Description of the multidimensional potential energy surface in fission of $^{252}$Cf and $^{258}$No

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The microscopic studies on nuclear fission require the evaluation of the potential energy surface as a function of the collective coordinates. A reasonable choice of constraints on multipole moments should be made to describe the topology of the surface completely within a reasonable amount of computing time. We present a detailed analysis of fission barriers in the self-consistent Hartree-Fock-Bogoliubov approach with the D1S parametrization of the Gogny nucleon-nucleon interaction. Two heavy isotopes representing different spontaneous fission modes - $^{252}$Cf (asymmetric) and $^{258}$No (bimodal) - have been chosen for the analysis. We have shown the existence of complicated structures on the energy surface that cannot be fully described in two-dimensional calculations. We analyze apparent problems that can be encountered in this type of calculations: multiple solutions for given constraints and transitions between various potential energy surfaces. We present possible solutions on how to deal with these issues.

Keywords: spontaneous fission, potential energy surface, microscopic methods, Cf-252, No-258

I. INTRODUCTION

The accurate description of collective nuclear motion from the ground state up to the scission point represents a crucial step to understand the fission of the atomic nucleus. An essential ingredient is the behavior of the binding energy of the nucleus as a function of the parameters characterizing the collective degrees of freedom. On its way from the initial ground state configuration to scission, the nucleus has to tunnel through a potential energy barrier determining the time scale of fission half-lives. Not only the height but also the width and the shape of the fission barrier are important for spontaneous fission half-lives estimations, while the topography of the potential energy surface (PES) is essential to determine fission dynamics. A detailed description of the theory of fission and challenges in this field can be found in the review papers: Refs. [1–3].

The first historical attempt to explain and describe the fission process was based on the semi-empirical liquid drop model assumptions [4] where the interplay between Coulomb repulsion and surface energy of a charged and deformed drop of nuclear matter is responsible for the splitting [5]. The success of this simple approach suggested that collective variables (in an intrinsic frame of the nucleus), associated with the shape evolution of a fissioning system, are a crucial ingredient in any microscopic analysis of fission process. The adiabatic approximation - based on the assumption that the time-scale of nucleons motion is much shorter than the time-scale of shape changes - allows obtaining a consistent description by considering just a small set of collective degrees of freedom well adapted to the shape evolution involved in fission.

Many theoretical papers describing the PES in heavy actinides have been published recently improving our knowledge of fission of heavy and super-heavy nuclei [6–21]. In those articles, one can distinguish two different approaches to describe the shape of the nucleus in the fission process. Both are based on the minimization of the energy along the different paths connecting the starting configuration (usually the ground state) with the scission configurations. In the first approach, which is mostly used with macroscopic-microscopic theories, a pre-defined class of nuclear shapes defined uniquely in terms of a given set of deformation parameters is used to define the set of accessible configurations to be used in the minimization of the energy. The number of parameters defines the dimensionality of the problem. An increasing number of dimensions increases the variety of the shapes used and, therefore, usually improves the calculation’s quality by providing lower energy solutions. This flexibility comes at the expense of calculating the energy for a huge number of points in the deformation space. On the other hand, the approach benefits from full control over the shapes characterizing the evolution of a nucleus from the ground state to scission. The alternative approach is mostly used by the microscopic self-consistent methods. In the self-consistent procedure, the wave functions along the fission path are determined by the minimization of the energy of the nucleus within a given set of constraints and assumed symmetries. The constraints only provide general guidelines for the nuclear density distribution and
do not fix its shape uniquely. For a given set of constraints, the nuclear shape is free to take any form among the allowed ones as to minimize the energy of the nucleus. The advantage of this procedure is that we do not have to worry if our space of deformation parameters is large enough to describe the shape adopted by the nucleus. Nevertheless, the results provided with this method are not always unique [22] as one can easily land for a given set of constraints in a local minimum instead of the absolute one. As a consequence, the self-consistent minimization procedure can produce several solutions with the same value of the constraints but different energies depending, for instance, on the starting wave function used in the solution of the variational equations. Those “multivalued” solutions are connected in a higher dimensional deformation space by a barrier separating them. A typical example, often seen in axially symmetric calculation constraining in the quadrupole moment, is the existence of two solutions with the same quadrupole moment but different values of the octupole moment in the region of the second barrier. The two coexisting minima are linked by a path going through the octupole moment in the parameter space. One of the unwanted consequences of this kind of situation is the possibility to jump between configurations when considering the behavior of quantities as a function of the current shape parameter. The leap is unphysical because one is skipping the path connecting the coexisting minima. When describing this situation, one talks about jumping from one fission valley to another. Whether the dynamics of fission justify this transition or it is just an artifact due to the limited number of constraints used to describe the fission path is a delicate issue that will be the subject of the present paper.

If the constraints are partially released, several different solutions may exist as local minima of the potential energy. In this case, one has to decide which of them should be considered in the analysis of fission. We may even encounter a situation where on the edge between two valleys, a fake or missing saddle can be found [22]. The first case occurs when two distinct nuclear shape configurations have got the same energy at some coordinate, and the fission paths are incorrectly linked together. The missing one means that minimizing the energy with a single constraint may pass over a saddle leading to another valley. The consequence of a wrong interpretation of the PES may have a non-negligible impact on the description of fission dynamics. The barrier heights may be improperly evaluated, and the fission valleys may be omitted or redundant.

It has been previously shown that non-geometrical constraints like the one associated with pairing correlations may strongly influence the fission dynamics scenario because of the strong dependence of the collective inertias on the inverse of the pairing gap [25–28]. As a consequence, the inclusion of the pairing degree of freedom can substantially modify the dynamical evolution of a collective wave packet. Moreover, this kind of constraint can play a central role if the least action principle is used instead of the least energy one to determine the fission path. The treatment of spontaneous fission using the least action principle and including the pairing degree of freedom leads to a substantial reduction of the spontaneous fission life time [25–28]. However, and despite its relevance, we are not considering the pairing degree of freedom in the present study.

This paper is devoted to the discussion of the choice of the multipole moments to be used as constraints for the calculation of the PES leading to fission in the self-consistent methods. The primary purpose is to determine which subspace of collective coordinates in a deformation space is sufficient for an accurate description of static properties of fissioning nuclei. We will analyze the mechanism of creating multiple solutions on the PES in the limited dimensionality of the space. The consequences of this behavior will be discussed. We will indicate regions where the discontinuity of the PES may be found.

To carry out our investigation, we have chosen two isotopes representing two different fission modes - asymmetric (254 Cf) [29–31] and bimodal (258 No) [32–33]. With this choice, we cover a broad and representative range of fission modes in heavy nuclei. The total half-life of the radioactive isotope 252 Cf is $t_{1/2} = 2.645(8) \text{y}$ with alpha decay as the dominant branch. Only 3.092(8)% of the fissioning nuclides undergo spontaneous fission. On the other hand, 258 No has a far shorter half live $t_{1/2} = 1.2(2)$ ms and fission is the principal decay channel [34].

## II. THEORETICAL FRAMEWORK

The present study has been carried out using the self-consistent constrained Hartree-Fock-Bogoliubov (HFB) method with the finite-range density-dependent nucleon-nucleon Gogny interaction. We use the well-reputed parametrization D1S [35] that has been extensively used in the literature to describe many different nuclear structure phenomena [36, 37] including the microscopic description of fission [38, 39].

In the HFB method [39, 40], the nuclear states are obtained as the solutions of the HFB equation, which is derived by requiring that the mean value of the routhian is a minimum:

$$\delta(\langle \Phi | \tilde{H} - \lambda_Z \tilde{Z} - \lambda_N \tilde{N} - \sum_{ij} \lambda_{ij} \tilde{Q}_{ij} | \Phi \rangle) = 0. \quad (1)$$

Here $\tilde{H}$ is the microscopic Hamiltonian, $\lambda_N$ and $\lambda_Z$ are the Lagrange multipliers used to fix the number of neutrons $N$ and protons $Z$, while $\lambda_{ij}$ are the Lagrange multipliers associated with the average value of the multipole moments $\tilde{Q}_{ij}$ with multipolarity $i$ and projection $j$. In this work the quadrupole ($Q_{20}$), octupole ($Q_{30}$), hexadecapole ($Q_{40}$) and triaxial quadrupole ($Q_{22}$) deformation parameters are considered. The equation is solved by expanding the creation and annihilation quasiparticle oper-
ators of the Bogoliubov transformation in a harmonic oscillator basis with oscillator length parameters optimized for each set of collective deformation parameters so as to minimize the binding energy. Most of the results are obtained in the axial regime with an axially symmetric deformed oscillator basis with \( N_\perp = 15 \) and \( N_z = 22 \). This basis is well suited to describe elongated shapes along the \( z \) axis as those typical of fission. Beyond mean-field, two-body kinetic energy correction and rotational energy correction are included in the calculation of the binding energy. In the calculations with non-zero triaxial multipole moment \( Q_{22} \) reflection symmetry is preserved, and therefore odd multipole moments are zero by construction and not considered in the discussion. For the “tri-axial” calculations an oscillator basis containing \( N = 18 \) shells is used.

The multipole moment operators are defined as

\[
\hat{Q}_{lm} = \frac{1}{\sqrt{2(1 + \delta_{m0})}} (\hat{M}_{lm} + r_m (-1)^m \hat{M}_{-m})
\]

with \( r_m = 1 \) if \( m \geq 0 \) and \(-1\) if \( m < 0 \). The raw multipole operators \( \hat{M}_{lm} \) are given by

\[
\hat{M}_{lm} = \sqrt{\frac{4\pi}{2l+1}} r^l Y_{lm}(\theta, \varphi)
\]

\[
= \sqrt{\frac{(l-m)!}{(l+m)!}} r^l P_{lm}[\cos(\theta)] e^{im\varphi},
\]

where \( Y_{lm} \) are spherical harmonics and \( P_{lm} \) are associated Legendre polynomials. Using the standard definition of the spherical harmonics we obtain \( Q_{20} = z^2 - \frac{1}{2}(x^2 + y^2) \), \( Q_{30} = z^3 - \frac{3}{2}(x^2 + y^2)z \), \( Q_{40} = z^4 - 3(x^2 + y^2)z^2 + \frac{5}{8}(x^2 + y^2)^2 \) and \( Q_{22} = \sqrt{3}/2(x^2 - y^2) \).

The computations were performed using the self-consistent HFB solver HFBaxial that uses the approximate second order gradient method [43] to solve the HFB equations and the formulas of [22] for an accurate evaluation of the matrix elements of the Gaussian central potential for the large basis required in fission. The program starts from an initial wave function and iteratively minimizes the energy subject to a given set of constraints. In this procedure, the shape of the nucleus is adjusted to fulfill the conditions imposed by the constraint parameters. Usually, the initial configuration is taken from a neighbor, previously computed, wave function. As the initial configuration is expected to be “close” to the sought solution this choice represents a way to decrease the number of iterations required in the minimization process and therefore, represents substantial computer time savings. The final solution may depend on the starting point in specific cases. This feature will be thoroughly discussed below.

As it has been mentioned in the Introduction, the use of a limited set of constraints always introduces some uncertainties in which wave functions belong to the neighborhood of which local minima. To help in the characterization of the different solutions of the HFB equation it is convenient to use a technique based on searching for discontinuities in the matter density distribution all over the PES. The so-called density distance \( D_{\rho\rho'} \) [22] has been used to detect such discontinuities in calculations considering the pair of shape parameters \( Q_{20} - Q_{30} \) as well as \( Q_{30} - Q_{40} \). For given configurations with matter density distributions \( \rho \) and \( \rho' \), the density distance is defined as:

\[
D_{\rho\rho'} = \int |\rho(r) - \rho'(r)| dr.
\]

Density distance remains small when nuclear shapes are similar, and it increases wherever there is a substantial change of nuclear shape for the two densities considered.

III. RESULTS

A. The PES in many coordinates

The theoretical description of fission is based on the analysis of the topography of the PES when represented as a function of the deformation parameters related to
FIG. 2. The PES of $^{252}$Cf (top) and $^{258}$No (bottom) as a function of $Q_{20}$ and $Q_{30}$ are shown as contour and color plots. Constant energy contours are plotted every 1 MeV. Asymmetric fission path is represented by a blue dashed line.

FIG. 3. The PES in $Q_{20} - Q_{22}$ plane for $^{252}$Cf (top) and $^{258}$No (bottom) are shown as contour and color plots. The iso-energy contour lines are plotted every 1 MeV. The dashed line shows the fragment of the fission path around the first barrier with non-zero triaxial deformation.

The elongation of the nucleus. More elaborated studies also include parameters related to reflection asymmetric shapes as they are required for the description of the asymmetry in fission fragment mass distribution. The inclusion of several shape parameters is also helpful in better characterizing not only the height but also the shape of the fission barrier. The shape of the fission PES of $^{252}$Cf and $^{258}$No are shown in Fig. 1 as a function of the quadrupole deformation. In Fig. 2, the PES maps in the quadrupole-octupole plane are displayed for the same isotopes. The mesh points used to obtain the maps are calculated every $\Delta Q_{20}=5$ b and $\Delta Q_{30}=4$ b$^{3/2}$.

The results presented in Fig. 2 have been calculated in the axial regime. However, non-axial shapes are crucial to describe the region of the first fission barrier correctly, and therefore we present the influence of triaxial deformations on the PES in Fig. 3. To simplify the calculation, reflection symmetry is preserved in these triaxial calculations, and therefore all the shapes have zero octupole moment. Usually, it is assumed that the information obtained from the aforementioned one- and two-dimensional plots together with the collective inertia is sufficient to describe the details of the fission process from the ground state till scission. Of course, they contain the key elements of the fission process like fission barrier heights and fragment mass asymmetry. Nevertheless, there are several limitations to this approach. First - the collective motion not only explores the minimum energy path (or the minimum action path) but also its neighborhood. There is a finite probability that the collective wave packet representing the evolution of the system towards fission explores regions close to the classical trajectory [45–47]. In this respect, the width of the valley, or - in other words - the stiffness of the potential energy, affects the spread of the collective wave packet and therefore the fragment mass distribution. Departure from the classical least energy fission path implies considering a broader set of nuclear shapes like those obtained by modifying the neck width and length or the shape of the pre-fragments. These variations can lead to a change of the obtained mass asymmetry at the scission point. Special care should be placed on a possible reduction of the neck thickness as it determines the scission...
FIG. 4. The PES of $^{252}\text{Cf}$ in a $Q_{30} - Q_{40}$ plane is shown as a contour and color plot. Constant energy contours are plotted every 2 MeV. The energy color scale is the same as in Fig. 2. See text for details.
FIG. 5. The same as in Fig. 4 but for $^{258}$No.
configuration.

Another problem is that points on the $Q_{20} - Q_{30}$ map are defined as local minima of the energy with given constraints on quadrupole and octupole moments. There is no guarantee that the minimum is unique. In fact, it was shown that sometimes there might exist multiple local minima in the energy \[48\]. These minima create different surfaces in the same place of the $Q_{20} - Q_{30}$ map. In such a case, one has to decide which of them should be taken under consideration for fission dynamics and, unfortunately, the answer is not straightforward.

Thus, we observe that other degrees of freedom may affect some aspects of the theoretical description of fission. It is even the case when a two-dimensional map in the self-consistent calculations is created from nuclear shapes optimized in the procedure of energy minimization, not just created by a two-parameter formula. To better describe and understand fission, one has to increase the size of the considered space of constraints on which the PES is spanned and look at it from a broader perspective. In this way, one should be able to compare all the available valleys and deduce which path should be preferred by the evolving system.

In order to extend the space of deformation, the most natural and most used coordinate is the next term in the multipole expansion: the hexadecapole moment $Q_{40}$, responsible for necking \[48\]. By decreasing the value of the hexadecapole moment, shapes with a thinner neck are obtained. The alternative option is applying the constraint on the neck parameter $Q_N$ \[39, 49\]. It produces the same effect as the scission region and very precise elsewhere.

To visualize a three-dimensional PES is a difficult task that can somehow be facilitated if one of the variables is kept fixed and the PES for the remaining two variables is plotted as a contour plot. Such a procedure has been followed in Fig. 7 for $^{252}$Cf and Fig. 8 for $^{258}$No where we show sections of the PES for fixed values of $Q_{20}$ as maps in the $Q_{30} - Q_{40}$ space. The black, blue, and red dots correspond to the least-energy fission paths found on the PES spanned on the $Q_{20} - Q_{30}$ space. The black dots correspond to the lowest-energy minimum, the blue ones stand for the next-in-energy local minimum, and the red dots indicate the post-scission minimum corresponding to two fragment solution. The blue, dashed lines show the results of 2-dimensional calculations, where the hexadecapole moment is self-consistently given by the minimization of the total HFB energy with double constraints on $Q_{20}$ and $Q_{30}$. The thick black line represents scission configurations and will be discussed below.

The analysis of the fission barrier in the next subsections will be based on all the above mentioned plots of the PES.

B. Detailed description of the PES

The fission barriers and the PESs obtained for the two nuclei considered agree with the expectations for nuclei in the heavy-actinides region. Both isotopes are prolate in their ground states with $Q_{30} = 16$ b. On the quadrupole-octupole map of the PES, one can see a fission valley heading towards large octupole deformation starting at the ground state. It describes super-asymmetric fission strongly related to cluster radioactivity \[50, 51\]. The minimum of the energy corresponding to this valley can be seen in Figs. 1 and 2 at $Q_{20} = 30, 40$ and 50 b and large octupole moments. The saddle point in the super-asymmetric valley reaches over 20 MeV and in heavy actinides, leads to an exotic decay mode \[51\], not observed experimentally. We will not discuss this type of fission here.

The first reflection-symmetric barrier is located at around $Q_{20} = 30 - 35$ b. It is well known that triaxial deformation reduces its height \[18, 19\]. In Figs. 1 and 3, we can see that the barrier width remains unchanged by including triaxiality but the sharp-peaked summit of the axial barrier is cut off by 4.7 MeV in $^{252}$Cf and 3.7 MeV in $^{258}$No. The fission barriers including triaxiality are 7.0 MeV and 7.3 MeV high, respectively. The experimental value for $^{252}$Cf is 5.3 MeV \[52, 53\]. Triaxial deformation of the fission path is relatively small $\gamma \leq 12^\circ$. At around $Q_{20} = 50$ b the nucleus goes back to fission through axial shapes, and triaxiality is negligible for larger elongations.

The modification of the landscape by including triaxial deformations is non-negligible, but its influence on the spontaneous fission half-life depends on the value of the collective inertia along the triaxial path as compared to the axial one. There are indications that triaxiality should not affect fission dynamics since the energy decrement at the saddle is compensated in the calculation of the collective action by the increase of the collective inertia and therefore, the tunneling probability is larger along the axial path \[10, 54\]. Please note that despite the similarity in barrier heights, the experimental fission half-lives of the two isotopes differ by 12 orders of magnitude \[55\]. The key to understanding this result, implying quite different barrier penetrabilities, is the existence of a second barrier in $^{252}$Cf that disappears in the $^{258}$No case, reducing the effective width of the total barrier dramatically. In consequence, theoretical fission half-lives are $\log_{10}(t_{1/2}/s) = 8.74$ for $^{252}$Cf and $\log_{10}(t_{1/2}/s) = -1.94$ for $^{258}$No (calculated in the axial regime). These values are less than one order of magnitude away from experimental data.

The second minimum can be found at an energy as low as 1.3 MeV above the ground state at $Q_{20} = 50$ b in $^{252}$Cf and 0.2 MeV below the ground state at $Q_{20} = 55$ b in $^{258}$No. In both isotopes, the shapes of the nucleus are axially and reflection symmetric in the second minimum. A well pronounced fission valley with non-zero octupole deformation opens up at larger elongation in both iso-
topes. The topography of the PES beyond this point is crucial for determining the fission fragments mass asymmetry and fission half-lives. The key factor is whether the nucleus would prefer to stay in the symmetric fission path or rather turn into the octupole valley. The substantial discrepancy between $^{252}\text{Cf}$ and $^{258}\text{No}$ can be found in the shape of the symmetric fission barrier and the shape of the energy surface around $Q_{20} = 100$ b for small octupole deformation. The difference is relatively small in absolute values but provides important consequences for the fission properties.

One can notice in the $^{252}\text{Cf}$ PES that around deformation ($Q_{20}, Q_{30}$) = (100 b, 0 b$^{1/2}$) a 4.5 MeV high second barrier arises, which blocks the symmetric fission channel in this isotope. In fact, from $Q_{20} = 70$ b, there is no local symmetric minimum on the PES (there is a peak not a saddle in the two-dimensional plot), and hence the barrier is plotted with a dash-dotted line in Fig. 1. In this region, remaining at zero octupole moment is energetically unfavorable as the potential energy grows 3.2 MeV above the second minimum and the asymmetric valley is easily reachable with small energy costs. We can see in Figs. 1 and 2 that the asymmetric valley starts already at $Q_{20} = 70$ b and the second saddle is at 3.1 MeV above the ground state (1.8 MeV above second minimum). Moreover, the energy in the asymmetric fission path rapidly decreases, reducing the barrier width.

In contrast, the second barrier in $^{258}\text{No}$, located at $Q_{20} = 65$ b, is flat with a height only 0.7 MeV above the second minimum (0.3 MeV above the ground state). It is almost completely hidden below the ground state and therefore does not contribute in a substantial way to the half-life, as it was mentioned above. At $Q_{20} = 90$ b the asymmetric valley opens up without any additional barrier (see Fig. 3). The fission process may proceed in the asymmetric mode, but the nucleus may as well stay at the reflection symmetric path without energetic costs. This fact explains the experimentally observed bimodal fission mass distribution with a small (5% abundance) component with high kinetic energy and mass symmetric distribution.

The topography of the $Q_{30} - Q_{40}$ planes given for fixed quadrupole moment and shown in Figs. 1 and 2 has quite a simple structure up to the region of the second barrier. We can see only one – or at most two – local minima in parabolic-shaped valleys. In the final phase of the fission process, the PES is far much complex. Already at $Q_{20} = 120$ b in both isotopes, we can see several branches of the fission valley with two or three local minima for the same quadrupole moment. The first one is octupole deformed. Its shape is depicted in the top panel of Fig. 4. It leads to asymmetric fission-fragment mass distribution, and therefore we refer to it as an asymmetric mode. The second one with $Q_{30} = 0$ b$^{1/2}$ and small values of $Q_{40}$ (around 50 - 70 b$^2$) is a natural continuation of the symmetric fission path. The nuclear shape consists here of two almost spherical pre-fragments, see the middle panel of Fig. 4. This one is often called a compact mode of fission. By stretching this configuration, we increase the distance between pre-fragments and make the neck thinner up to its disappearance. The compact path is continued after scission with two separated fragments. For a two-fragment solution, further increasing of the quadrupole moment leads to an increase of the distance between daughter nuclei instead of a shape change. The minimum of the energy is obtained for a configuration with a small mass asymmetry between fragments and, in consequence, a small octupole deformation.

The third minimum also corresponds to reflection symmetric shapes, but the hexadecapole moment takes much larger values, over 90 b$^2$. In this configuration, pre-fragments are not well disentangled. The shape is almost cylindrical, cucumber-like with a small reduction of thickness in the region of the neck (bottom panel of Fig. 6). This solution is called symmetric elongated mode. Small reflection asymmetry can also be found here, especially for large quadrupole moments. The corresponding fission path is the highest in energy, and it survives up to a very large elongation of the nucleus as the neck is not formed and a rupture of the system is not possible without a substantial energy cost. Calculations with the Skyrme energy density functional suggest that this fission path is energetically comparable with an asymmetric path around the second barrier in the nuclei from the region of heavy actinides and may play an important role in fission.

We should stress here that the crossing of fission paths in Fig. 1 cannot be interpreted as a possible place of bifurcation or configuration change. This is a typical example of a fake saddle point. The fact that two or even three lines have the same energy for the same quadrupole moment does not mean that they represent the same or similar shapes of the nucleus. As one can see in Fig. 6 the differences in the nuclear density distribution between fission paths are usually huge.

The existence of two local minima and surrounding local valleys (e.g. compact and symmetric elongated) at the same quadrupole and octupole deformation leads straight to the multiplication of the surfaces on the traditional elongation–mass asymmetry maps, like in Fig. 2. The blue dashed lines in Figs. 4 and 5 indicate solutions corresponding to the local minimum of the energy for fixed $Q_{20}$ and $Q_{30}$, i.e. these data could be used to create the PES map in the ($Q_{20}, Q_{30}$) space. Mixing values coming from different valleys may lead to an ambiguous and often erroneous interpretation of the calculated results which might eventually suggest contradictory conclusions. As the surfaces are often similar in energy, the choice of the surface would likely be a matter of a random selection by a numerical procedure or an arbitrary decision of the researcher. There is also the risk of an accidental change of the surface. This effect could easily be omitted in the analysis of fission as the graphical plotting programs are likely to smooth out sharp ridges. The application of the density distance parameter described below in Subsection 4.1.1 can be useful to prevent these...
The density distribution of $^{258}$No at $Q_{20} = 140$ b (left) and $Q_{20} = 200$ b (right) in various fission paths: asymmetric (top), compact before and after scission (middle) and elongated symmetric (bottom).

In the analysis of Figs. 4 and 5 various scenarios for reaching pre-scission configuration can be envisaged. The scission line is visible in these plots for $Q_{20} \geq 120$ b as a black line (consequence of plotting many closed energy contour lines) separating single shapes (above) from two-fragments configuration (below). The rapid change on the energy is a consequence of the strong dependence of the neck with multipole moment parameters: slight changes lead to a strong reduction of the neck and eventually to the splitting of the nucleus (see discussion below).

Beyond the region of the second fission barrier ($Q_{20} = 100$ b), the PES goes down towards scission. The pre-scission line, i.e. the line of the most elongated shapes before the rupture of the neck, is clearly seen at Fig. 2 as a few MeV high cliff that separates the fission valley from the two-fragments configuration. There are several ways of reaching a scission configuration: The first is through a symmetric compact mode. Increasing elongation leads to a relatively smooth shape evolution from pre- to post-scission configuration. Nevertheless, even if a energy fall is not noticed, an abrupt change in the nuclear density distribution around the neck region is visible (e.g. see 255Fm case). The two dimensional $Q_{30} - Q_{40}$ sections of the PES between $Q_{20} = 120$ b and 130 b in $^{252}$Cf and between 150 b to 160 b in $^{258}$No do not differ substantially among them despite a few MeV energy drop in the minimum of the valley. It indicates that the pre- and post-scission density distributions of the whole system are relatively similar despite the neck rupture. Another, most intuitive, way of reaching a scission point from the asymmetric fission valley is by going along the fission path (marked with the blue dashed line in Figs. 1 and 2 and black dots in Figs. 4 and 5) to the largest possible quadrupole moment. As the energy decreases simultaneously with increasing elongation, the largest gradient indicates this is the most probable fission scenario. The large mass asymmetry $A_H/A_L \sim 140 - 142/112 - 116$ obtained before the neck rupture in this point corresponds to the experimentally observed most probable fission fragment asymmetry.

The two scenarios presented above for the evolution of the nuclear shape assume that the system remains on the fission paths presented in Fig. 1. Therefore, only one or two particular shapes of the nucleus are taken at scission. Such analysis can explain the fission modes observed in the experiment, but it is insufficient to reproduce the details of the fission fragment mass distribution. The reason is that on its way from the saddle to scission, the collective wave packet may explore different configurations away from the lowest energy fission path, still fulfilling the condition of the descending energy but not with the largest gradient. In this way, every configuration of the scission line in the neighborhood of the asymmetric fission valleys which are visible in Fig. 3 is accessible, of course with a reduced probability. These configurations can be observed in Figs. 4 and 5.

For $Q_{20} \geq 140$ b the post-scission compact minimum in the south-west corner of each panel has got lower energy than on the asymmetric path. The latter valley seems to be soft in the direction towards the first one, and the ridge separating them does not exceed 2 MeV. Those figures indicate that the exit points from the asymmetric fission valley are available already at relatively small octupole moments and with a smaller asymmetry of nuclear shapes than at the end of the asymmetric fission path.

Two additional aspects of this scenario must be pointed out. First, a scission point is accessible at much less elongated nuclei than at the end of the asymmetric fission path. In some lighter nuclei, where a scission point is above the ground state energy, this would reduce the width of the barrier. In consequence, tunneling probability and the half-lives can be substantially shortened. Second, at smaller quadrupole moment, an exit point from the asymmetric valley at low octupole moment may be ended not in fusion valley but in the compact fission valley before scission. This is another mechanism of feeding the symmetric mode of fission. Thus, the dynamical calculations of the fission mass yields for $^{252}$Cf, where only quadrupole and octupole deformations were taken under consideration, showed a small contribution for the symmetric mass division.
FIG. 7. The density distance function $D_{\rho \rho'}$ (in logarithmic scale) given by Eq. (4) between two neighboring configurations in a deformation space $Q_{20} - Q_{30}$ of $^{252}\text{Cf}$ (top) and $^{258}\text{No}$ (bottom). Contour lines for the energy are plotted every 5 MeV for better identification of the different regions of the PES.

C. Surface discontinuity and density distance

As mentioned in Section II, the density distance is an appropriate quantity to check the consistency of the PES and pinpoint possible discontinuities of the surface that may lead to false conclusions concerning fission dynamics. In Fig. 7 we have plotted, for each point in the $(Q_{20}, Q_{30})$ plane, the largest of the two density distances computed for the two configurations $(Q_{20} + \Delta Q_{20}, Q_{30})$ and $(Q_{20}, Q_{30} + \Delta Q_{30})$. The figures look pretty similar for both isotopes and a few regions of large $D_{\rho \rho'}$ can be identified:

A - first barrier;
B - around the second minimum;
C - between symmetric and asymmetric valley at $Q_{30} \sim 15 \text{ b}^{3/2}$;
D - bordering asymmetric valley at large octupole deformation;

E - scission line.

We will denote these regions as “regions of discontinuities” due to the large difference in densities corresponding to neighboring points indicating on possible abrupt change of configuration.

The first region of discontinuity (A) is encountered already at the first barrier. The nucleus has a double cone (diamond) shape on the up-going part of the barrier, whereas a two-center structure is created beyond the maximum of the barrier, as it can be seen in the left panels of Fig. 8. Both density distributions are clearly different with a significant jump in hexadecapole moment. A sharp peak of the first fission barrier also indicates a sudden change of configuration, and the fake or missing saddle mentioned above is usually present [22] because two solutions can be found for the same quadrupole moment around the peak. The density distance calculated in this region does not take into account the influence of triaxiality discussed in Subsection III A that eliminates discontinuities.

In the right panels of Fig. 8, the region (D) of enhanced density distance is observed. As we can see, there is no discontinuity here but only a change of the hexadecapole moment can be observed in this region. The source of this kink can be explained by looking at Figs. 4 and 5. The valleys plotted in the $Q_{30} - Q_{40}$ planes around $Q_{20} =$
FIG. 9. Fragments of the PES of $^{252}$Cf at fixed $Q_{20} = 50$ b, 70 b, 90 b and 110 b.

140 b lie along a more or less straight line with a slope of the order of 1. We determine the localization of the bottom of these valleys by minimization with a constraint on the octupole moment (marked by blue dashed lines). This procedure sometimes does not give the correct value that is obtained by following the direction of the gradient along $Q_{30}$ and $Q_{40}$ that determines the bottom of the valley. As a consequence of the improper determination of the bottom of the valley using a constraint on the octupole moment, large increases in the value of $Q_{40}$ can be noticed between $Q_{30} = 50$ b $^{3/2}$ and 55 b $^{3/2}$ in Fig 8. No real discontinuity of the surface is found here, but rather a problem with the precise numerical evaluation of the bottom of the valley and therefore no important physics is missed here.

The regions (C) and (D) should be discussed together as they separate the compact symmetric and the asymmetric fission valleys. A first look at the PES in Fig. 1 reveals a seemingly smooth surface: no sharp ridges or sudden energy changes. Therefore, it comes as a surprise to find a discontinuity here. To solve this puzzle, one has to use a magnifying glass: in Figs. 9 and 10 we have plotted a blown-up view of the sections of both valleys in $^{252}$Cf and $^{258}$No, respectively. The step size in these calculations was reduced to $\Delta Q_{30} = 1$ b $^{3/2}$ with starting point from the nearest mesh point with smaller or larger octupole moment.

In the left columns of Figs. 9 and 10 the PES in the second minimum is plotted. In this case, the energy grows up smoothly with increasing mass asymmetry. Only a small bending in octupole moment can be noticed. The PES picture at $Q_{20} = 70$ b, in the region (B) of discontinuity, is completely different, see panels in the second column. We find a kink in the energy curve at a relatively small octupole deformation. At this point, a clear change of configuration takes place as the neck, clearly visible for near reflection symmetry shapes, is not pronounced anymore in more asymmetric shapes. Also, the hexadecapole moment jumps from $Q_{40} = 25$ b$^{2}$ to 35 b$^{2}$. It is easy to distinguish here the compact valley from the elongated asymmetric one. Moreover, in $^{252}$Cf, the asymmetric valley can be extended towards lower octupole moments up to zero. This is the germ of the symmetric elongated fission valley. Discontinuity in the region (B) is not a significant problem in the description of fission as a transfer from the second minimum to the asymmetric valley requires a few additional MeV of energy, which practically blocks such evolution.

Increasing the quadrupole moment, we find a space between regions (B) and (C) in Fig. 7. Its impact is also visible in Figs. 9 and 10 at $Q_{20} = 90$ b. Here, the PES as a function of $Q_{30}$ is continuous again. Hexadecapole mo-
ment gradually increases indicating a smooth connection between the compact and asymmetric valleys. The transfer between configurations is possible as a consequence of decreasing the energy of the asymmetric minimum. The tiny part of the symmetric elongated surface can be noticed only very close to reflection symmetric shapes.

The rightmost panels of Figs. 9 and 10 describe the region (C) of discontinuity. Despite the same values of the quadrupole and octupole moments and the similarity of energies, the hexadecapole moments and the shapes of the nucleus are considerably distinct in both configurations. In the compact symmetric mode, two pre-fragments are separated by a thin neck. In the asymmetric mode, the density distribution is more uniform along the symmetry axis. In both isotopes, the compact mode is limited to hexadecapole moments in the range from $Q_{40} = 50 \, \text{b}^2$ to $60 \, \text{b}^2$ whereas the asymmetric mode is described by much higher values, over $65 \, \text{b}^2$. In $^{252}\text{Cf}$, the compact valley created by increasing the octupole moment ends with a sudden drop into the asymmetric valley. In this nucleus, by decreasing octupole moment in the calculations of consecutive mesh points in the asymmetric valley, one may reach zero octupole moment in a configuration characteristic for the elongated symmetric valley. The transition from the compact to the asymmetric valley is an analogue of the scission line discontinuity described below. In $^{258}\text{No}$ both surfaces meet at the same energy, and the elongated symmetric part can not be determined at $Q_{20} = 110 \, \text{b}$. In region (C), in both isotopes, transfer to the asymmetric valley is energetically favorable.

The transition between configurations in this region is usually overlooked. It is easy to link both valleys when the mesh points are scattered by 4 or 5 $\text{b}^{3/2}$, which is usually a reasonable choice while producing the PES maps. The similarity of the energy slopes as well as the fact that increasing octupole moment on the compact valley beyond its end, leads to a solution in the asymmetric one (by applying the self-consistent energy minimization) enhances the chances of making mistakes. The discontinuity in the region (C) signals the frontier between the compact mode surface in the symmetric second minimum region and the symmetric second barrier.

Looking at the energy section maps in Figs. 4 and 5 we find that the discontinuity between symmetric and asymmetric surfaces discussed above is a good example of missing saddles as discussed by Dubray and Regnier [22]. In three-dimensional PES, the problem of a rapid change of configurations disappears.

Finally, a commonly known discontinuity is localized in the region (E) of the scission line. There is a huge difference in pre-scission and post-scission configurations. It
FIG. 11. The same as in Fig. 7, but for the PES at fixed $Q_{20}$ in a deformation space $Q_{30} - Q_{40}$ of $^{252}$Cf at $Q_{20} = 70$ b (top), at $Q_{20} = 130$ b (middle) and $^{258}$No at $Q_{20} = 160$ b (bottom). Contour lines of equal energy are plotted every 5 MeV for better identification of the different regions of the PES.

is very hard or even impossible to find a continuous link by using constraints on multipole moments to control the nuclear shape. Applying constraints on the neck parameter $Q_N$ may help to provide the continuous surface on the scission line [49, 50].

Let us discuss now the source of the scission line cliff obtained in the self-consistent calculations. The asymmetric valley in two-dimensional space is built of configurations which are local minima along all the directions orthogonal to the ones of the constraints. In consequence, decreasing the neck thickness (or hexadecapole moment) leads to increasing the energy of the system even though the ruptured nucleus is energetically favorable. The height of the barrier separating the asymmetric path from the no-neck solution reduces to zero with increasing quadrupole moment. Beyond the pre-scission line, any shape of the nucleus is unstable against neck rupture, i.e. the energy monotonically decreases with decreasing neck thickness. The energy minimization procedure cannot find a stable solution with a neck. The gradient of the energy directs the system towards post-scission configuration with much lower energy in the self-consistent process. Of course, the cliff on the scission line does not mean that in Nature the neck disappears instantly, but only that a further thinning of the neck should occur without increasing the elongation of the system.

The concept of density distance can also be applied to the PES given as a function of the octupole and hexadecapole moments for fixed $Q_{20}$ values. An example of the results is presented in Fig. 11. Here again, the discontinuity at the scission line is clearly visible. The density distance is also enhanced in some other regions of the PES quite randomly scattered on the surface. Its values are relatively small in comparison to the scission line ones. The only characteristic region of larger density distance separates elongated symmetric valley from the compact one.

D. Multiple solutions

We have already shown that the description of fission in terms of a one-dimensional or even a two-dimensional PES may lead to many misunderstandings. Two or more different configurations can be obtained in the same location of the PES in those cases. This problem has been observed while discussing the region between the compact symmetric and the asymmetric valleys. Similar issues can arise if one analyses the so-called fusion channel with two separate fragments. Decreasing the quadrupole moment of the system in this region leads to approaching fragments which are much closer than what can be achieved in the scission configuration. In consequence, the fusion valley covers a much larger area than presented in Fig. 2. This surface, mostly "hidden" under the asymmetric fission valley from Fig. 2 is shown in Fig. 12. Only in the lowest quadrupole deformation region, the fragments are close to each other, and Coulomb energy is so high that the fusion valley climbs up above the fission one. Since the global energy minimum for a given quadrupole moment may be in the post-scission configuration, an important physical problem appears. Should we take this solution as part of the PES leading to fission or rather keep staying in the fission valley as long as it is possible.

Two alternative approaches can be found in Fig. 1 of Ref. [60] by Regnier et al. and Fig. 1 of Ref. [58] by Warda et al. Both Figures show the PES of $^{258}$Fm calculated with the same model and interaction (HFB theory and Gogny D1S force). Nevertheless, the shape of the asymmetric fission valley is different. In the first plot, it is narrow and equipotential (the lines are mainly horizontal), whereas in the second case, the asymmetric valley is wide and the lines of constant energy are rather vertical. The source of the difference comes from the distinct strategy of selecting the local minima for the
FIG. 12. The same as in Fig. 2 but for the fusion valleys are plotted.

surface. Regnier et al. selected the lowest of the local minima for the given constraints. Warda et al. put more attention to the continuity of the changes in the shape and preservation of the valley in which a nucleus was in the previous phase of evolution. In the first approach, the scission line is localized at a much lower elongation, and the PES includes a larger part of the fusion valley.

We would like to stress that, unexpectedly, both figures give the correct surface in two dimensions showing the importance of considering multidimensional PESs. Restricting the deformation space to just one, two or three dimensions simplifies the interpretation of the results as well as its graphical representation, but it always hides information and can veil our understanding of the nature of the fission process.

We would like to point out that one can observe an internal structure of the PES in the fusion channel. The surface is usually smooth with mass and deformations of the fragments gradually evolving with octupole moment. A rapid drop in the energy indicates an abrupt change of the fragment configuration.

The extended fusion valley can also be seen in Fig. 5, where, for fixed quadrupole moments, the PES as a function of the octupole and hexadecapole moments are plotted. Again we can see the fusion valley even at low quadrupole moments. It extends towards much larger hexadecapole moments than it was shown in Figs. 4 and 5. This analysis provides one more, not very optimistic, conclusion. Applying a triple constraint (on quadrupole, octupole and hexadecapole moments) and preparing a three-dimensional surface in the self-consistent calculation does not guarantee the uniqueness of the solution. We still can obtain completely distinct shapes of the density distribution depending on the initial configuration.

IV. CONCLUSIONS

We have investigated the fission barriers of two heavy actinide nuclei: $^{252}$Cf and $^{258}$No using the self-consistent microscopic approach. The calculations were made using multiple constraints on the quadrupole, octupole, and hexadecapole moments. A detailed analysis has shown a complicated structure of the potential energy surface at large quadrupole deformations of the nucleus. The competition between local minima at a given quadrupole moment: compact, elongated and symmetric elongated determines the fission mode and the experimentally observed fragment mass distribution. We have shown that the scission may occur at a quadrupole deformation smaller than the one at the end of the fission path in the minimum of the valley on the potential energy surface.

The calculations using three constraints give a much more complete description of the potential energy surface. Nevertheless, it is possible to find distinct solutions corresponding to the same values of the quadrupole, octupole, and hexadecapole moments. These configurations create various layers of the potential energy surface in the same place of two- or three-dimensional maps. It makes the description of the fission even more complicated.

Reducing the full space of deformation to two-dimensions creates a potential energy surface that is not continuous. Rapid changes of the configuration of density distribution may be found even at seemingly smooth surfaces. We therefore conclude that the jumps between surfaces must be discussed in the analysis of the fission process.

The present analysis is based on the HFB approximation, but it also applies to any constrained, self-consistent type of calculations. Problems with multiple minima and surface discontinuities also affect macroscopic-microscopic models, although it is much easier to control the whole spectrum of nuclear shapes there.

The discussion of the determination of the potential energy surface is not the only relevant issue in the analysis of fission. Many other aspects also have a significant impact on the dynamics of this process. We should mention here the influence of the inertia parameter and pairing degrees of freedom that shall also be investigated in the future.
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