The Scission Point Configuration and the Multiplicity of Prompt Neutrons

F.A. Ivanyuk\textsuperscript{a,b,*}, S. Chiba\textsuperscript{b}, Y. Aritomo\textsuperscript{b}

\textsuperscript{a}Institute for Nuclear Research, Prospect Nauki 47, 03680 Kiev, Ukraine
\textsuperscript{b}Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro, Tokyo 145-0061, Japan

Abstract

We defined the optimal shape which fissioning nuclei attain just before the scission and calculated the deformation energy as function of the mass asymmetry and elongation at the scission point. The calculated deformation energy is used in quasi-static approximation for estimation of the mass distribution of fission fragments, total kinetic and excitation energy of fission fragments, and the total number of prompt neutrons. The calculated results reproduce rather well the experimental data on the position of the peaks in the mass distribution of fission fragments, the total kinetic and excitation energy of fission fragments. The calculated value of neutron multiplicity is somewhat larger than experimental results.

1. Introduction

In the theory of nuclear fission the quasistatic quantities like the potential energy surface, the ground state energy and deformation, and the fission barrier height are commonly calculated within the macroscopic-microscopic method Strutinsky (1966); Brack et al. (1972). In this method the total energy of the fissioning nucleus consists of two parts, macroscopic and microscopic. Both parts are calculated at a fixed shape of the nuclear surface. In the past a lot of shape parameterizations were proposed and used. A good choice of the shape parameterization is often a key to the success of the theory. Usually, one relies on physical intuition for the choice of the shape parameterization.

A method to define the shape of the nuclear surface which does not rely on any shape parameterization was proposed by V. Strutinsky in Ref. Strutinsky et al. (1963). In this approach the shape of an axial, left-right symmetric nucleus was defined by looking for the minimum of the liquid-drop energy under the additional restrictions that fix the volume and elongation of the drop.

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\* Corresponding author.
E-mail address: ivanyuk@kinr.kiev.ua

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Recently the method was further developed by incorporating the axial and left-right asymmetry, and the neck degree of freedom of the nuclear shape, see Ivanyuk (2014) and references therein.

The important result of the Strutinsky procedure Strutinsky et al. (1963) is the possibility to definite in a formal way the scission point as the maximal elongation at which the nucleus splits into two fragments.

Having at one’s disposal the shape and the deformation energy at the scission point we evaluated the measurables of the fission experiments: the mass distribution, total kinetic and excitation energy of fission fragments, and the multiplicity of prompt neutrons.

2. Optimal shapes

In Strutinsky et al. (1963) the shape of nucleus is described by rotation of some profile function $\rho(z)$ curve around the $z$-axis. A formal definition of $\rho(z)$ was obtained looking for the minimum of the liquid-drop energy, $E_{LD} = E_{surf} + E_{Coul}$, under the constraint that the volume $V$ and deformation $R_{12}$ are fixed,

$$\frac{\delta}{\delta \rho} \left[ E_{LD} - \lambda_1 V - \lambda_2 R_{12} \right] = 0, \quad \text{with} \quad V = \pi \int_{z_1}^{z_2} \rho^2(z)dz, \quad R_{12} = \frac{2\pi}{V} \int_{z_1}^{z_2} \rho^2(z)dz. \quad (1)$$

The deformation parameter $R_{12}$ was chosen in Strutinsky et al. (1963) as the distance between the centers of mass of the left and right parts of the nucleus, see (1). The $\lambda_1$ and $\lambda_2$ in (1) are the corresponding Lagrange multipliers.

Since both Coulomb and surface energy are functionals of $\rho(z)$ the variation in (1) results in an equation for $\rho(z)$,

$$\rho \rho'' = 1 + (\rho')^2 - \rho (\lambda_1 + \lambda_2 |z| - 10x_{LD} \Phi_3) \left[ 1 + (\rho')^2 \right]^{\frac{3}{2}}. \quad (2)$$

Here $\Phi_3$ is the Coulomb potential at the nuclear surface and $x_{LD}$ is the fissility parameter of the liquid drop.

By solving Eq. (2) for given $x_{LD}$ and $\lambda_2$ ($\lambda_1$ is fixed by the volume conservation condition) one obtains the profile function $\rho(z)$ which we refer to as the optimal shape. These shapes correspond to the lowest possible energy of liquid drop with a given volume and elongation $R_{12}$. Varying the parameter $\lambda_2$ one obtains a full variety of shapes ranging from a very oblate shape (disk, even with central depression) up to two touching spheres.

The results of calculations show that the deformation $R_{12}$ of optimal shapes is limited by some maximal value $R_{12}^{(crit)}$. Above this deformation the solutions of (2) for mono-nuclear shapes do not exist. This maximal deformation was interpreted by Strutinsky et al. (1963) as the scission point. Having at one’s disposal the shape and the deformation energy at the scission point one can try to evaluate the measurables of the fission experiments like the mass distribution, total kinetic and excitation energy of fission fragments, the multiplicity of prompt neutrons.

3. The potential energy surface and the mass distribution of fission fragments

For the accurate calculation of the deformation energy the account of shell effects is essential. In order to calculate the shell correction the optimal shape was expanded in series in deformed Cassini ovaloids (up to 20 deformation parameters were included). For the shape given in terms of Cassini ovaloids the single-particle energies and the shell correction $\delta E$ were calculated by the Pashkevich (1971) code with deformed Woods-Saxon potential.

Figs. 1a,b show the total (liquid-prop plus the shell correction including the shell correction to the pairing energy)

$$E_{def} = E_{def}^{LD} + \delta E, \quad \text{with} \quad \delta E = \sum_{n,p} (\delta E_{shell}^{(n,p)} + \delta E_{pair}^{(n,p)}) \quad (3)$$

definition energy for $^{180}\text{Hg}$ and $^{236}\text{U}$. The summation in (3) is carried out over the protons ($p$) and neutrons ($n$).

The unexpected mass-asymmetric distribution of fission fragments for beta-delayed fission of $^{180}\text{Hg}$ was reported in Andreyev et al. (2010). In Figs. 1a,b only the liquid-drop part of deformation energy is shown beyond the scission point. In Figs. 1c,d the deformation energy of compact shapes was extrapolated beyond the scission point. In case of $^{180}\text{Hg}$ the lowest energy at the scission point corresponds to the fragment mass number $A_H = 100$ and $A_L = 80$, what coincides with the experimental results Andreyev et al. (2010). One can see also that beyond the scission point the minimum of deformation energy moves towards the symmetric splitting. The knowledge of the scission point is
important for the dynamical calculations. If one would continue the dynamical calculations up to the shape with zero neck one would get for $^{180}$Hg the mass-symmetric distribution of fission fragments.

For the calculation of the mass distribution one has to rely on some assumption on the fission process. Solving of a dynamical problem for the fission process is very time consuming. Having at one’s disposal only the potential energy surface one could nevertheless try to estimate the observables measured in the experiments. Keeping in mind that fission is a slow process, one could assume that during the fission process the state of the fissioning nucleus is close to statistical equilibrium; i.e., each point $q_i$ on the deformation energy surface is populated with a probability given by the canonical distribution,

$$P(\alpha, q_i) = e^{-\left(\frac{E(\alpha, q_i)}{T_{\text{coll}}} - Z\right)}$$

with $Z \equiv -T_{\text{coll}} \log \sum_i e^{-\left(\frac{E(\alpha, q_i)}{T_{\text{coll}}}\right)}$. (4)

Here $T_{\text{coll}}$ is a parameter characterizing the width of the distribution (4) in the space of deformation parameters. The $\alpha$ is the mass asymmetry of the fissioning system and $q_i$ are the rest of the collective parameters.

The normalized mass distribution of the fission fragments $Y(\alpha)$ can be expressed then in terms of the deformation energy at the critical deformation $R_2^{(\text{crit})}$.

$$Y(\alpha) = \sum_i P(\alpha, R_2^{(\text{crit})}, q_i).$$

The calculated mass distributions of the fission fragments for some nuclei are shown in Fig. 2. For these nuclei the experimental information is available, see Ghys et al. (2014) and references therein. On average the experimental results are reproduced by calculations rather well.
Fig. 2. The mass distribution of fission fragments calculated with $T_{\text{coll}} = 1.5 \text{ MeV}$ in (4) for zero intrinsic excitation energy $E_x$. The red line for $^{198}\text{Hg}$ was calculated for $E_x = 10.9 \text{ MeV}$, see Itkis et al. (1989). The heavy dots in $^{236}\text{U}$ panel show the measured data, Zeynalov et al. (2006).

4. The total kinetic energy and the neutron multiplicity

In the above calculations the shape at the scission point was defined by the minimization of the liquid-drop energy. The shell correction was added afterwards. In order to introduce an additional freedom for the shape of fissioning nucleus it was suggested by Ivanyuk (2014) to carry out the minimization of the liquid-drop energy with additional constraints

$$E = E_{LD} - \lambda_1 V - \lambda_2 \tilde{R}_{12} - \lambda_3 \tilde{\delta} - \lambda_5 Q_{2L} - \lambda_6 Q_{2R}. \quad (6)$$

Here $Q_{2L}$ and $Q_{2R}$ are the quadrupole moments of the left and right parts of nucleus. The $\tilde{R}_{12}$ and $\tilde{\delta}$ are the smoothed constraining operators for the elongation and mass asymmetry, see Ivanyuk (2014). The scission point configuration becomes, thus, dependent on Lagrange multipliers $\lambda_5$ and $\lambda_6$. The population of the points in $\{\lambda_5, \lambda_6\}$ space is fixed by the distribution (4).

The comparison of the calculated $TKE$ for a few fission reaction with the available experimental results is shown in Fig. 3. In these calculations we define $TKE$ as the sum of the Coulomb interaction of spherical fragments immediately after scission and the prescission kinetic energy $KE_{pre}$,

$$TKE = -\langle E_{\text{Coul}}^{(\text{int})}(\alpha) \rangle + TKE_0, \quad \text{with} \quad \langle E_{\text{Coul}}^{(\text{int})}(\alpha) \rangle \equiv \frac{1}{2} \sum_i Z_L Z_H e^2 \frac{Z_L Z_H e^2}{R_{12}^{(\text{crt})}(\alpha, q_i)} P(\alpha, q_i) \sum_i P(\alpha, q_i), \quad (7)$$

where $eZ_L$ and $eZ_H$ are the charges of light and heavy fragments. The summation in (7) is carried out over $\lambda_3$ and $\lambda_6$. Like in Ivanyuk (2014) we define the $TKE_0$ from the energy balance $E_{gs}(A_L + A_H) + B_n = E_{jbs} + TKE_0$, i.e. we assume the "complete acceleration": the energy difference between the saddle and scission turns into the kinetic energy of relative motion of fragments. The opposite extreme case would be the assumption of overdamped motion: all the energy difference between the saddle and scission turns into heat, with no prescission kinetic energy. The comparison of the calculated and measured values of $TKE$ shown in Fig. 3 is in favor of "complete acceleration". Without contribution from $TKE_0$ the $TKE$ (dashed curve in Fig. 3) would be too small.

The calculated $TKE$ is rather close to experimental data. The position of the maximum of $TKE$ and the drop at symmetric splitting are also well reproduced. This can be considered as a confirmation that the potential energy just before scission and the mean value of $\langle R_{12}^{(\text{crt})} \rangle$ are defined correctly.
Once $TKE$ is known, the total excitation energy $TXE$ can be found from the energy balance,

$$E_{gs}(A_L + A_H) + B_n = E_{gs}(A_L) + E_{gs}(A_H) + TKE + TXE$$

(8)

One can see from (8) that $TKE$ and $TXE$ are two parts of the total energy release $Q$. $TKE + TXE = Q$, where $Q$-value is the difference of the ground state energies $Q = E_{gs}(A_L + A_H) + B_n - E_{gs}(A_L) - E_{gs}(A_H)$. The $Q$-value does not depend on dynamics, it can be calculated within the macroscopic-microscopic method or taken from the existing databases. Since the experimental value of $TKE$ is rather well reproduced by the present calculations, the calculated total excitation energy $TXE = Q - TKE$ should be also quite accurate.

The fragments are deexcited by the emission of neutrons and $\gamma$-rays. When the excitation energy is smaller than the neutron separation energy $S_n$, the $\gamma$-quanta are emitted. The energy available for $\gamma$-ray emission varies from $S_n$ to zero. So, on average the excitation energy available for neutron emission is given by $E_x - S_n/2$. The average value of the total number $\bar{\nu}_{tot}$ of prompt neutrons can be estimated by the relation

$$\bar{\nu}_{tot} \approx \langle TXE \rangle / \bar{S}_n - 1/2, \quad \text{with} \quad \langle TXE \rangle = \sum_{A_H} [Q(A_H) - TKE(A_H)] Y(A_H) \quad \text{and} \quad \bar{S}_n = 5.7 \text{ MeV}.$$  

(9)

To calculate the dependence of $\bar{\nu}$ on the fragment mass number $A$ one needs to know how the excitation energy is shared between the fragments. Here we assume that the excitation energy of light and heavy fragments immediately after the neck rupture is the same, for details, please, see Ivanyuk et al. (2014).

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Fig. 3. The total kinetic energy (7) calculated with (solid lines) and without (dashed line) account of fragments prescission energy. The experiments results (solid circles) are taken from Sergachev et al. (1968); Hambsch et al. (1989); Tsuchiva et al. (2000); Allaert et al. (1982); Nishio et al. (1995); Ramaswami et al. (1977). The $Q$-value for fission of $^{232}$Th, $^{235}$U, $^{239}$Pu and $^{245}$Cm are shown by dotted lines.

Fig. 4. (a) the excitation energy available for prompt neutron evaporation (open circles) and the experimental results for neutron multiplicity Apalin et al. (1998); Nishio et al. (1998) multiplied by neutron separation energy; (b) the calculated value of total neutron multiplicity (9) (open squares) and the experimental results (Ohsawa, 2008) (solid squares).
In Fig. 4a we compare the excitation energy available for the prompt neutron emission, $E_x - 0.25S_{2n}$, with the experimental value of neutron multiplicity Apalin et al. (1998); Nishio et al. (1998) multiplied by the half of two-neutron separation energy $S_{2n}$ (in order to remove the rapid fluctuations due to the odd-even effect in $S_n$). One can see that there is some discrepancy up to 5 MeV at large mass asymmetries, but on the average the saw-tooth structure is rather well reproduced.

The comparison of calculated $\bar{\nu}_{tot}$ with the available experimental results is shown in Fig. 4b. On average the dependence of $\bar{\nu}_{tot}$ on the proton number of fissioning nuclei is qualitatively reproduced. The calculated value of $\bar{\nu}_{tot}$ are however larger than experimental by 0.5-0.9. The source of this discrepancy can be related to the use of a very simple estimate (9) for the neutron multiplicity and use of the quasistatic approximation (4) for the mass distribution.

5. Summary

The calculations presented in this contribution show that the optimal shape prescription offers a good possibility to define the shape of fissioning nuclei just before the scission. This information can be used for the evaluation of the quantities which are measured in fission experiments like the mass distribution, the total kinetic and excitation energies of fission fragments, and the multiplicity of prompt neutrons. The calculated distribution of the total kinetic energy for fission of $^{232}$Th, $^{235}$U, $^{239}$Pu and $^{248}$Cm was found to be in a rather good agreement with experimental data. The dependence of the total multiplicity of prompt neutrons on the proton number of the fissioning nucleus is qualitatively reproduced. The mass distributions of fission fragment are reproduced on average rather well. For a more accurate description of mass distribution the dynamical approach to the fission process seems necessary.

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