Fission rate in multi-dimensional Langevin calculations

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(Received 26 September 2006; revised manuscript received 4 April 2007; published 25 June 2007)

Experimental data on nuclear dissipation have often been interpreted using one-dimensional model calculations of the Langevin or Fokker-Planck type. In the present work, the influence of the dimensionality of the deformation space on the time dependence of the fission process has been investigated in a systematic and quantitative way. In particular, the dependence of the transient time and the stationary value of the fission rate on the number of collective coordinates involved in Langevin calculations is investigated for the one-body and two-body dissipation mechanisms. We show that the results of Langevin-type calculations change appreciably if the deformation space is extended up to three dimensions.

DOI: 10.1103/PhysRevC.75.064614 PACS number(s): 25.85.−w, 05.10.Gg

I. INTRODUCTION

The dynamical formulation of the fission process as the passage over a saddle point from a "metastable" region (around the nuclear ground state) to a "stable" region (corresponding to the separated fission fragments) is the specific case of a rather general problem appearing in many fields of statistical mechanics and chemistry. One of the earliest mathematical formulations of this kind of problem was given by Becker and Döring [1] concerning the formation of drops in a supersaturated vapor. The first to consider the dynamics of nuclear fission was Kramers [2]. He based his consideration on the Brownian motion in a potential well.

In all these studies, the problem was treated using only one collective variable. Furthermore, only the asymptotic quasistationary stage of the process was investigated. Later, important progress has been made to overcome these restrictions. The efforts were undertaken in two directions: on the one hand, the dimensionality of the problem was extended. In 1956 Brinkmann [3] generalized Kramer's work to n dimensions. More elaborate studies on the statistical theory of the decay of metastable states of a multi-dimensional system were made later, e.g., by Landauer and Swanson [4], and Langer [5,6]. Similar studies, directly dedicated to the nuclear-fission problem were performed by Weidenmüller and Jing-Shang [7,8], and Brink and Canto [9]. On the other hand, the time behavior of the decay process was explicitly explored. Grangé, Jun-Qing, and Weidenmüller [10] considered the transient effects in nuclear fission, occurring during the relaxation of the system to quasiequilibrium. Many other papers of these and other authors followed, investigating this problem in more detail.

All these studies were performed on the basis of the integral form of the stochastic equation of the Fokker-Planck type. These investigations remained rather schematic and approximate, mostly due to the limitations of the technical methods for solving these equations. In the special problem of the statistical decay of a metastable state in many dimensions, the studies were essentially limited to quadratic approximations to the multi-dimensional potential and to isotropic mass and friction tensors, not depending on the collective coordinates. Under these restrictions, the influence of the variation of the width of the potential in the directions perpendicular to the decay path along the decay path has been demonstrated, see [7] and references therein.

An important technical step forward toward more realistic calculations of the decay process was made by Abe, Grégoire, and Delagrange [11], introducing the differential form of the stochastic equation of the Langevin type. In the following, this approach allowed to overcome the above-mentioned restrictions. Thus, explicit calculations of individual trajectories on a complex multi-dimensional potential-energy surface with realistic inertial and friction forces enabled studying much more complex systems. For one specific case, Wada, Carjan, and Abe [12,13] have calculated the fission decay using Langevin equations in two dimensions. They came to the conclusion that the transient time is not significantly changed, while the quasistationary flux is enhanced by only 15% compared to the one-dimensional calculation. The same result that the two-dimensional fission rates are slightly larger than the one-dimensional ones was obtained in the Langevin calculations made by Fröbrich and Tillack [14]. They also speculated that the inclusion of additional collective coordinates would again influence the rate.

The Langevin calculations have recently been extended up to three dimensions for specific studies on fission dynamics by several authors [13,15,16]. However, dedicated studies on the influence of the dimensionality of the dynamical model on the calculated results are scarce up to now, and they have been performed up to two dimensions only. The present work applies the Langevin calculations in three dimensions to this problem for the first time and investigates it in a systematic and quantitative way.

Apart from the general understanding of the fission process, the dimensionality of the model calculations is also of importance for the interpretation of experimental observables. By comparing experimental data with different theoretical descriptions, one hopes to conclude on the validity of the physics involved in the considered theoretical models. For this purpose, however, one should be sure that technical restrictions of the model calculations, such as the dimensionality of the considered model space, do not have any significant influence on the results.

Although the specific conditions of our calculations and thus our quantitative results apply to the problem of nuclear fission, the importance of the present study is much more general, because it shows the qualitative importance of including all relevant collective variables for obtaining realistic results for the decay of a metastable state in many dimensions. These results have general importance, as in many areas of physics, chemistry and biology one is dealing with transport processes, which can be described using multi-dimensional Langevin or Fokker-Planck equations.

II. DYNAMICAL MODEL

Experimental data on nuclear dissipation have often been interpreted using one-dimensional Langevin models, where only one parameter is used for the description of the possible shapes of the fissioning nucleus. This is usually an elongation parameter, which describes the evolution of the shape of the nucleus from the spherical configuration up to the scission configuration of touching fragments. Such one-dimensional calculations simplify the theoretical treatment and reduce the ensemble of possible shapes of the fissioning nucleus, since they do not need large computational time and could be used for the investigations of the prescission particle emission and time characteristics of the fission process. However, almost all the problems of collective nuclear dynamics are essentially multi-dimensional. For example, for the correct description of the experimentally observed mass-energy distribution of fission fragments at least three independent shape parameters are needed [15,16]: the elongation parameter, the parameter which describes the appearance of the neck in the shape of the nucleus, and the mass-asymmetry parameter. Therefore, such an important characteristic as the fission rate R is investigated in the present work using Langevin calculations with different numbers of collective coordinates involved in the dynamical consideration for the two most frequently used dissipation mechanisms: one-body and two-body.

In the dynamical calculations we applied the well-known $\{c, h, \alpha\}$ parametrization [17]. In cylindrical coordinates the surface of the nucleus is given by

$$\rho_s^2(z) = \begin{cases} (c^2 - z^2)\left(A_s + Bz^2/c^2 + \dfrac{\alpha z}{c}\right), & B \geqslant 0; \\ (c^2 - z^2)\left(A_s + \dfrac{\alpha z}{c}\right)\exp(Bcz^2), & B < 0, \end{cases} \tag{1}$$

where z is the coordinate along the symmetry axis and ρ_s is the radial coordinate of the nuclear surface. In Eq. (1) the quantities B and A_s are defined by

$$B = 2h + \frac{c-1}{2};$$
$$A_s = \begin{cases} c^{-3} - \dfrac{B}{5}, & B \geqslant 0; \\ -\dfrac{4}{3}\dfrac{B}{\exp(Bc^3) + \left(1 + \frac{1}{2Bc^3}\right)\sqrt{-\pi Bc^3}\,\mathrm{erf}(\sqrt{-Bc^3})}, & B < 0. \end{cases} \tag{2}$$

In Eqs. (1) and (2), c denotes the elongation parameter, the parameter h describes the variation in the thickness of the neck for a given elongation of the nucleus, and the parameter of the mass asymmetry α determines the ratio of the volumes of the future fission fragments.

The coupled Langevin equations have the form:

$$\begin{aligned} \frac{dq_i}{dt} &= \mu_{ij} p_j, \\ \frac{dp_i}{dt} &= -\frac{1}{2} p_j p_k \frac{\partial \mu_{jk}}{\partial q_i} - \frac{\partial F}{\partial q_i} - \gamma_{ij}\mu_{jk} p_k + \theta_{ij}\xi_j(t), \end{aligned} \tag{3}$$

where $\mathbf{q}$ is the vector of collective coordinates, $\mathbf{p}$ is the vector of conjugate momenta, $F(\mathbf{q}) = V(\mathbf{q}) - a(\mathbf{q})T^2$ is the Helmholtz free energy, $V(\mathbf{q})$ is the potential energy, $m_{ij}(\mathbf{q})$ ($\|\mu_{ij}\| = \|m_{ij}\|^{-1}$) is the tensor of inertia, $\gamma_{ij}(\mathbf{q})$ is the friction tensor. The normalized random variable $\xi_j(t)$ is assumed to be a white noise. The strength of the random force θ_{ij} is given by $\sum \theta_{ik}\theta_{kj} = T\gamma_{ij}$. The temperature of the "heat bath" T has been determined by the Fermi-gas model formula $T = (E_{\text{int}}/a(\mathbf{q}))^{1/2}$, where E_{int} is the internal excitation energy of the nucleus, and $a(\mathbf{q})$ is the level-density parameter, which has been taken from the work of Ignatyuk *et al.* [18]. The repeated indices in the equations above imply summation over the collective coordinates.

As collective coordinates we have used the parameters $\mathbf{q} = (q_1, q_2, q_3)$, which are connected with the shape parameters c, h, and α by $q_1 = c, q_2 = (h + 3/2)/(\frac{5}{2c^3} + \frac{1-c}{4} + 3/2)$, and $q_3 = \alpha/(A_s + B)$, if $B \geqslant 0$, or $q_3 = \alpha/A_s$, if $B < 0$. The advantage of using the collective coordinates $\mathbf{q} = (q_1, q_2, q_3)$ instead of the (c, h, α) parameters is discussed in Refs. [16,19].

During a random walk along the Langevin trajectory in space of the collective coordinates, the energy conservation law has been used in the form $E^* = E_{\text{int}} + E_{\text{coll}} + V$. Here E^* is the total excitation energy of the nucleus, $E_{\text{coll}} = 0.5 \sum \mu_{ij} p_i p_j$ is the kinetic energy of the collective degrees of freedom. The inertia tensor was calculated by means of the Werner-Wheeler approximation for incompressible irrotational flow [20]. The potential energy of the nucleus was calculated within the framework of a macroscopic model with finite range of the nuclear forces [21]. In the present analysis we have used one-body dissipation [22] based on the "wall" and "wall-plus-window" formulas, and two-body dissipation [20] with the two-body friction constant $\nu_0 = 2 \times 10^{-23}$ MeV s fm^{-3}. In order to investigate only the influence of the dimensionality of the model on the calculated results, we carry out Langevin calculations with some simplifications. We started modeling the fission process from the spherical compound nucleus assuming that the intrinsic degrees of freedom are thermalized. The calculations have been done for zero angular momentum. The evaporation of the prescission light particles was not considered in the present analysis. Shell corrections have also been neglected. Of course, all these effects have important influence on the fission process, but in the present study we are particularly interested in the importance of the dimensionality of problem, and, therefore, we want to keep all other effects as simple as possible. The fission rate was calculated as $R(t) = -1/N(t)dN(t)/dt$, where $N(t)$ is the number of trajectories which did not escape beyond the saddle at time t. This procedure is similar to that used in many previous studies [12–14] for calculations of fission rates. Usually, $R(t)$ is analyzed in terms of the stationary value R_{st} and the transient time τ_{tr}. The transient time τ_{tr}, as defined in Ref. [23], is the time needed for the $R(t)$ to reach 90% of the stationary value. The dynamical calculations have been performed for the compound nucleus ^{248}Cf at two excitation energies $E^* = 30$ MeV and 150 MeV. The potential energy for the nucleus ^{248}Cf is presented in Figs. 1 and 2. In Fig. 1 the potential energy is presented in collective coordinates (q_1, q_2) for symmetric fission. The potential energy in the collective coordinates (q_1, q_3) is presented in Fig. 2 for the parameter h equal to zero.

It is useful to introduce here the notion of a boundary of the metastable region around the ground state in the space of collective coordinates. We define this boundary as the water divide in the multi-dimensional potential-energy landscape

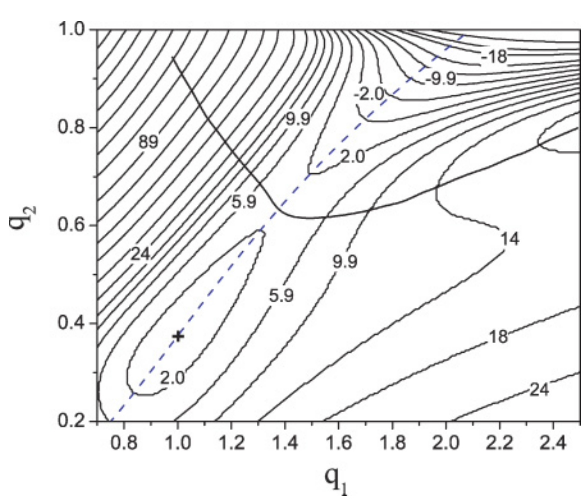

FIG. 1. (Color online) The potential energy surface for the compound nucleus ^{248}Cf in the collective coordinates q_1 and q_2. The dashed curve corresponds to the case of $h = \alpha = 0$. The numbers at the contour lines indicate the potential energy in MeV. The cross corresponds to the spherical deformation. The solid curve corresponds to the water divide, which separates the metastable region from the stable region; for more details, see text.

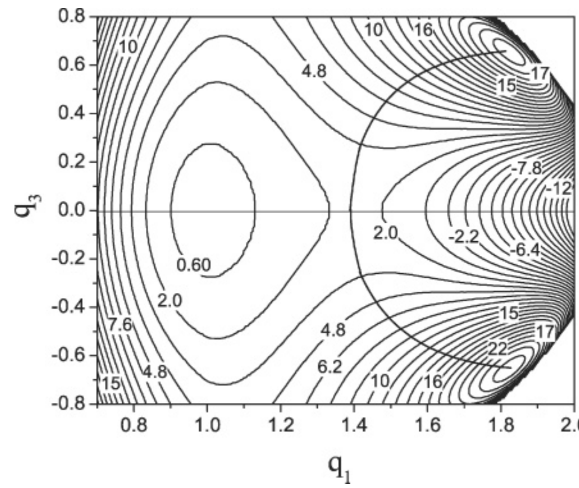

FIG. 2. The potential energy surface for the compound nucleus ^{248}Cf in the collective coordinates q_1 and q_3. The parameter h is fixed and equal to zero. The numbers at the contour lines indicate the potential energy in MeV. The solid curve corresponds to the water divide, which separates the metastable region from the stable region.

[24]. It is a curve in the two-dimensional case and a surface in the three-dimensional case. The saddle point, defined as the lowest barrier dividing the metastable region from the stable region, is a point on this water divide, and thus the water divide is the most natural generalization of the saddle point to the multi-dimensional case.

In order to find the water divide in the multi-dimensional case, dynamical Langevin calculations have been performed in the overdamped regime and without random force. In these calculations the components of the friction tensor were multiplied by a constant factor in such a way that the reduced friction coefficient $\beta = \gamma/m$ was larger than 50×10^{21} s^{-1} for all possible deformations in the space of collective coordinates. Under such conditions, the motion will be mainly determined by the potential and the friction tensor, while the influence of the mass tensor can be neglected. Moreover, by neglecting the random force, the motion will be deterministic, and any initial deformation chosen on the grid of collective coordinates will either end in the spherical shape or in some scission configuration. Thus, one can determine for every point in the space of collective coordinates whether it belongs to the metastable region or the stable (scission) region, and, as a result, to find the boundary (saddle deformations) between them in the multi-dimensional case. Please note that when determining the boundary of the quasibound region it is important to take into account the friction tensor, as due to its dependence on the collective coordinates the motion does not follow the direction of the steepest descent.

III. RESULTS AND DISCUSSION

In the present analysis, one-dimensional, two-dimensional, and three-dimensional Langevin calculations have been performed. The one-dimensional Langevin calculations have been carried out using only the elongation parameter c, while the parameters h and α have been set to zero. Such

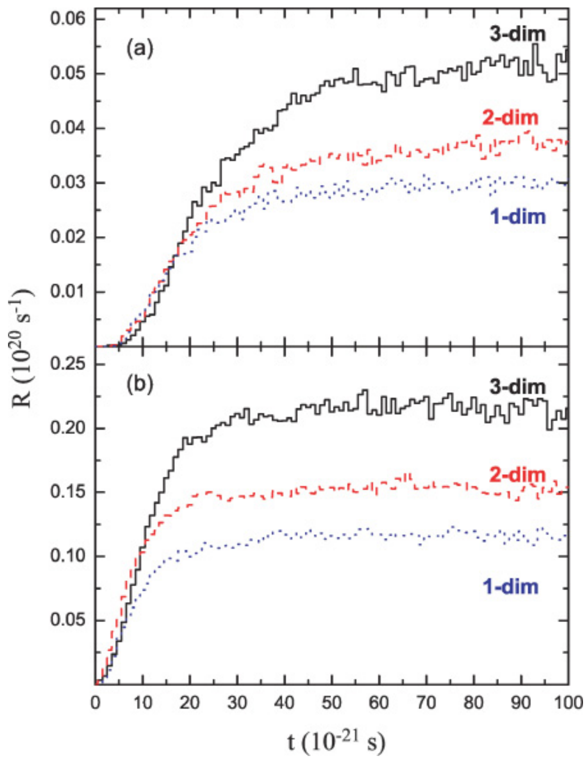

FIG. 3. (Color online) The fission rate calculated for the nucleus ^{248}Cf in the case of one-body dissipation for excitation energy $E^* = 30$ MeV (a) and $E^* = 150$ MeV (b). The solid, dashed, and dotted curves correspond to the three-, two-, and one-dimensional Langevin calculations, respectively.

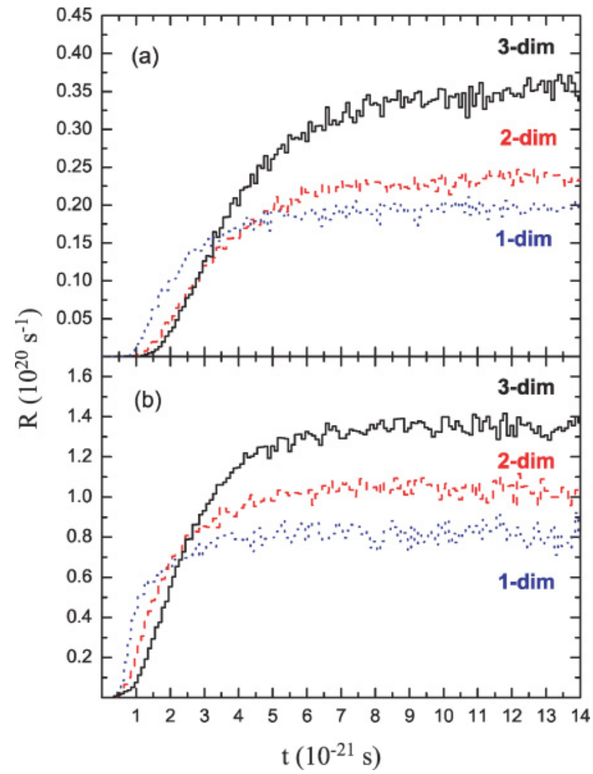

FIG. 4. (Color online) The same as in Fig. 3, but for the case of two-body dissipation.

calculations will approximately correspond to the bottom of the fission valley and will follow the dashed line in Fig. 1. The two-dimensional Langevin calculations have been performed using the q_1 and q_2 collective coordinates, and the parameter q_3 has been set to zero. Such two-dimensional Langevin calculations describe the symmetric fission. The three-dimensional Langevin calculations have been performed using the collective coordinates q_1, q_2, and q_3. The results of the calculations for the nucleus ^{248}Cf are presented in Figs. 3 and 4 for the case of the one-body and two-body dissipation, respectively.

One can see from these figures that the stationary value of the fission rate R_{st} increases after introducing new collective coordinates in the dynamical consideration. The stationary value of the fission rate in the one-dimensional case R_{st}^{1d} is about 20% lower than in the two-dimensional R_{st}^{2d} case and about 50% lower as compared to the three-dimensional R_{st}^{3d} case, regardless of the excitation energy or the friction mechanism. The change in the stationary value of the fission rate when going from the one-dimensional to the multi-dimensional description can be caused by both static and dynamic characteristics of the fission process. Weidenmüller and Jing-Shang have discussed in Ref. [7] the influence of the geometry of the fission valley on the calculated value of the stationary fission rate. They have shown that if the fission valley gets wider as one approaches the saddle-point configurations, the multi-dimensional stationary value of the fission rate will increase as compared to the one-dimensional value. The opposite is to expect if the fission valley gets narrower when approaching the saddle-point configurations [7]. Apart from these static arguments, in multi-dimensional Langevin calculations the stationary value of the fission width will also be influenced by the dependence of the mass and friction tensors on the chosen collective variables. The combination of all these effects leads to the differences between the one- and multi-dimensional calculations seen in Figs. 3 and 4.

On the other hand, our results show that the stationary values of the fission rate are larger in the case of two-body dissipation as compared to one-body dissipation. In fact, the collective energy at saddle point deformations averaged over Langevin trajectories $\langle E_{\rm coll}\rangle$ is lower in the case of one-body dissipation than in the case of two-body friction. The $\langle E_{\rm coll}\rangle$ has the following values: $\langle E_{\rm coll}^{1d}\rangle = 1.36$ MeV, $\langle E_{\rm coll}^{2d}\rangle = 2.07$ MeV, and $\langle E_{\rm coll}^{3d}\rangle = 2.65$ MeV in the calculations with one-body friction. In the case of two-body dissipation the $\langle E_{\rm coll}\rangle$ has the following values: $\langle E_{\rm coll}^{1d}\rangle = 1.46$ MeV, $\langle E_{\rm coll}^{2d}\rangle = 2.58$ MeV, and $\langle E_{\rm coll}^{3d}\rangle = 3.6$ MeV. The available phase space determined from energy conservation does not depend on the dissipation mechanism and is the same for the calculations with one-body and two-body frictions. Nevertheless, as one can see from the $\langle E_{\rm coll}\rangle$ values, the fissioning systems in the calculations with two-body friction are more mobile compared to the case of one-body viscosity and, as a result, populate larger phase space at saddle-point deformations. This fact results in larger values of the fission rate in the model calculations with two-body dissipation as compared to the calculations with one-body dissipation.

From the results shown in Figs. 3 and 4 we can also discuss the influence of the number of collective coordinates involved in the Langevin calculations on the transient time. When *two-body dissipation* is assumed, the transient time shows a clear dependence on the dimensionality of the model space. The lowest transient time is obtained in one-dimensional calculations τ_{tr}^{1d} and the largest in three-dimensional calculations τ_{tr}^{3d}. In the one-dimensional case, the fissioning system can oscillate only in fission direction, and the energy is transferred only between the elongation degree of freedom and the heath bath. Thus, the Langevin trajectory follows the dashed line shown in Fig. 1. In multi-dimensional calculations, the fissioning system has more freedom. During the random walk in multi-dimensional space, the fissioning system can significantly deviate from the one-dimensional Langevin trajectory, and the energy can be transferred not only between the elongation degree of freedom and the heat bath, but also between the elongation variable and additional collective variables. Therefore, in average, the motion in the fission direction could be slowed down as compared to the one-dimensional case, and, consequently, the fissioning system would need more time in order to reach the saddle-point configurations in the multi-dimensional case than in the one-dimensional case. This could be the reason why τ_{tr} in the multi-dimensional case is larger than τ_{tr}^{1d}. In the calculations performed with *one-body dissipation*, the sensitivity of the transient time τ_{tr} to the dimensionality of the model space is still present but strongly reduced. As discussed above, the fissioning systems in the calculations with one-body friction are less mobile compared to the case of two-body viscosity and, as a result, populate a more restricted region in deformation space. Therefore, the motion in multi-dimensional space deviates less from the one-dimensional Langevin trajectory. This could result in a lower sensitivity of τ_{tr} to the dimensionality of the model space. However, this discussion could only provide a few qualitative arguments. One should not forget that the stationary value of the fission rate and the transient time are also decisively determined by the complex dependence of the mass and friction tensors on the collective coordinates.

One could raise the question whether is it sufficient to consider three dimensions for a realistic description of the fission process. This question is equivalent to the task to divide the degrees of freedom in a limited number of collective variables, which are explicitly treated, and a heat bath, which represents all the other degrees of freedom. According to the derivation of the Fokker-Planck or the Langevin equations, this division should be performed on the base of the time scale of the dynamics of the system. The heat bath should contain only those degrees of freedom which vary fast compared to the collective degree of freedom we are interested in. Obviously, a one-dimensional calculation, which treats dynamically only the elongation of the nucleus, does not fulfill this requirement, because the time scales of neck formation and mass-asymmetry are comparable with the motion in fission direction. Langevin calculations previously performed [15,16] have shown that for the correct description of the experimentally observed mass-energy distribution of fission fragments at least three independent shape parameters are needed: the elongation parameter, the parameter which describes the appearance of the neck in the shape of the nucleus, and the mass-asymmetry parameter. Thus, we can assume that in the present work the most relevant degrees of freedom are included, and, thus, the results of the three-dimensional calculations are much more realistic than the results of the one- or two-dimensional analysis. At the end, we would like to mention that some other authors [25–28] have used five or six shape parameters for the description of different features of the fission process. These additional shape parameters could also be dynamically treated in the Langevin calculations, and their possible influence on the time behavior of the fission flux could be studied. This is beyond the scope of the present work.

IV. CONCLUSIONS

Our three-dimensional Langevin calculations with realistic potential and inertial forces as well as friction tensors given by one-body and two-body dissipation, respectively, have shown that the inclusion of three dimensions can have substantial influence on the time behavior and on the quasistationary value of the fission flux if compared to the results of a one-dimensional model. We have also performed calculations of the fission rate at the saddle point using the last-passage-time concept [29], and we came to the same conclusions concerning the influence of the model dimensionality on the fission process. Our results are particularly important for the conclusions about nuclear dissipation, deduced from the comparison of experimental results with model calculations, which are performed in restricted deformation space. One may suppose that qualitatively the same conclusion is valid for other problems in statistical physics and chemistry on the decay of metastable states of multi-dimensional systems, which might be revisited with the powerful modern tools of Langevin calculations.

ACKNOWLEDGMENTS

We would like to thank Drs. G. D. Adeev, A. Ya. Rusanov, and A. V. Karpov for stimulating and useful discussions, and correspondence. One of us (P.N.N.) is grateful to the Humboldt foundation for the financing of the stay at GSI, Darmstadt.

[1] R. Becker and W. Döring, Ann. Phys. (Leipzig) **24**, 719 (1935).
[2] H. A. Kramers, Physica **7**, 284 (1940).
[3] H. C. Brinkmann, Physica (Amsterdam) **22**, 149 (1956).
[4] R. Landauer and J. A. Swanson, Phys. Rev. **121**, 1668 (1961).
[5] J. S. Langer, Phys. Rev. Lett. **21**, 973 (1968).
[6] J. S. Langer, Ann. Phys. (NY) **54**, 258 (1969).

[7] H. A. Weidenmüller and Z. Jing-Shang, J. Stat. Phys. **34**, 191 (1984).
[8] Z. Jing-Shang and H. A. Weidenmüller, Phys. Rev. C **28**, 2190 (1983).
[9] D. M. Brink and L. F. Canto, J. Phys. G: Nucl. Phys. **12**, L147 (1986).
[10] P. Grangé, L. Jun-Qing, and H. A. Weidenmüller, Phys. Rev. C **27**, 2063 (1983).
[11] Y. Abe, C. Grégoire, and H. Delagrange, J. Phys. (Paris) **47**, C4-329 (1986).
[12] T. Wada, N. Carjan, and Y. Abe, Nucl. Phys. **A538**, 283c (1992).
[13] Y. Abe *et al*., Phys. Rep. **275**, 49 (1996).
[14] P. Fröbrich and G.-R. Tillack, Nucl. Phys. **A540**, 353 (1992).
[15] A. V. Karpov, P. N. Nadtochy, D. V. Vanin, and G. D. Adeev, Phys. Rev. C **63**, 054610 (2001).
[16] G. D. Adeev *et al*., Fiz. Elem. Chastits At. Yadra **36**, 732 (2005) [Phys. Part. Nucl. **36**, 378 (2005)].
[17] M. Brack *et al*., Rev. Mod. Phys. **44**, 320 (1972).
[18] A. V. Ignatyuk *et al*., Yad. Fiz. **21**, 1185 (1975) [Sov. J. Nucl. Phys. **21**, 612 (1975)].
[19] P. N. Nadtochy and G. D. Adeev, Phys. Rev. C **72**, 054608 (2005).
[20] K. T. R. Davies, A. J. Sierk, and J. R. Nix, Phys. Rev. C **13**, 2385 (1976).
[21] A. J. Sierk, Phys. Rev. C **33**, 2039 (1986).
[22] J. Blocki *et al*., Ann. Phys. (NY) **113**, 330 (1978).
[23] K.-H. Bhatt, P. Grangé, and B. Hiller, Phys. Rev. C **33**, 954 (1986).
[24] B. Hayes, Am. Sci. **88**, 481 (2000).
[25] J. R. Nix, Nucl. Phys. **A130**, 241 (1969).
[26] U. Brosa, S. Grossmann, and A. Müller, Phys. Rep. **194**, 167 (1990).
[27] M. C. Duijvestijn, A. J. Koning, and F.-J. Hambsch, Phys. Rev. C **64**, 014607 (2001).
[28] P. Möller, D. G. Madland, A. J. Sierk, and A. Iwamoto, Nature (London) **409**, 785 (2001).
[29] J.-D. Bao and Y. Jia, Phys. Rev. C **69**, 027602 (2004).