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Scission Configurations for StI and StII Fission Modes in the Reaction $^{235}$U($n_{th}$, f)

N. Carjana,b,∗, F.-J. Hambshc,F. A. Ivanyukd, P. Taloue

aNational Institute for Physics and Nuclear Engineering “Horia Hulubei”, Reactorului 30, RO-077125, POB-MG6, Magurele-Bucharest, Romania
bCentre d’Etudes Nucleaires de Bordeaux - Gradignan,UMR F 5797, CNRS/IN2P3 - Universite Bordeaux 1, BP 120, 33175 Gradignan Cedex, France
cInstitute for Reference Materials and Measurements, 2440 Geel, Belgium
dInstitute for Nuclear Research, Kiev, Ukraine
eLos Alamos National Laboratory, Los Alamos, NM 87544, USA

Abstract

Two scission configurations that can explain the fission fragment properties of the principal fission modes, short (StI) and standard (StII), in the reaction $^{235}$U($n_{th}$, f) are presented. These configurations are very close to the optimal scission shapes defined with three constraints: on fragment elongation, mass asymmetry and neck radius. They are subsequently approximated by the modified Cassini ovals in order to calculate fission fragment properties such as mass yields, excitation energies of individual fragments and total kinetic energies. For each configuration a comparison is made with the same quantities obtained from experimental data after decomposition into contributions from three fission modes.

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1. Introduction

Although neither generally accepted nor fully proven, the concept of fission modes is a useful and elegant way to analyse the experimental fission-fragment distributions by the deconvolution of the fission yield for a given total kinetic energy (TKE) and mass split ($A_L/A_H$) of the primary fragments using, for each mode, a product of two Gaussians (Knitter et al., 1987; Hambsch et al., 1989). To account for the Q-value limitation on the high TKE side (Brosa et al., 1990) the Gaussian was replaced by a distribution slightly asymmetric with respect to $TKE_{max}$.

Usually three fission modes (StI, StII and SL) are enough to explain the experimental data. This means that there are only three simultaneous independent-processes that divide the fissioning nucleus in two fragments. It is a considerable simplification over considering each mass division as a separate process.

∗ Corresponding author
Email address: carjan@theory.nipne.ro (N. Carjan)
From theoretical point of view, this concept implies that there are three valleys in the potential energy surface that a fissioning nucleus takes, with different probabilities, during its descent from the saddle point to the scission point. The bottoms of these valleys lead to three most probable just-before scission (JBS) configurations that mark the moment when the neck rupture starts. At that moment the properties of the primary fission fragments are set for each fission mode and should be inferred from the properties of these three scission configurations.

As a new argument in favour of the existence of StI and StII in $^{236}_{\text{U}}$, we propose in the present study two energetically preferred configurations that are characterized by an elongation and a mass asymmetry that agree with the most probable TKE and $A_L/A_H$ for each mode obtained after the deconvolution of the yields $Y(\text{TKE}, A)$ measured in the reaction $^{235}_{\text{U}}(n_{\text{th}}, f)$.

Moving perpendicular to the elongation in the mass asymmetry direction we calculate the distributions $Y(A), \langle \text{TKE}\rangle(A)$ and $\Delta E_{\text{def}}(A)$. Here, the $\Delta E_{\text{def}}$ is the deformation energy liberated during scission which, due to the extremely diabatic neck rupture, is assumed to be transformed into fragments’ excitation.

The partition of the total excitation energy $E_{\text{exc}}(A)$, that the fragments already have immediately after scission, between the light and the heavy fragments $E_{\text{exc}}(L(H))$ is calculated both in the thermalization hypothesis ($T_L = T_H$) (Madland and Nix, 1982) and in the sudden approximation (Carjan et al., 2007). Then we calculate the extra-deformation energy immediately after scission (IAS) $\Delta E_{\text{def}}(L(H))$ for each fragment (L or H) separately by the Strutinsky shell-correction approach (Brack et al., 1972).

This allows to estimate the energy available to emit prompt neutrons. We compare it with the energy cost for the same emission estimated from the measured neutron multiplicities. Comparing available energy with energy cost we avoid the debate on the emission mechanism: statistical, dynamical or both. Finally, we add the excitation energy of the light and of the heavy fragments to obtain the total excitation energy $\text{TXE}$.

Fig. 1. (a) potential energy of deformation just before scission corresponding to the StII configuration (upper) as a function of the fragment mass $A$ and the resulting fragment mass distribution (lower). The dotted curve is the StII yield taken from deconvoluted experimental data; (b) calculated total excitation energy of the primary fragments immediately-after scission compared with the same quantity extracted from experimental data for ST II fission mode. The St II mass yield is also plotted for orientation.

2. Standard II Scission Configuration

It was shown (Ivanyuk, 2009; Carjan et al., 2012) that the Cassini ovals with deformations $\alpha, \alpha_1$ reproduce well the shapes of fissioning nuclei (we call them optimal shapes) obtained by the minimization of liquid-drop energy without a specific shape parametrization (Strutinsky et al., 1963).

It has been also pointed out that nuclear shapes around scission described by Cassini ovals ($\alpha=0.985$ and 1.001) explain well the most probable mass division ($A_L=95$) of the most abundant (StII) fission mode in $^{236}_{\text{U}}$ (Carjan et al., 2010,b).
The lower part of Fig. 1a shows that the whole mass distribution is quite well reproduced assuming statistical equilibrium for the collective degrees of freedom normal to the fission direction (Nöremberg, 1969), in particular for the mass asymmetry:

$$Y(A) \propto e^{-E_{jbs}^{\text{def}}(A)/T_{\text{coll}}},$$

(1)

and $T_{\text{coll}} = 1.5 \text{ MeV}$.

A small deviation of the calculated distribution from Gaussians is noticed. The more pronounced drop towards symmetry is a general feature since the slope of the potential (upper part of Fig. 1a) is always larger there than towards larger mass asymmetries. However, pure Gaussian mass-distributions, exclusively used in the deconvolution, is an accepted approximation that reduces the number of parameters in the fit.

Therefore we dispose of a sequence of scission shapes defined by $A_L/A_H$ to describe the characteristics of the main (St II) fission mode. Below we use these shapes to calculate the total excitation energy available in the primary fragments to emit prompt neutrons and $\gamma$-rays for each fragment pair $(A_L, A_H)$:

$$\text{TXE}_{\text{St II}} = E_{\text{ias}} + \Delta E_{\text{ias}}^{\text{def}}(L) + \Delta E_{\text{ias}}^{\text{def}}(H)$$

(2)

where

$$E_{\text{ias}} = E_{\text{jbs}}^{\text{def}} - E_{\text{def}}^{\text{ias}} + (B_n - B_f).$$

(3)

The $B_n = 6.545 \text{ MeV}$ and $B_f = 5.670 \text{ MeV}$ are the neutron binding energy and the height of the 2nd saddle in $^{236}_{144}$U, respectively. The $\Delta E_{\text{ias}}^{\text{def}} = E_{\text{jbs}}^{\text{def}} - E_{\text{def}}^{\text{ias}}$ is the potential energy liberated during scission that goes all into excitation due to the non-adiabaticity of the process Rizea and Carjan (2013).

In Eq. (2) a superfluid descent (no dissipation) from saddle to just-before scission is assumed. In sub-barrier fission the coupling of the fission motion to the internal degrees of freedom is weak during this descent (Nifenecker et al., 1965; Börner and Gönnenwein, 2012; Rizea and Carjan, 2012) and this weakness is accentuated by the existence of the pairing gap (Ivanyuk and Hofmann, 1999).

The IAS and ground-state energies for each fragment $E_{\text{ias}}^{\text{def}}(L)$ or $E_{\text{ias}}^{\text{def}}(H)$ and $E_{\text{gs}}^{\text{def}}(L)$ or $E_{\text{gs}}^{\text{def}}(H)$ are calculated as the sum of the liquid drop energy plus the shell correction (including the correction to the pairing energy). The ground state shape was parametrised in terms of distorted Cassini ovaloids. The values of deformation parameters $\alpha_2 - \alpha_6$
were found by the minimization of the energy with respect to the variation of these parameters. For the IAS configuration (the Cassinian oval with $\alpha = 1.001$) the shapes of light and heavy fragments were fitted separately by the Cassinian ovals with 10 deformation parameters. Details on the Strutinsky shell-correction prescription used to estimate the deformation energies are given in Ref. (Carjan et al., 2012).

In Fig. 1b we compare the average total excitation energy Eq.(2) for St II mode with the results extracted from experimental data after decomposition into fission modes. The agreement is only partial namely from $A_H = 118$ to 136 and from 150 to 160. At very large mass asymmetries the disagreement can be blamed on extremely low statistics but the one around $A_H = 140$ is a problem.

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3. Standard I Scission Configuration

Judging from the mean TKE values extracted from experimental data for StI, StII and SL fission modes, one can deduce that the StI (SL) scission configuration is more compact (elongated) than the one for StII.

The nuclear shapes defined in terms of Cassini ovals used in the previous section are close to the optimal shapes with two constraints (on elongation and on mass asymmetry) (Carjan et al., 2012). The fragment deformation (or the neck size) for a given overall-elongation and mass asymmetry attains the ”most favored” value which results from the minimum of the potential energy condition. To obtain more compact or more elongated configuration one has to add, in the optimal shapes procedure, another constraint fixing, e.g. the hexadecapole deformation. Using \( \lambda_4 Q_4 \) as an additional constraint allows to vary the deformation of the fragments. However, at large value of \( \lambda_4 \) the \( \lambda_4 Q_4 \) constraint results in unphysical shapes.

Another possibility to vary the neck size is to fix the amount of matter in the neck region by introducing the constraining function \( f_4 \) of the type Warda et al. (2002); Ivanyuk (2013)

\[
f_4 = \frac{1}{V} \int dV \rho^2(z) \exp \left[ -\left( \frac{z - z_{neck}}{\Delta z} \right)^2 \right].
\]

with \( \Delta z = 0.25 \times R_0 \).

In this case the profile function \( \rho(z) \) is found by the minimization of the LD energy under four constraints

\[
\frac{\delta}{\delta \rho} \left( E_{LD} - \lambda_1 V - \lambda_2 \tilde{R}_{12} - \lambda_3 \tilde{\delta} - \lambda_4 f_4 \right) = 0,
\]

with

\[
\tilde{R}_{12} \equiv \frac{\pi}{V} \int \sqrt{(z - z_{neck})^2 + (\Delta z)^2} \rho^2(z) d\zeta, \quad \tilde{\delta} \equiv \frac{\pi}{V} \int \frac{z - z_{neck}}{\sqrt{(z - z_{neck})^2 + (\Delta z)^2}} \rho^2(z) d\zeta.
\]
The minimization of the LD energy (5) leads to the integro-differential equation for \( \rho(z) \),

\[
\rho'' = 1 + (\rho')^2 \rho \left\{ V + \lambda_2 \frac{\sqrt{\left(z - z_{\text{neck}}\right)^2 + (\Delta z)^2}}{\sqrt{\left(z - z_{\text{neck}}\right)^2 + (\Delta z)^2}} + \lambda_3 \frac{z - z_{\text{neck}}}{\sqrt{\left(z - z_{\text{neck}}\right)^2 + (\Delta z)^2}} \right. \\
\left. + \lambda_4 \exp \left[ - \frac{\left(z - z_{\text{neck}}\right)^2}{\Lambda z} \right] + 10 x_{LD} \Phi_2(z) \right\} \left[ 1 + (\rho')^2 \right].
\]

(7)

Here, the Lagrange multiplier \( \lambda_1 \) is fixed by the volume conservation condition, the \( \lambda_2, \lambda_3 \) are 'responsible' for the elongation and the mass asymmetry and the fourth constraint has the requested consequence for the neck size of the optimal scission shape. Depending on the sign of \( \lambda_4 \) the scission shapes become more elongated or more compact as can be seen in Fig. 4.

To describe the JBS shapes for StI we choose the optimal scission shapes (7) that correspond to \( \lambda_4 = -0.5 \). For IAS shapes we choose two spheres in the centers of mass of the JBS fragments. With this configuration the Coulomb interaction energy for StI is calculated in Fig. 3.

The potential energy of deformation JBS is represented in the upper part of Fig. 5a as a function of the fragment mass \( A \) and the resulting fragment mass distribution (lower). The dotted curve is the StI yield taken from deconvoluted experimental data; (b) potential energy of deformation corresponding to two spherical fragments (upper) as a function of the fragment mass \( A \) and the resulting fragment mass distribution (lower). The dotted curve is the StI yield taken from deconvoluted experimental data.

![Fig. 5. (a) potential energy of deformation just before scission corresponding to the StI configuration (upper) as a function of the fragment mass A and the resulting fragment mass distribution (lower). The dotted curve is the StI yield taken from deconvoluted experimental data; (b) potential energy of deformation corresponding to two spherical fragments (upper) as a function of the fragment mass A and the resulting fragment mass distribution (lower). The dotted curve is the StI yield taken from deconvoluted experimental data.](image)

An equation similar with Eq. (2) can be used to estimate the total excitation energy of the primary fragments in the StI fission mode. In this case \( \Delta E_{\text{def}} \) is the difference between the shell-corrected deformation energy JBS and IAS (upper parts of Figs. 5a and 5b, respectively) and \( \Delta E_{\text{ias}}(L(H)) \) is the shell corrected energy of spherical fragments. The result is plotted in Fig. 6a together with the same quantity extracted from experimental data after decomposition in fission modes. One notices the same overall qualitative agreement as for StII (Fig. 1b). However, in the mass range spanned by StI (i.e., around \( A_H = 134 \)), the agreement is better.

The division of the excitation energy between the L and the H fragments is plotted in Fig. 6b. \( S_n/2 \) is subtracted in order to obtain only the energy available for emitting prompt neutrons (and no \( \gamma \) rays). It is again compared with the energy cost extracted from experimental data. In this case, the partition of \( E_{\text{ias}} \) is given by the thermalization hypothesis \( T_L = T_H \). The good agreement indicates that the IAS fragments are close to spheres.
4. Usefulness and Implications

Our present theoretical study of scission configurations for different fission modes is of triple utility:

1) It provides deformation parameters for shell model calculations before, during and after the rupture of the neck connecting the nascent fragments making microscopic calculations possible for each fission mode. Any realistic scission model needs this information.

2) It brings physical input into the decomposition of the experimental data into contributions from each fission mode. For instance an asymmetric mass distribution, a prescission kinetic energy that depends linearly on mass asymmetry and a Coulomb interaction between fragments calculated with finite-size charge distributions should be included in this decomposition. Moreover it provides non-arbitrary initial values for all parameters used in the $\chi^2$ minimization making this procedure more reliable. Depending on the confidence level we have in our estimates, we can fix some parameters reducing the number of degrees of freedom in the fit. Any future fission-mode analysis should take these predictions into account.

3) It challenges the common idea that there is one and only one configuration of the fissioning nucleus at scission that can explain on average all fission observables that are determined at this last fission stage such as: total kinetic energy of the fission fragments, their masses, their angular momenta, their excitation energies and all properties of ternary particles and prompt neutrons.

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References