On the topographical properties of fission barriers

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Abstract

The fission barrier, given as the difference between the saddle-point and ground-state masses, plays a mandatory role in determining the survival probability of fissile nuclei. While the ground-state mass is strongly influenced by the shell correction, according to the topographic theorem the saddle-point mass should be rather close to its macroscopic value. In the present paper, the topographical properties of fission barriers have been investigated within the macro-microscopic approach. The range of the validity of the topographic theorem was studied in a quantitative way. It is shown that the conditions for the validity of the topographic theorem are fulfilled at the inner barrier, while at the outer saddle-point, deviations caused by the presence of shell effects of the nascent fragments have been found.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The fission barrier is a crucial characteristic for the analysis of the fission process and, in particular, for estimating the survival probability of excited compound nuclei. The experimental determination of the height of the fission barrier is a rather complicated procedure requiring also some theoretical assumptions, for instance on the nuclear level densities. The experimental data on the height of the fission barriers available at the moment are restricted to about hundred data points (see, e.g., [1–3] and references therein), with relative uncertainties which are often several orders of magnitude larger than the uncertainties in the experimental ground-state masses. Moreover, the values for the same nuclei differ by as much as 1 MeV.

Difficulties are also present in the theoretical description. The realistic determination of the saddle-point deformation and, consequently, of the height of the fission barrier requires using at least three degrees of freedom describing the elongation of the nucleus, deformation and mass asymmetry. Additional degrees of freedom, e.g. neck thickness or deformations of the two nascent fragments are also important for the fission process. Finding the characteristic
points in such a multidimensional space can in some cases be very difficult and time consuming. The most often used models applied for the calculation of potential-energy landscapes and for the determination of the ground-state masses and fission barriers are: the standard macro-microscopic approach, e.g., [4–8], the extended Thomas–Fermi model with effective Skyrme force, e.g., [9], and microscopic models based on self-consistent Hartree–Fock calculations (both relativistic and non-relativistic), e.g., [10, 11]. The first two types of models are based on the Strutinsky shell-correction method [12, 13] for the microscopic part, while the macroscopic part is obtained applying a variant of the liquid-drop or droplet model (in the standard macro-microscopic model) or by convolution of the energy-density functional (in the Thomas–Fermi method). In the extended Thomas–Fermi method both the macroscopic and the microscopic parts of the potential energy are calculated consistently. Hartree–Fock calculations have the advantage to find the complex shape, which allows for the highest binding energy with a given constraint. However, the optimization process can lead to discontinuities in the shape along a coordinate defining the constraint, leading to severe problems in defining a characteristic quantity of the potential-energy landscape like the fission saddle [14]. The flooding algorithm [9, 14], which is the most powerful approach for this purpose, can only yield reliable results, if calculations are made in a controlled multidimensional deformation space, e.g. with the standard macro-microscopic approach.

In discussing different properties of the nuclear-potential-energy surface, Myers and Swiatecky have introduced the topographic theorem [6]. According to this theorem, due to the specific topological properties of the potential-energy landscape around the fission saddle, the saddle-point mass given as the sum of the ground-state mass and the height of the fission barrier should be a smooth function of different macroscopic quantities of the nucleus, e.g. neutron number, proton number or fissility. In other words, although the shell effects can considerably change the saddle-point deformation compared to predictions of a macroscopic model, the difference between the macroscopic and macro-microscopic saddle-point mass should be very small, much smaller than the ground-state shell-correction energy. If so, then the mass at the fission threshold should be essentially a macroscopic quantity, which gives rather direct information on some important global macroscopic properties of nuclei.

The topographic theorem was used in [1, 15], where the validity of different theoretical predictions of the fission barriers in the experimentally unexplored regions has been examined by means of a detailed analysis of the isotopic trends of the available experimental saddle-point masses given as the sum of the ground-state mass and the height of the fission barrier. It was argued that models which predict strong variations of the difference between experimental saddle-point mass and model-calculated macroscopic saddle-point mass, would not be able to give realistic predictions for nuclei in regions far from stability.

Another consequence of the topographic theorem is that the saddle-point mass can be calculated within some macroscopic model, once the parameters of the macroscopic model have been well established. This would simplify and speed up the calculation significantly, because only the ground-state mass should be found in the full macro-microscopic calculations taking into account the shell correction for determining the fission barrier.

Some rather qualitative theoretical arguments for the validity of the topographic theorem have been given in [6] considering the specific properties of a saddle point in the potential energy in multidimensional (at least two-dimensional) space. The saddle point is characterized by a maximum along a cut in the fission direction in this space and minima along cuts in all other directions, which are perpendicular to the fission direction. It was argued [6] that shell effects, which modulate the potential-energy surface with periodic oscillations in all directions, change the threshold energy only little, if the wavelengths of the microscopic variations of the potential-energy are ‘small’ compared to the wavelength of the corresponding macroscopic
variations. Small regions with positive shell corrections do not increase the threshold sizably, because the system can avoid this region by moving around. Small regions with negative shell corrections do not decrease the threshold neither. By relating the order of the macroscopic wavelength to the nuclear size and the order of the microscopic wavelength to the typical wavelength of the quantized nucleons, Myers and Swiatecki estimated a value of \( \approx A^{-1/3} \) for the ratio of microscopic and macroscopic wavelengths, which seemed to be small enough for the topographic theorem to be valid for heavy nuclei.

The topographic theorem has also been empirically validated [6, 16] by comparing the experimental values of the fission-saddle masses with the predictions of different macroscopic models. The authors of [6, 16] concluded that the absolute values of the shell correction to the saddle-point mass should be below \( \sim 2 \text{ MeV} \).

It is the aim of the present work to investigate the conditions for the validity of the topographic theorem on the mathematical level in a quantitative way. The quantitative limit of the ratio of the microscopic and macroscopic wavelengths for the validity of the theorem will be determined. This will be done on the base of a schematic macro-microscopic model, where the wavelengths can be varied to a large extent that is impossible in a realistic macro-microscopic model. These conditions will be compared with the situation in nuclei by means of a realistic model calculation.

2. Details of the calculation

The potential energy of a deformed nucleus can be calculated as

\[
V_{\text{pot}}(A, Z; R, \vec{\beta}, \eta) = M(A, Z; R, \vec{\beta}, \eta) - \text{normalization constant},
\]

where \( M \) is the system mass (the system can be either a mononucleus or two separated nuclei), which depends on the nucleon composition \( A \) and \( Z \), elongation of the mononucleus \( R \) (distance between mass centers of the nascent fragments), various deformation parameters \( \vec{\beta} \) (ellipsoidal deformations of the nascent fragments in our case) and mass asymmetry \( \eta \). By using the normalization constant usually either the macroscopic (liquid-drop) part of \( M \) is normalized to zero for the spherical shape of the compound nucleus or the total potential energy is set to be zero in the entrance channel of, e.g. a fusion reaction for the ground-state deformations of the target and projectile at infinite distance between them.

2.1. Macro-microscopic model

According to the arguments given in section 1, we used a standard macro-microscopic model to determine the properties of the potential-energy landscape which are relevant for the validity of the topographic theorem. In the standard macro-microscopic model based on the Strutinsky shell-correction method [12, 13] the system mass is given by

\[
M(A, Z; R, \vec{\beta}, \eta) = M_{\text{LDM}}(A, Z; R, \vec{\beta}, \eta) + \delta E(A, Z; R, \vec{\beta}, \eta).
\]

Here \( M_{\text{LDM}} \) is the liquid-drop mass which reproduces the smooth part of the dependence of the mass on deformation and nucleon composition. The second term \( \delta E \) is the microscopic shell correction (including pairing correction) which is usually calculated using the Strutinsky shell-correction method. It gives a non-smooth behavior of \( M \) due to irregularities in the shell structure.

We calculate the macroscopic mass \( M_{\text{LDM}} \) in the framework of the finite-range liquid-drop model [4, 5, 17] (FRLDM). The shell correction is obtained applying the well-known two-center shell model developed in [18–20].
In spite of the fact that the standard macro-microscopic approach works well for the ground-state and saddle-point deformations, it (being applied to the whole system) fails in the region of the Coulomb barrier in the entrance channel of the fusion reaction and also in the region of two well-separated nuclei [6, 14, 21, 22]. The standard model cannot describe correctly the transition from the potential energy of the mononucleus to the potential energy of separated nuclei. An extended macro-microscopic approach was proposed in [21, 22] for the simultaneous analysis of deep-inelastic collisions, quasifission and fusion–fission processes. The mentioned problem of the standard model was solved within the extended macro-microscopic approach. In the region of nuclear deformations under discussion (saddle-point deformation) and especially for heavy nuclei the extended macro-microscopic model coincides with the standard one. Thus, in the present paper we will use the standard model described above.

The two-center parametrization [20] has been chosen for the description of nuclear shapes. It has five free parameters. It is possible, consequently, to define five independent degrees of freedom determining the shape of the nucleus. We use the following set of them: \( R \) – the distance between mass centers of the nascent fragments or separated nuclei; their ellipsoidal deformations \( \delta_1 \) and \( \delta_2 \); \( \eta = (A_2 - A_1)/(A_2 + A_1) \) – the mass asymmetry parameter (\( A_1 \) and \( A_2 \) are the mass numbers of the fragments) and \( \epsilon \) – the neck parameter. This parametrization is quite flexible and gives realistic shapes for the fission as well as for the fusion process [20]. However, inclusion of all five degrees of freedom of the two-center parametrization complicates the calculations significantly and it is almost beyond our computational possibilities. In order to decrease the number of collective parameters we use one unified dynamical deformation \( \delta \) instead of two independent variables \( \delta_1 \) and \( \delta_2 \) (see [21] for more details). The fixed value of the neck parameter \( \epsilon \approx 0.35 \) was recommended in [23] for studying the fission process within the two-center shape parametrization. We used this value in the calculation of the potential energy and further determination of fission barriers. Thus, the calculations of the potential-energy landscape were performed in the three-dimensional deformation space \( \{R, \delta, \eta\} \).

Figure 1 shows the dependence of the shell correction on elongation \( R \) and mass asymmetry \( \eta \) for the nucleus \( ^{238}\text{U} \). Cuts for constant elongation (near the compound-nucleus ground state and near scission) and cuts for constant mass asymmetry (at mass symmetry and in the bottom of one of the asymmetric fission vallies) are also shown. These figures clearly visualize the two basic topological properties of the shell correction: first, near the ground state the shell correction is an oscillating function of the chosen deformation parameters. We will refer to this part of the shell correction as the compound-nucleus shell correction. When the deformation is increased, and we go away from the ground state, the amplitude of the oscillations of the compound-nucleus shell correction decreases. Second, coming closer to the scission region, where the neck connecting the nascent fragments is already well pronounced, the shell effects corresponding to the final fission fragments appear gradually. After the shell effects of the nascent fragments have established completely, the shell correction becomes independent of the relative distance between the fragment centers-of-mass \( R \), but still depends on the other deformation parameters. As we will see below, these two features play a crucial role for the validity of the topographic theorem and, in particular, determine different topographical properties of the inner and outer saddle points.

The influence of the fragment shell effects was widely discussed in the literature (see e.g. [7, 24–26]). It was found in [24] that in the region of actinides the fragment shells are present and, therefore, influence the mass-asymmetry deformation already at the outer saddle point. The presence of the shell effects of the nascent fragments is proved to be associated with the appearance of a neck in the shape of the fissioning nucleus. When the nucleus starts to develop a neck, it is more probable that the wavefunctions have a knot in the center of the system. This
Figure 1. Shell-correction energy for the $^{238}$U nucleus in the coordinates $(R, \eta)$. The numbers at the contour lines give values of the shell correction in MeV. The cuts of the contour plot are made at constant values of $R$ (6.2 fm and 18 fm) and $\eta$ (0 and 0.14) shown by thick white lines. Types of the lines correspond to those of the cuts. The dash-dotted curve on the upper graph is the macroscopic potential for symmetric mass split $\eta = 0$. The table contains the characteristic wavelengths extracted from these figures (for the definition of the scaled elongation parameter $r$, see the text).

means that the wavefunctions resemble already the wavefunctions in the separate fragments. This may explain why the shell effects observed at larger elongations show only little variation as a function of elongation. Our findings also confirm the previous results: the outer saddle is already influenced by the nascent fragment shells.

For the quantitative investigation of the topographic theorem one needs to know the values of the wavelengths of both the shell correction and the macroscopic potential energy. We define them using the procedure visualized in figure 1 (we describe the procedure for the two-dimensional case, but it can be easily extended for more dimensional deformation space):

(i) First, we find the position of the ground state of a nucleus ($R_{g.s.}$ and $\eta_{g.s.}$) as a global minimum of the potential energy.

(ii) Second, we make cuts of the shell correction energy at the constant values $R = R_{g.s.}$ and $\eta = \eta_{g.s.}$ as shown in figure 1. Along these cuts near the ground state we fix positions of two successive minima or maxima in each direction. The distances between each pair
of these points give us the corresponding wavelengths of the shell-correction oscillations $\lambda^{(0)}_{\text{CN}}$ and $\lambda^{(0)}_{\text{CN}}$. Some uncertainty resides in this definition, because the shell-correction oscillations are not exactly periodic, and one can define the wavelength as the distance between two successive maxima or minima or doubled distance between minimum and maximum nearest to the ground state. This induces an uncertainty of about 10–20% that is not important for the present study.

(iii) In order to determine the wavelength of shell-corrections oscillation in the region of separated fragments $\lambda^{(0)}_{\text{CN}}$ and $\lambda^{(0)}_{\text{fr}}$, the cuts should be done in the vicinity of $R = R_{\text{scission}}$, where $R_{\text{scission}}$ is the distance of the mass centers, corresponding to two touching shapes.

(iv) Analyzing the macroscopic potential energy one can find the positions of the ground state $(\eta)$ to those of the macroscopic part. Since the landscape of the macroscopic energy has only one such characteristic length scale associated with the positions of the ground state and the saddle point, we need to establish a length-scale correspondence between all the deformation degrees of freedom. A consistent way to do this is through matching the curvatures of the potential energy. In other words, we assume that if the curvatures of the macroscopic potential energy in the two directions are the same (in some chosen units) then these two coordinates are similar, and the value of the characteristic wavelength obtained in one direction can also be used for the other one.

The following values were estimated for the rigidities of the macroscopic potential energy at the ground state of the nuclei around uranium: $C_{R} = 3.5$ MeV fm$^{-2}$ and $C_{\eta} = 50$ MeV with respect to the elongation $R$ and mass-asymmetry $\eta$, respectively. Introducing a new dimensionless elongation $r = R/(4 \text{ fm})$ one has $C_{r} \approx C_{\eta} = 50$ MeV. Thus, in what follows we will use the parameters $r$ and $\eta$ which are similar in the sense described above. Finally, we have for these coordinates: (i) for the wavelength of the shell-correction oscillation in $r$ direction: $\lambda^{(0)}_{\text{CN}} \approx 0.6$. (ii) For the macroscopic energy: $\tilde{\lambda} \approx 2$ and the distance between the ground state and the saddle point is $\tilde{\lambda}_{\text{CN}} \approx 8 \text{ fm}$. (iii) The characteristic length-scale of undulations of the macroscopic mass in $R$ direction deduced from the doubled distance between the ground state and the saddle point is $\tilde{\lambda}_{\text{CN}} \approx 8 \text{ fm}$. For the further discussion we need the ratios of the wavelengths of the shell-correction oscillations in both directions $(R$ and $\eta$) to those of the macroscopic part.

We draw the following quantitative conclusions from figure 1: (i) the variation of the shell effects in mass asymmetry occurs with a wavelength $\lambda^{(0)}_{\text{CN}} \approx 0.6$ near the ground state of the compound nucleus and $\lambda^{(0)}_{\text{fr}} \approx 0.2$ at scission. (ii) In the elongation direction one can observe two regions with rather different characteristics. For compact shapes, the shell effects show rapid oscillations with a wavelength of about $\lambda^{(0)}_{\text{fr}} \approx 2–2.5 \text{ fm}$. When the shape becomes necked-in with increasing elongation, the shell correction almost does not depend on $R$. The corresponding wavelength in the elongation direction goes to infinity $\lambda^{(0)}_{\text{fr}} \rightarrow \infty$. (iii) The characteristic length-scale of undulations of the macroscopic mass in $R$ direction deduced from the doubled distance between the ground state and the saddle point is $\tilde{\lambda}_{\text{fr}} \approx 8 \text{ fm}$. For the further discussion we need the ratios of the wavelengths of the shell-correction oscillations in both directions $(R$ and $\eta$) to those of the macroscopic part. Since the landscape of the macroscopic energy has only one such characteristic length scale associated with the positions of the ground state and the saddle point, we need to establish a length-scale correspondence between all the deformation degrees of freedom. A consistent way to do this is through matching the curvatures of the potential energy. In other words, we assume that if the curvatures of the macroscopic potential energy in the two directions are the same (in some chosen units) then these two coordinates are similar, and the value of the characteristic wavelength obtained in one direction can also be used for the other one.

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We also estimated how much the ratios $\lambda^{(0)}_{\text{CN}}/\tilde{\lambda}$, $\lambda^{(0)}_{\text{CN}}/\tilde{\lambda}$, and also in deformation direction $\lambda^{(0)}_{\text{CN}}/\tilde{\lambda}$ vary throughout the periodic table. For a given beta-stable nucleus we found these three ratios to be approximately equal. The value varies from 0.1 for $Z^{2}/A = 31$ to 0.4 for $Z^{2}/A = 39$. The fact that the ratios corresponding to different degrees of freedom are found to be practically equal means that the ratio is a characteristic of a nucleus itself and not of a specific deformation parameter. Therefore, we may introduce a ratio, common for all the deformation parameters, $\lambda_{\text{CN}}/\tilde{\lambda}$, which has the range of variation $0.1 \leq \lambda_{\text{CN}}/\tilde{\lambda} \leq 0.4$. 

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2.2. Schematic macro-microscopic model

This observation motivates us to construct a schematic model which reproduces the qualitative features of real nuclei. On the top of the macroscopic potential there are shell effects in the compact region which show a periodic variation in the elongation direction and in mass asymmetry with about the same wavelength ratio with respect to the variation of the macroscopic potential. In addition, the amplitude of the shell effect attenuates in the elongation direction. For necked-in shapes, the shell effects in mass asymmetry continue to be subject to periodic variations, while they are almost constant in elongation direction.

We construct a two-dimensional potential-energy surface in the coordinates ‘elongation’ \( r \) (\( l(r) \)) and ‘mass-asymmetry’ \( \eta \). We do not include the third coordinate ‘deformation’ (or more of them) that we have in the realistic macro-microscopic model, because otherwise the model will lose its transparency. In subsection 3.1, we will discuss the influence of the third dimension on the results obtained with the two-dimensional model.

The macroscopic mass is parametrized by a parabolic function with rigidity \( C_\eta \) in \( \eta \) direction and by two smoothly joined parabolas with rigidities \( C_{gs} \) and \( C_{sd} \) in \( r \) direction:

\[
M_{\text{LDM}}(r, \eta) = \frac{C_\eta \eta^2}{2} + \begin{cases} 
\frac{C_{gs} (r - r_{gs})^2}{2}, & r < r_1; \\
V_B - \frac{C_{sd} (r - r_{sd})^2}{2}, & r \geq r_1,
\end{cases}
\]

(3)

where \( r_{gs} \) and \( r_{sd} \) are the positions of the ground state and saddle point, respectively; \( V_B \) is the value of the fission barrier in the schematic macroscopic model; and \( r_1 \) is the point where the two parabolas join. Thus, we have four free parameters: \( C_\eta, C_{gs}, r_{gs} \) and \( r_{sd} \). The values of the other two parameters \( r_1 \) and \( C_{sd} \) are determined from the condition of continuity of the potential energy and its derivative with respect to \( r \) at \( r = r_1 \). The mass-asymmetry parameter changes in the range \([-1, 1]\). The positions of the ground state and saddle point in the schematic LDM were chosen as \( r_{gs} = 0 \) and \( r_{sd} = 1 \). For the rigidities of the potential energy we used values obtained in the standard macro-microscopic model corresponding to the region of uranium: \( C_\eta = C_{gs} = 50 \text{ MeV} \).

The shell correction is parametrized by

\[
\delta E(r, \eta) = A_{\text{CN}} \cdot \cos \left( 2\pi \frac{r - r_{gs} - \Delta r}{\lambda_{CN}^{(r)}} \right) \cdot \exp \left[ -\left( \frac{r - r_{gs}}{l_{CN}^{(r)}} \right)^2 \right]
\times \cos \left( 2\pi \frac{\eta}{\lambda_{CN}^{(\eta)}} \right) \cdot \exp \left[ -\left( \frac{\eta}{l_{CN}^{(\eta)}} \right)^2 \right]
\]

\[
+ A_{t} \cdot \left[ 1 - \exp \left[ -\left( \frac{r - r_{gs}}{l_{t}^{(r)}} \right)^2 \right] \right] \cdot \cos \left( 2\pi \frac{\eta}{l_{t}^{(\eta)}} \right) \cdot \exp \left[ -\left( \frac{\eta}{l_{t}^{(\eta)}} \right)^2 \right].
\]

(4)

Here, the first term gives the shell correction near the ground state of the compound nucleus. It consists of two cosine functions and exponential damping terms, which model the shell correction in \( r \) and \( \eta \) directions with the characteristic length-scale of the shell oscillations \( \lambda_{CN}^{(r)} \) and \( \lambda_{CN}^{(\eta)} \), and damping factors \( l_{CN}^{(r)} \) and \( l_{CN}^{(\eta)} \), correspondingly. The quantity \( A_{\text{CN}} \) is the amplitude of the shell-correction term in the spherical shape of the compound nucleus. We assume that the position of the minimum of the shell correction may differ in general from the minimum of the macroscopic potential. This difference is taken into account by the phase-shift parameter \( \Delta r \). Thus, for \( A_{\text{CN}} < 0 \) the ground state of the compound nucleus (the minimum of the total
potential) is located at $\eta = 0$ and somewhere in between $r = r_{gs}$ and $r = r_{gs} + \Delta r$. The second term in (4) is responsible for the shell effects in the nascent fragments. They show up in the region of large deformations, while the compound-nucleus shell effects vanish with deformation. The fragment shell correction has the amplitude $A_{fr}$, and it is modeled again by a cosine function with exponential damping. The corresponding shell-oscillation length scale and damping factor are $\lambda^{(n)}_{fr}$ and $l^{(n)}_{fr}$, respectively.

An example of the potential energy (both the macroscopic and full macro-microscopic) for the $^{238}$U nucleus is shown in figure 2. The same potentials obtained within the schematic model are shown in figure 3. The typical values of the ratios extracted above from the standard macro-microscopic model in the uranium region of nuclei are: $\lambda^{(r)}_{CN}/\tilde{\lambda} \simeq \lambda^{(n)}_{CN}/\tilde{\lambda} \simeq 0.3$ and $\lambda^{(n)}_{fr}/\tilde{\lambda} \simeq 0.1$. These values were assumed in figure 3. Comparing with the realistic macro-microscopic potential we see that the schematic model gives reasonable potential energies describing the main features of the realistic ones.

3. Results and discussions

For the determination of the saddle point we applied the ‘flooding’ procedure [9, 14]. Step by step ‘water’ is added to the ground-state region, and we control the ‘wet’ region of the potential energy surface. The procedure is finished when the scission region becomes wet. This minimal height of the water column equals the value of the fission-barrier height.

It was pointed out that while the compound nucleus deforms from its ground state to scission, a neck in the nuclear shape appears and the mononucleus decays into two fragments when the system looses stability against neck variation. With increasing deformation, the oscillating compound-nucleus shell correction vanishes, and the shell effects associated with the nascent fragments establish. Consequently, the dependence of the shell correction on the elongation $r$ gradually disappears for the highly deformed mononucleus, and it vanishes completely asymptotically for two well-separated nuclei.
Due to the presence of shell effects on the smooth LDM ‘background’, the topography of the LDM saddle point is considerably changed. With the increase in the fissility of the fissioning system, the position of the LDM saddle point moves to smaller deformation. This, combined with the oscillatory behavior of shell effects as a function of deformation, will result in different fission-barrier structures depending on the size of the system. In the mass region $A \approx 230$ two barriers are present: the inner barrier (or A) is closer to the ground-state configuration, while the outer one (or B) is closer to the scission point. For nuclei well above or well below this region, only one barrier determines the fission process, A or B, respectively. Thus, in the following we will discuss the validity of the topographic theorem for these different configurations.

3.1. Calculations within the schematic macro-microscopic model

Using the schematic macro-microscopic model (3), (4) we investigated both the inner and the outer barrier. First, we performed calculations with the amplitude of the fragment shell correction $A_f = 0$. This case can be interpreted as that of the inner barrier, when the nucleus deformation at the saddle point is rather small and shell effects of the nascent fragments do not influence the fission barrier. For this calculation we also switch off the damping of the shell effects with deformation ($l_{CN}^{CM} = l_{CN}^{CM} \rightarrow \infty$), because the inner barrier is quite close to the ground state of the compound nucleus and, therefore, the shell effects in the inner saddle point are almost as strong as in the ground state. Results of these calculations for $A_{CN} = -10$ MeV are shown in figure 4. The white curve in figure 4(a) and the vertical lines in figures 4(b)–(d) specify the range of $\lambda_{CN}/\tilde{\lambda}$ where the difference between macro-microscopic and macroscopic saddle-point masses does not exceed 1.5 MeV. Note that the topographic theorem should be valid for any value of the phase-shift $\Delta r$. Therefore, this parameter was varied in figures 4(b)–(d). Any large value found for $M - M_{LDM}$ in these figures disproves the validity of the topographic theorem. In figure 4(c) the curves corresponding to the different values of $\Delta r$ coincide with each other, therefore, the case of $\Delta r = 0$ is only shown.
Figure 4. Difference between the saddle-point masses obtained in the schematic macro-microscopic ($M$) and macroscopic ($M_{LDM}$) models. All the plots are obtained with $A_{CN} = -10$ MeV, $A_{fr} = 0$ and $l_{CN}^{(\eta)} = l_{fr}^{(\eta)} \to \infty$. Part (a) shows the values in the two-dimensional fold $\lambda_{CN}/\tilde{\lambda}$ versus $\lambda_{CN}/\tilde{\lambda}$ for a fixed phase-shift parameter $\Delta \sigma_1 r = 0$. Parts (b), (c) and (d) display the values along some linear cuts in (a) with different values of $\Delta \sigma_1 r$.

Figures 4(b) and (c) show that it is not sufficient for the validity of the topographic theorem if only one of these ratios is small. The most physically interesting case is shown in figure 4(d), because we found the ratios of the shell correction oscillation wavelengths to that of the macroscopic potential to be equal for different degrees of freedom.

We see that the macroscopic saddle-point mass deviates from the macro-microscopic saddle-point mass by less than 1.5 MeV for the ratio $\lambda_{CN}/\tilde{\lambda} < 0.5$. The situation in nuclei with a ratio $0.1 \leq \lambda_{CN}/\tilde{\lambda} \leq 0.4$ lies inside this region, although it reaches almost to the border for heavy nuclei. It means that the topographic theorem should be valid for the inner barrier. This would also imply that for nuclei in the fissility region $Z^2/A > 36$, for which the inner barrier is the highest barrier, the saddle-point mass should be essentially a macroscopic quantity. Moreover, we obtain the better agreement with the topographic theorem the smaller $\lambda_{CN}/\tilde{\lambda}$ is. This follows from the general properties of the topographic theorem.

Then, we considered the case of $A_{fr}^{(\eta)} \neq 0$. This corresponds to the case where the fission barrier is the outer barrier and shell effects of the nascent fragments influence it. The obtained results are shown in figure 5. The parameters are the following: $A_{CN} = -2$ MeV, $l_{CN}^{(\eta)} = l_{fr}^{(\eta)} = 1$ and $l_{CN}^{(\eta)} = l_{fr}^{(\eta)} = 0.3$. The amplitude of the fragment shell correction is $A_{fr} = 10$ MeV for (a) and (c) and $A_{fr} = -10$ MeV for (b) and (d). Since in our schematic
Figure 5. Difference between the saddle-point masses obtained in the schematic macro-microscopic ($M$) and macroscopic ($M_{LDM}$) models. All the plots were obtained with $\lambda_{CN} = -2$ MeV, $k_{CN}^{(f)} = k_{CN}^{(i)} = 1$ and $\eta_{CN}^{(f)} = \eta_{CN}^{(i)} = 0.3$. The amplitude of the fragment shell correction is $A_{fr} = 10$ MeV for cases (a) and (c) and $A_{fr} = -10$ MeV for (b) and (d). The plots (a) and (b) were calculated with a constant value of $\lambda_{fr}^{(i)}/\tilde{\lambda} = 0.1$.

model the fragment shell effects establish gradually, the amplitude (for the chosen values of the parameters) around the macroscopic saddle-point constitutes $\sim 60\%$ of the value $A_{fr}$.

Even for small values of the ratios of the wavelengths we find substantial deviations of the LDM saddle-point mass from the full macro-microscopic mass. The deviation depends strongly on the amplitude of the fragments shell correction. We may conclude that in general the topographic theorem is not valid for the outer barrier. This means that the application of the topographic theorem to the case when the outer fission barrier is higher than the inner one (nuclei lighter than uranium) is not well justified from the mathematical point of view.

One more conclusion that we draw from the performed analysis concerns the sign of the deviation $M - M_{LDM}$. For the inner barrier one may expect mostly positive values of $M - M_{LDM}$ in accord with the most physically interesting case shown in figure 4(d). In contrast, with the exception of $A_{fr} > 0$ and large values of $\lambda_{fr}^{(i)}$ (figure 5(c)), all differences in the case of the outer barrier are negative. One may understand this result (see illustration in figure 6) by considering the topographical properties of the outer barrier caused by the fragment shells. Since the fragment shells do not vary as a function of elongation, the landscape at the outer saddle is characterized by gorges and ridges in elongation direction. Therefore, the outer
saddle is found in one of the gorges close to mass symmetry. This means that the true saddle-point energy tends to be systematically lower than the liquid-drop saddle.

Let us discuss how the third dimension influences the results obtained above within the two-dimensional schematic macro-microscopical model. One may assume that the coordinate $r$ was chosen along the bottom of the fission valley of the macroscopic potential. It means that the position and the height of the macroscopic fission barrier do not change if we include the third deformation degree of freedom in the two-dimensional schematic model. The saddle-point mass in the three-dimensional macro-microscopic calculations can only decrease or stay the same in comparison with the two-dimensional model, because the system may find an energetically more favorable way in three-dimensional space than in the two-dimensional one. Our calculations show that this gain in energy (the difference between the two-dimensional and three-dimensional saddle-point masses) does not exceed 0.6 MeV for reasonable values of the schematic model parameters. As the difference between macro-microscopic and macroscopic saddle-point masses $M - M_{\text{LDM}}$ obtained in the three-dimensional model would be, depending on the values of the model parameters, 0–0.6 MeV lower than in the two-dimensional calculations, the conclusions that were obtained on the base of the two-dimensional schematic model will also be valid if additional degrees of freedom are included.

### 3.2. Calculations within the realistic macro-microscopic model

In the previous section, using a schematic model we have shown in a quantitative way that the constancy of the shell effects as a function of elongation in the necked-in region is in conflict with the validity of the topographic theorem. However, for compact shapes, the topographic theorem should be fulfilled for values $\lambda_{\text{CN}}/\tilde{\lambda} \leq 0.5$. Values in the range $0.1 \leq \lambda_{\text{CN}}/\tilde{\lambda} \leq 0.4$ are found in nuclei. We have performed three-dimensional calculations of the potential energy for 30 nuclei. The results of these calculations are summarized in figure 7. The macroscopic saddle-point masses are compared with the macro-microscopic ones in figure 7(a) and with the experimental saddle-point masses in figure 7(b). We see that the macroscopic model provides rather good agreement of the saddle-point mass both with the experimental data and with the macro-microscopic saddle-point masses in the whole analyzed region of nuclei.

According to our conclusions from the schematic model calculation for the nuclei lighter than uranium (where the outer barrier is the highest one) the conditions of the topographic theorem are not fulfilled. Therefore, one may expect an increase of the deviation of the saddle-point mass from its macroscopic value with decreasing nucleus mass number, because
the saddle point moves toward scission, and the fragment shell effects influence its topological properties more and more. Nevertheless, a substantial deviation is not observed neither in our calculations nor in the previous ones [33, 34]. In our opinion it is explained by the following: a deviation of the saddle-point mass from the macroscopic value cannot exceed the amplitude of the shell correction. The shell corrections, which have been found to influence the fission process most strongly, correspond to $Z$-numbers 50 and 82 and $N$-numbers 82 and 126 for spherical nuclei and $N \simeq 86$ for deformed ones. However, the fission valleys determined by these magic numbers are located for the light fissioning nuclei at large mass asymmetries and, hence, have almost no influence on the topological properties of the saddle point. One may draw the same conclusion analyzing, e.g., the mass distributions of fission fragments for light fissioning nuclei. In [35], the influence of the shell effects on the fission-fragment mass distributions formed in low-energy fission of nuclei from $^{198}$Ir to $^{213}$At was observed, but it was found that this influence is rather small due to weak shells mainly present in the considered mass region. It saves us from the large deviations from the macroscopic saddle-point mass even in the region of light nuclei regardless that the topographic theorem is no more valid here.

As was discussed above, the difference $M - M_{\text{LDM}}$ is expected to be mostly negative for lighter nuclei with the fission barrier located at the outer saddle point and positive in the case of the inner barrier. This tendency is also seen in figure 7(a) when comparing the saddle-point masses of the macro-microscopic model with those of the macroscopic model. We find mostly negative values for $Z^2/A < 36$ and positive values for $Z^2/A > 36$. The same tendency can be seen in figure 4 of [33] and figure 6 of [34], where a transition from negative values to slightly positive values is also found around $Z^2/A \simeq 36$.

4. Conclusions

The topographic theorem [6] states that the saddle-point mass should be close to its macroscopic value. It happens when the shell correction has an oscillating behavior in all deformation directions with substantially smaller wavelengths in comparison with the characteristic length scale of the undulations of the macroscopic potential energy. At the same time, the fission barrier, which is the difference of the saddle-point mass (the macroscopic quantity according to the topographic theorem) and the ground-state mass, is strongly influenced by the shell correction at the ground state.
In the present work, we have studied the validity of the topographic theorem in a quantitative way. Calculations performed with a realistic macro-microscopic model have shown that the properties of the potential-energy landscape in fissioning nuclei are characterized by the ratio of the wavelengths of microscopic and macroscopic variations $\lambda_{\text{CN}}/\tilde{\lambda}$ as a function of elongation, and/or mass asymmetry in the order of 0.1–0.4 in the compact region. For necked-in shapes, these ratios are quite different: the value of $\lambda_{\text{fr}}/\tilde{\lambda}$ as a function of mass asymmetry is about 0.1, while as a function of elongation it amounts to much higher values. Calculations, performed with a schematic model, have shown that, for the validity of the topographic theorem, this ratio should be smaller than 0.5. Thus, we can conclude that for the compact saddle-point configurations, corresponding to the inner barrier, the topographic theorem is valid. In contrast, from the mathematical point of view, for more necked-in saddle-point configurations, corresponding to the outer barrier, the conditions of the topographic theorem are not fulfilled. Since for nuclei in the actinide region with a fissility parameter $Z^2/A$ larger than 36 the inner barrier is the higher one, the topographic theorem is expected to be valid for these nuclei within 1.5 MeV. Thus, we can conclude that for these nuclei the fission-saddle mass is essentially a macroscopic quantity. This is a very peculiar case, because the vast majority of nuclear observables are strongly influenced by microscopic effects like shell structure and pairing correlations. For nuclei with lower fissility parameter, the mathematical conditions for the validity of the topographic theorem are not fulfilled, because the shape at the fission barrier is characterized by a neck. In this case, the shell effects on the path from saddle to scission resemble already the shells in the separated fragments and, thus, vary only little as a function of elongation. However, the macro-microscopic barrier may still be rather close to the macroscopic barrier also for these lighter nuclei, because the strong shell effects, responsible for the appearance of the asymmetric fission channels, loose their influence for nuclei with $A < 226$.

Following these results we can also conclude that the method proposed in [1, 15] for testing the validity of different theoretical descriptions of the fission saddle-point mass in the experimentally unexplored regions is well justified, and that it thus can be used for fixing the isotopic trends in the parameters of different macroscopic models. This finding is extremely important for applications in astrophysics.

Some remarks should also be added concerning the applicability of the topographic theorem in the case of superheavy nuclei. There is no reason for the theorem to be not valid, but one needs to locate the position of the macroscopic saddle point properly. The macroscopic fission barrier in this region is zero, and therefore, the macroscopic saddle point coincides with the macroscopic ground state. This means that the saddle-point mass (which is determined by the shell correction) should be close to the macroscopic mass of the spherical nucleus. However, as pointed out by Swiatecki et al [16], a systematic correction to the macroscopic saddle-point mass should be taken into account, which is connected with the fact that the macroscopic energy at the true saddle point is systematically below the macroscopic energy in the spherical shape. This correction is smaller for nuclei with a spherical ground state and larger for deformed nuclei.

Calculation of the potential energy for any nuclear system can be done at the web server [37] with a free access.

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References


[32] Habs D 1977 *Habilitationsschrift* (Heidelberg: Max-Planck-Institut)