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Dynamical Modeling of the Nuclear Fission Process at Low Excitation Energies

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Abstract

Two recipes for modeling the dynamics of the nuclear fission process are known in literature. The underlying equations contain the driving, dissipative, and random forces. The two recipes are mostly different in the prescriptions for the driving force. In this work we carefully compare these driving forces and the resulting fission rates. It turns out that the rates may be very close or strongly different depending on the value the shell correction to the nuclear deformation energy. We give arguments in favor of one of the recipes.

Keywords

Nuclear Fission, Dynamical Modeling, Stochastic Differential Equations, Fermi Gas Model

1. Introduction

Numerous experiments related to the nuclear fission process [1,2], in particular those aiming for discovering new superheavy elements [3-5], require practical and reliable numerical modeling of fission dynamics at low excitation energies. The most important physical quantity characterizing the fission process, although not observable, is the fission rate which is by definition

$$R(t_i) = \frac{1}{N_{tot} - N_f(t_i)} \frac{N_f(t_i) - N_f(t_{i-1})}{\Delta t}, \tag{1}$$

$$N_f(t_i) = \sum_{j=1}^{i} \Delta N_f(t_j). \tag{2}$$

Here $\Delta N_f(t_j)$ is the number of trajectories reached the scission point during the time interval $\Delta t = t_j - t_{j-1}$; $N_f(t_i)$ is the number of trajectories reached the scission point until the time moment t_i.

Presently the dynamical modeling of fission is mostly performed by solving numerically the stochastic differrential equations with the white noise. In the simplest one dimensional case these equations read

$$dq = pm^{-1}dt \tag{3}$$

$$dp = -\eta m^{-1} pdt + fdt + \sqrt{2\eta T} \cdot dW \tag{4}$$

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Here dt is the time interval during which the collective coordinate (deformation parameter) q and its conjugate momentum p increase by dq and dp, respectively; W is the Wiener process whose increment dW obeys the normal distribution with the variance dt ($dW \sim \sqrt{dt}$); η and m are the friction and inertia parameters, respectively. For the sake of simplicity we consider η and m to be deformation independent ($\beta = \eta / m$).

The driving force can be calculated by two methods. The first one is a generalization [6] of the thermodynamical approach, which was developed for the one dimensional problem in [7,8] and later was extended to the multidimensional case in [9]. Note that this method is applied, except [6], for the high excitation energies when the shell correction to the nuclear Potential Energy (V, PE) and to the single particle Level Density Parameter (a, LDP) is believed does not play a role. The driving force calculated using this approach, f_I, is defined as a proper derivative of a thermodynamical potential:

$$f_I = -\left(\frac{\partial F}{\partial q}\right)_T = T\left(\frac{\partial S}{\partial q}\right)_E \tag{5}$$

is the Helmholtz free energy, $S(q,E)$ is the nucleus entropy, and E is its total excitation energy. Within the framework of the Fermi gas model, the entropy reads

$$S(q,E) = 2\left[a(q,U)U(q)\right]^{1/2} \tag{6}$$

The intrinsic excitation energy U is related to E and PE as follows:

$$U(q) = E - V(q) = E - V_L(q) - V_S(q) \tag{7}$$

Here $V_L(q)$ and $V_S(q)$ are the smooth (liquid drop) part of PE and the shell correction, respectively. According to [10] the LDP can be written as

$$a(q,U) = a_L(q)\left\{1 + g(U)V_S(q)U^{-1}\right\} \tag{8}$$

The function $g(U)$ reaches unity when U becomes large enough:

$$g(U) = 1 - \exp(-kU) \tag{9}$$

$k = 0.054\ \text{MeV}^{-1}$. The deformation dependence of the smooth part of the LDP is defined as follows [10]: $a_L(q) = a_1 A + a_2 A^{2/3} B_s(q)$. Here A is the nucleus mass number, $a_1 = 0.073\ \text{MeV}^{-1}$ and $a_2 = 0.095\ \text{MeV}^{-1}$, $B_s(q)$ is the dimensionless nuclear surface area.

Using Equations (5), (7) and (8) we obtain for the driving force the following expression

$$f_I = -V_L' - V_S' + a_E' T^2 \tag{10}$$

The prime denotes the derivative with respect to the coordinate, the subscript "E" indicates that the derivative must be taken keeping E constant.

Within the framework of the second approach [11,12] the driving force f_{II} is calculated according the formula, which (using our notations) reads

$$f_{II} = -V_L' - (1-g)V_S' \tag{11}$$

Equations (10) and (11) look very much different. One hardly can expect to find the fission rates similar if f_I and f_{II} are used in Equation (4). In order to check whether the rates are different indeed we construct a schematic PE which reproduces the main distinct features of the PE of ^{236}U-nucleus. This schematic $V(q)$ is shown in **Figure 1** along with $V_L(q)$ and $V_S(q)$.

One sees clearly the double humped structure of the fission barrier which is well known for the actinide nuclei [13].

We modeled the fission process applying Equations (3), (4) and the driving forces f_I and f_{II}. The PE of **Figure 1** was used for the modeling. The initial conditions corresponded to the Brownian particles at rest at the left minimum of the PE. Typical fission rates resulted from this modeling according to Equation (1) are shown in **Figure 2**. Although the quasistationary rate R_{DII} exceeds R_{DI} by some 20%, one can expect much larger difference considering Equations (10) and (11).

In order to figure out the reason for this surprisingly small difference let us transform Equation (10). The derivative of the LDP reads:

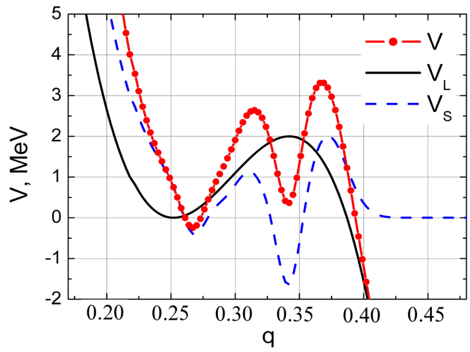

Figure 1. The schematic PE for ^{236}U (curve with dots) as a function of collective coordinate along with its components: the smooth (solid curve) and shell correction (dashed curve) parts.

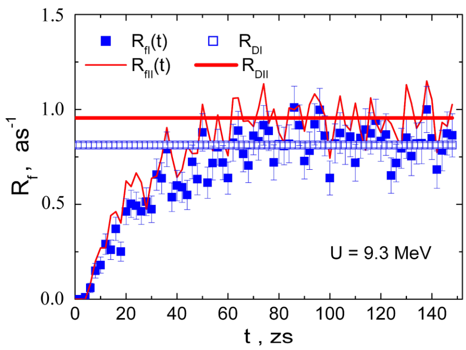

Figure 2. The dynamical fission rates calculated for ^{236}U according to Equation (1) versus modeling time. The horizontal lines indicate the quasistationary values of the rates.

$$\left(\frac{\partial a}{\partial q}\right)_E = a_L\left[\frac{g'\cdot V_S}{U}+\frac{g\cdot V_S'}{U}-\frac{g\cdot V_S\cdot U'}{U^2}\right]+a_L'\frac{g\cdot V_S}{U} \tag{12}$$

Keeping in mind that $U'=-V_L'-V_S'$ and $g'=kU'\exp(-kU)$ we convert Equation (10) to the form

$$f_I=-V'+a_L'\varepsilon+\frac{U}{1+\varepsilon}\left[\frac{V_SkV'}{U}-\varepsilon kV'+\frac{g\cdot V_S'}{U}-\frac{\varepsilon V'}{U}\right] \tag{13}$$

Here $\varepsilon=g(U)V_S(q)U^{-1}$ turns out to be a small parameter not exceeding 0.1 in the region of the barrier at $U>10$ MeV in particular because in the considered case $V_S(q)$ is in order of 2 MeV. Omitting in (13) the terms obviously proportional to ε we arrive at the formula

$$f_I=f_{II}+V_SkV_L'+V_SkV_S'+g\cdot V_L' \tag{14}$$

Since k^{-1} is about 20 MeV, in Equation (14) the terms containing $kV_S(q)$ are rather small. The last term is small because $V_L(q)$ is rather smooth (see **Figure 1**). We believe that this derivation explains relatively small difference between f_I and f_{II} resulting in small difference between the corresponding fission rates in **Figure 2**.

We also have considered the case of a nucleus with the large shell correction at the ground state, namely the double magic lead-208. The PE of **Figure 3** was used for the modeling in this case. The absolute value of the shell correction is now about 12 MeV. The way of modeling **Figure 4**. One sees that in this case R_{DII} exceeds R_{DI} by factor of 2 whereas the conventional value of the intrinsic excitation energy at which the shell correction ceases to manifest itself (and consequently R_{DII} and R_{DI} must converge) is about 60 MeV.

It is worthwhile to discuss and illustrate what does the smearing of the shell correction exactly mean. Within the framework of the first recipe, it turns out that one can calculate the fission rate ignoring completely the shell correction in the PE (*i.e.* using V_L instead of V in Equation (7)) and in the LDP (*i.e.* using a_L instead of a in Equation (6)). The corresponding fission rate R_{DIL} must converge with R_{DI} as E increases. This is seen in **Figure 5** where the quasistationary rates resulting from dynamical modeling are shown. In order to quantify the convergence between R_{DIL} and R_{DI} we have calculated the fractional difference $R_{DI}/R_{DIL}-1$. It has turned out that the difference goes to zero reaching circa −10% at $E=60$ MeV as it is known for the statistical rates.

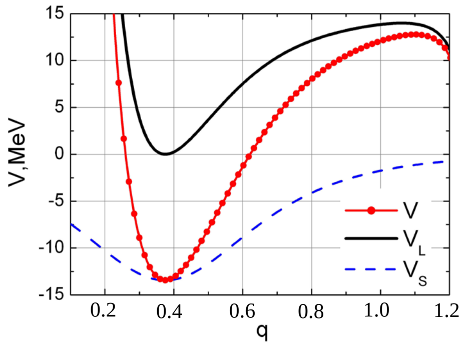

Figure 3. The schematic PE for ^{208}Pb (curve with dots) as a function of collective coordinate along with its components: the smooth (solid curve) and shell correction (dashed curve) parts.

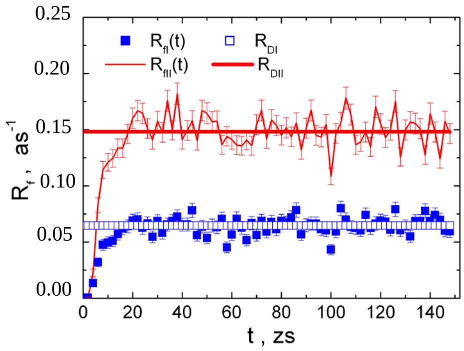

Figure 4. The dynamical fission rates calculated for ^{208}Pb according to Equation (1) versus modeling time. The horizontal lines indicate the quasistationary values of the rates.

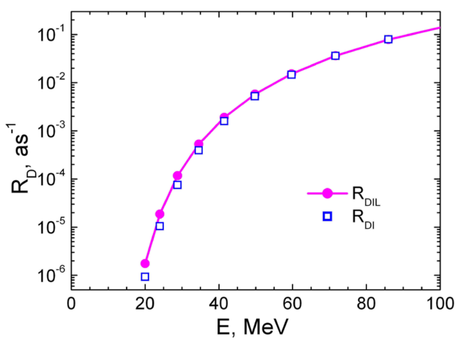

Figure 5. The dynamical quasistationary fission rates calculated for ^{208}Pb nucleus accounting for the shell correction (squares) and ignoring those (line with circles).

Within the framework of the second recipe, the convergence is not reached because the reference point for the excitation energy always include the potential energy with the shell correction (see Equation (6) of [12]).

To finalize, we have compared two approaches for calculating the driving force for the nuclear fission process at low excitation energies when the shell effects are expected to be significant. We have found that in the case of uranium-236 nucleus the quasistationary decay rates R_{DI} and R_{DII} resulting from these approaches are rather close (the difference is about 20%). This is however just because for this nucleus the shell correction is small in comparison with the typical energy $k^{-1} = 18.5$ MeV controlling the smearing out the shell effects. For the lead-208 nucleus with larger value of the shell correction, the difference between R_{DI} and R_{DII} reaches factor of 2. This is significantly larger than the difference between the rates calculated within the frame work of the first approach with and without the shell correction. Since the first approach is based on the thermodynamical arguments, we are inclined to make favor to it in comparison with the second one.

Acknowledgements

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