of the non-Markovian renormalization of the stiffness coefficient (18).

In addition to the numerical calculations of the fission rate, we have suggested the non-Markovian extension of the classical Kramers result for the escape rate over the parabolic barrier. We have shown that the memory effects are manifested in the Kramers rate formula (49) as a modification of the system's stiffness at the barrier top,  $C \rightarrow C + C'_{0,B}$ . Such kind of modification reduces the fission rate  $R_f$  in the long-time correlation regime, improving the agreement of the Kramers rate formula (49) with the result of exact solution of the non-Markovian Langevin equation of motion (1); see the dashed line in Fig. 7.

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