



Modelling of low energy fission of atomic nuclei

A. Dobrowolski, B. Nerlo-Pomorska, K. Pomorski, A. Zdeb

Instytut Fizyki, Uniwersytet Marii Curie Skłodowskiej, 20-031 Lublin, Poland.

J. Bartel, H. Molique, C. Schmitt

Institut Pluridisciplinaire Hubert Curien, CNRS-IN2P3, 67-200 Strasbourg,

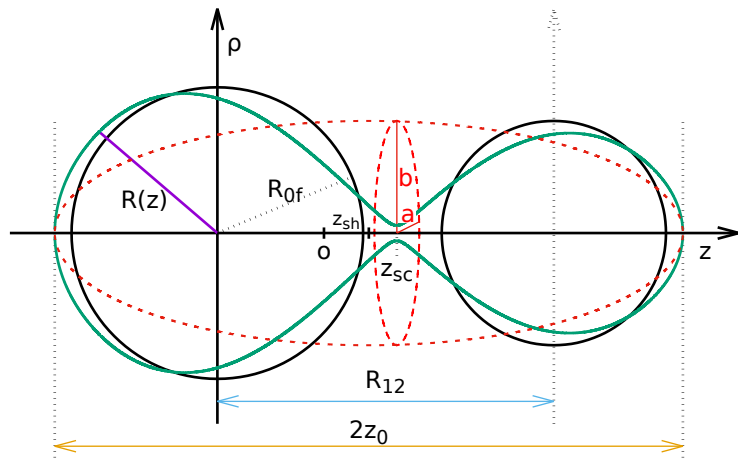
France.

Project No. 08-131

Program:

- Fourier over Spheroid parametrization of fissioning nuclei shapes,
- Some examples of the 4D macroscopic-microscopic PES's,
- Mass and Total Kinetic Energy of fragments obtained within the 3D Langevin dissipative dynamics,
- Charge equilibration mode at the scission configuration,
- Neutron emission from the fragments,
- Transition from asymmetric to compact-symmetric fission in Fermium isotopes - more detailed study of spontaneous fission,
- Spontaneous fission lifetimes of heavy and super-heavy nuclei,
- Plans for the future:
 - fission yields of hot nuclei,
 - searching of shape isomers and shape coexistence in Pt-Hg nuclei,
 - more detailed study of the spontaneous fission lifetimes.

New Fourier-over-Spheroid (FoS) shape parametrization *



$$\rho^2(z, \varphi) = \frac{R_0^2}{c} f\left(\frac{z-z_{sh}}{z_0}\right) \frac{1-\eta^2}{1+\eta^2+2\eta \cos(2\varphi)},$$

Function $f(u)$ defines the shape of the nucleus having half-length $c = 1$:

$$f(u) = 1 - u^2 - \sum_{k=2,4}^{\infty} \left\{ a_k \cos\left[\frac{(k-1)\pi}{2}u\right] + a_{k+1} \sin\left[\frac{k\pi}{2}u\right] \right\},$$

where $-1 \leq u \leq 1$ and $a_2 = a_4/3 + a_6/5 + a_8/7 + \dots$

The first two terms in $f(u)$ describe a circle, a_2 ensures **volume conservation** for arbitrary deformation parameters $\{a_3, a_4, \dots\}$. The parameter c determines the **elongation** of the nucleus keeping its volume fixed, while a_3 and a_4 describe the **reflectional asymmetry** and the **neck size**, respectively, while the higher order terms regulate the **deformation of fragments**.

The half-length is $z_0 = cR_0$ and $-z_0 + z_{sh} \leq z \leq z_0 + z_{sh}$, where the shift

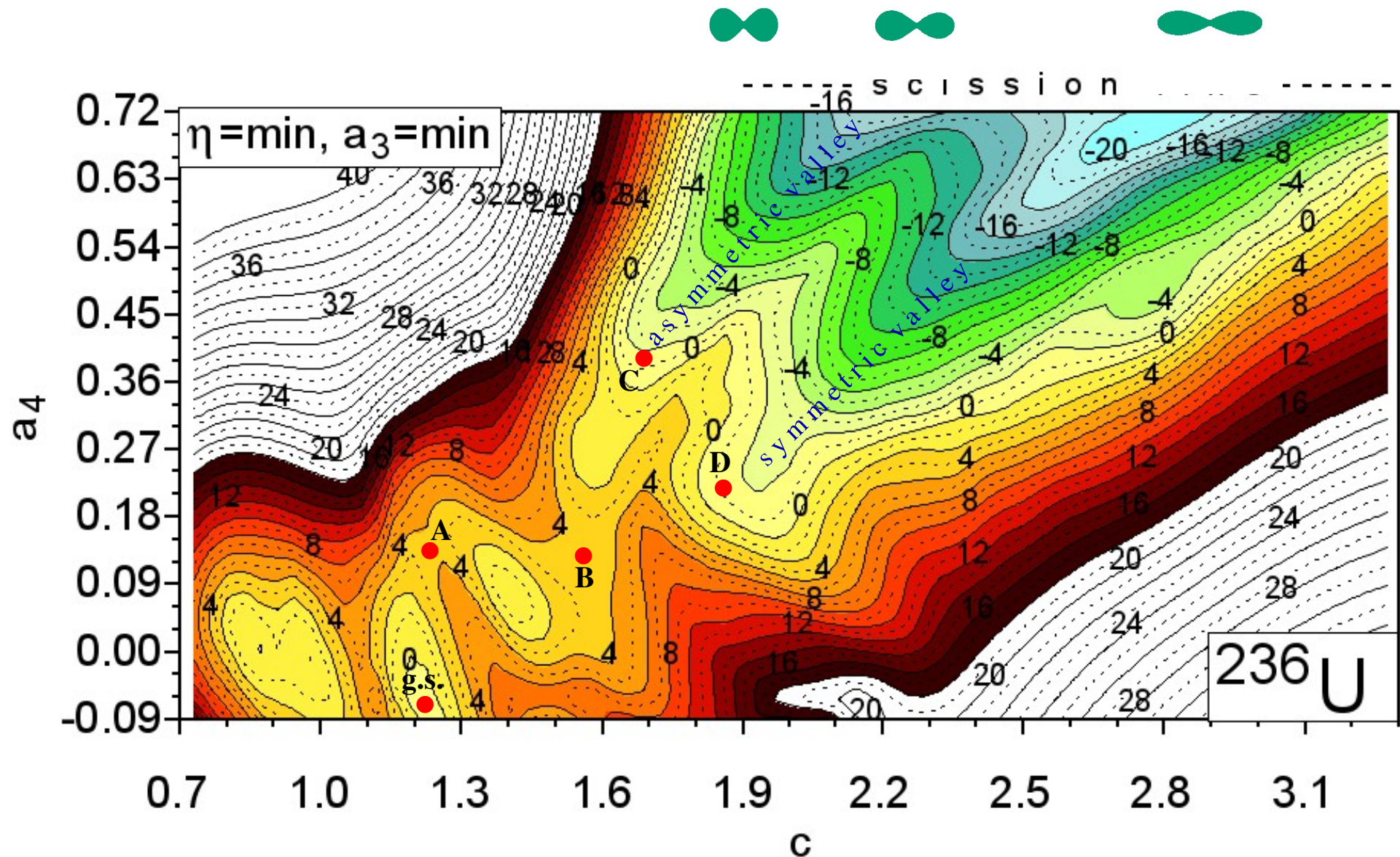
$$z_{sh} = -\frac{3}{4\pi}z_0 \left(a_3 - \frac{a_5}{2} + \frac{a_7}{3} - \dots \right)$$

places the nuclear **center of mass** at the origin of the coordinate system.

The parameter $\eta = (b - a)/(b + a)$ describes a possible, here elliptical, **non-axial deformation** of a nucleus. It is similar, but more general than the **γ -deformation** of Åge Bohr.

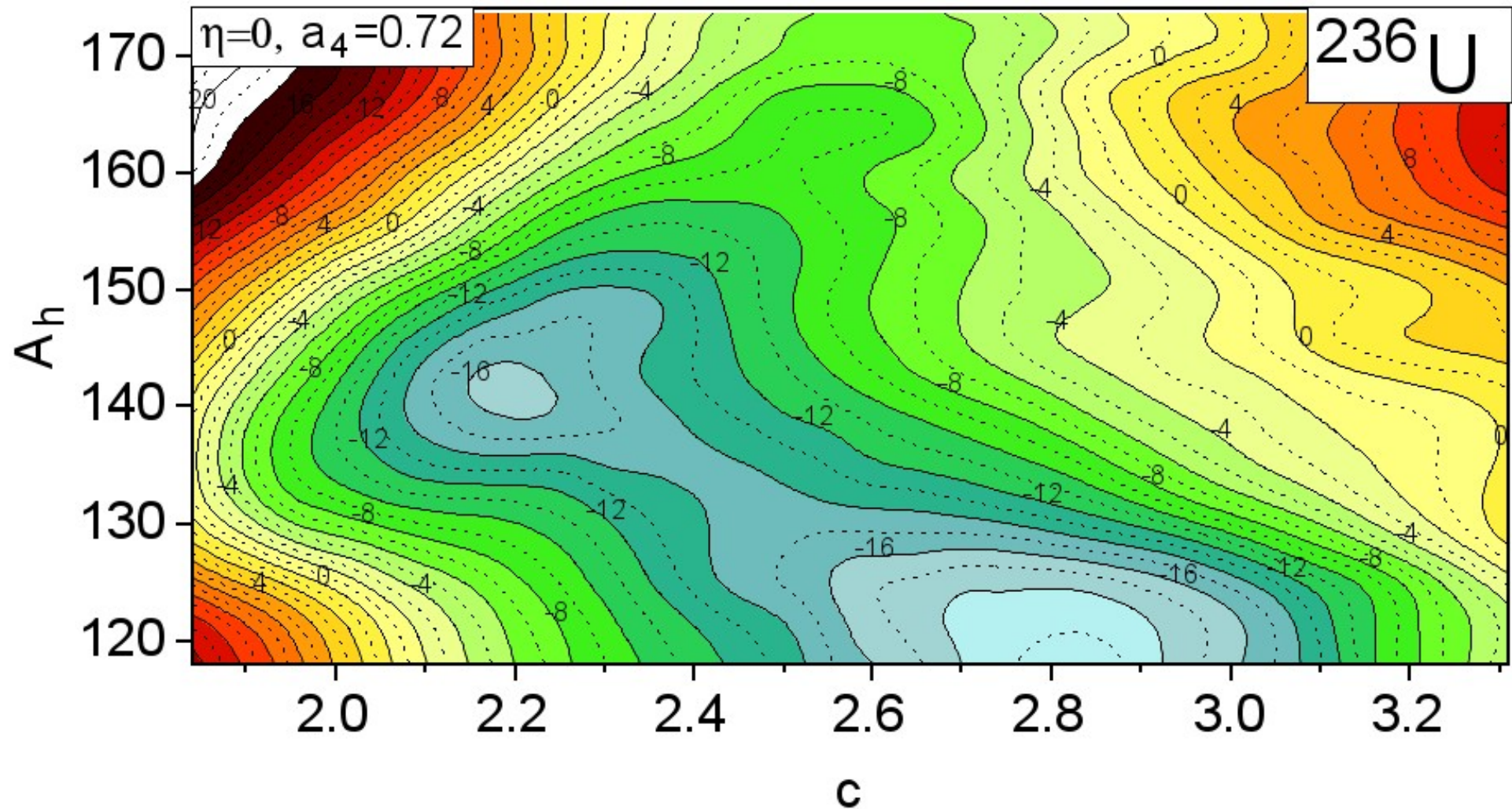
*K. P., B. Nerlo-Pomorska, C. Schmitt, Z.G. Xiao, Y.J. Chen, L.L. Liu, J. Bartel, PRC **107**, 054616 (2023).
C. Schmitt, K. P., B. Nerlo-Pomorska, J. Bartel, Phys. Rev. C **95**, 034612 (2017)
K. P., B. Nerlo-Pomorska, J. Bartel, Phys. Scr. **92**, 064006 (2017).

Potential energy surface of ^{236}U



Potential energies of even-even actinide and SH nuclei are evaluated within the **macro-micro** method using the **LSD** formula for the macroscopic energy, while the microscopic one is obtained using the **Yukawa-folded** mean-field potential and the **Strutinsky** and **BCS** methods.

Potential energy surface of ^{236}U around scission



The **mass of the heavy fragment** is found to be $A_h \approx \frac{A}{2}(1 + 1.01 a_3)$ and in our parametrization it is independent on c value. The **Langevin** and **Master** equations describe the fission dynamics and the emission of the post-fission neutrons.

Langevin equations for the fission process*

The dissipative fission dynamics is governed by the **Langevin equation** which in the generalized coordinates ($\{q_i\}$, $i = 1, 2, \dots, n$) has the following form:

$$\frac{dq_i}{dt} = \sum_j [\mathcal{M}^{-1}(\vec{q})]_{ij} p_j \quad \text{friction and random forces}$$

$$\frac{dp_i}{dt} = -\frac{1}{2} \sum_{j,k} \frac{\partial [\mathcal{M}^{-1}(\vec{q})]_{jk}}{\partial q_i} p_j p_k - \frac{\partial V(\vec{q})}{\partial q_i} - \sum_{j,k} \gamma_{ij}(\vec{q}) [\mathcal{M}^{-1}(\vec{q})]_{jk} p_k + F_i(t) ,$$

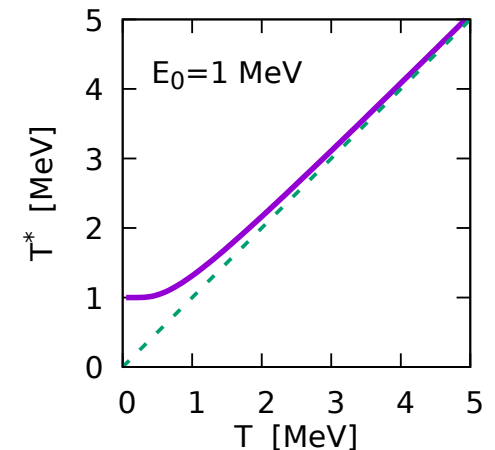
Here $V(\vec{q}) = E_{\text{pot}}(\vec{q}) - a(\vec{q})T^2$ is the **free-energy** of fissioning nucleus having temperature T and the single-particle level density parameter $a(\vec{q})$ while \mathcal{M}_{ij} and γ_{ij} are the **mass** and **friction tensors**. The vector $\vec{F}(t)$ stands for the **random Langevin force** which couples the collective dynamics to the intrinsic degrees of freedom and is defined as:

$$F_i(t) = \sum_j g_{ij}(\vec{q}) G_j(t) ,$$

where $\vec{G}(t)$ is a **stochastic function** which **strength** $g(\vec{q})$ is given by the **diffusion tensor** $\mathcal{D}(\vec{q})$ defined by the **generalized Einstein relation**:

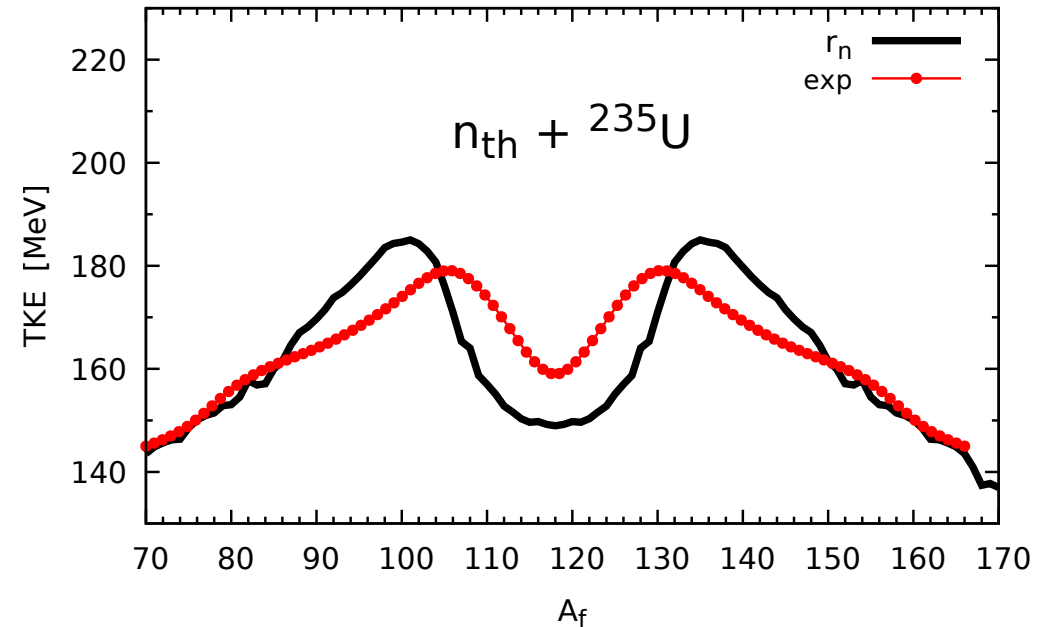
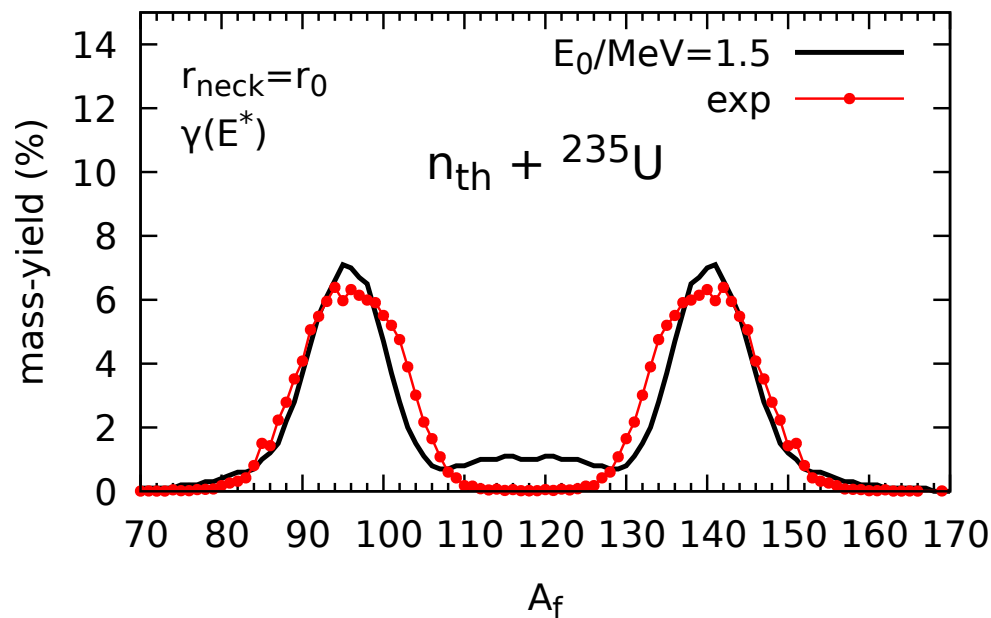
$$\mathcal{D}_{ij} = T^* \gamma_{ij} = \sum_k g_{ik} g_{jk} .$$

Here $T^* = E_0 / \tanh(E_0/T)$ and E_0 is the **zero-point collective energy**, while T is obtained from the **energy conservation law**: $E^*(\vec{q}) = a(\vec{q})T^2 = E_{\text{init}} - E_{\text{coll}}$.



* H.J. Krappe and K.P., *Nuclear Fission Theory*, Lecture Notes in Physics, Vol. 838, Springer Verlag, 2012.

Example of mass and TKE yields got by the 3D Langevin calculation*

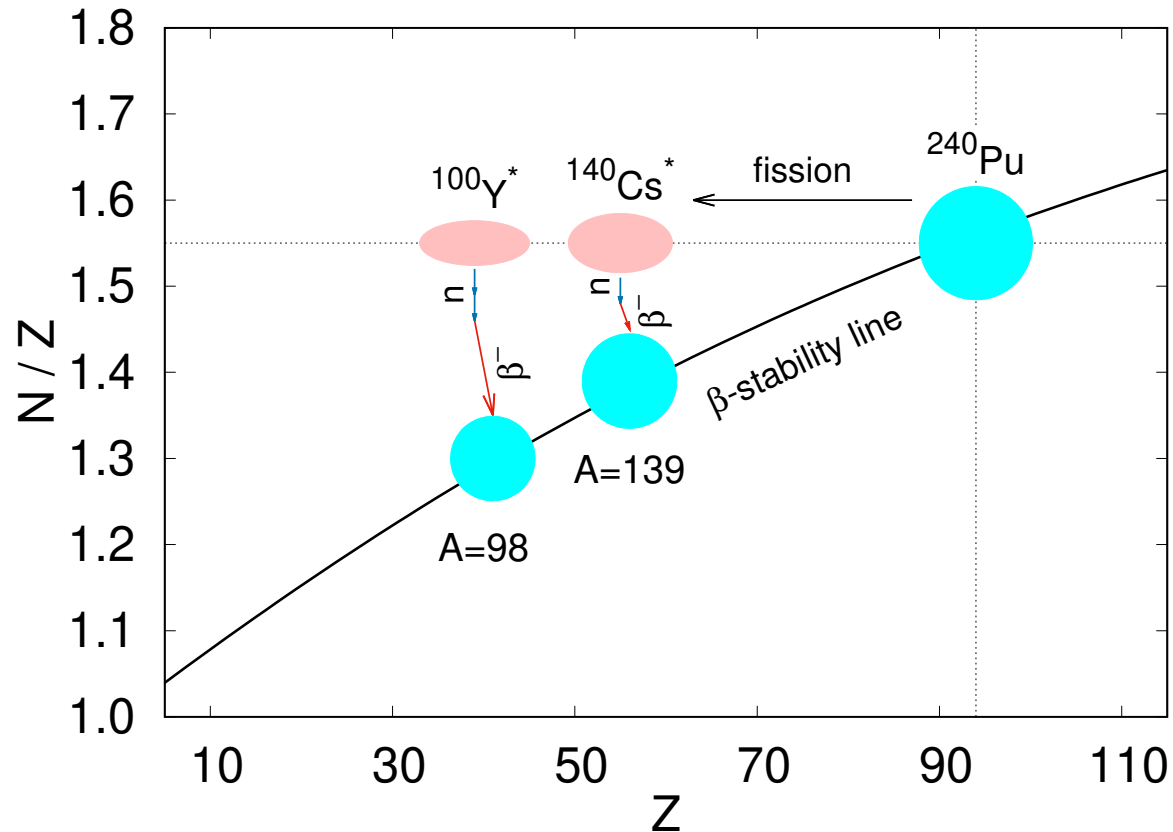


Total kinetic energy (TKE) of the fragments $E_{\text{kin}}^{\text{frag}}$ is given by the sum of the Coulomb repulsion energy (V_{Coul}), the nuclear interaction energy of fragments (V_{nuc}), and the pre-fission kinetic energy of the relative motion ($E_{\text{kin}}^{\text{Coll}}$) evaluated at the scission point (q_{sc}):

$$E_{\text{kin}}^{\text{frag}} = E_{\text{Coul}}^{\text{rep}}(q_{\text{sc}}) + V_{\text{nuc}}(q_{\text{sc}}) + E_{\text{kin}}^{\text{coll}}(q_{\text{sc}}) .$$

* K. P., B. Nerlo-Pomorska, C. Schmitt, Z.G. Xiao, Y.J. Chen, L.L. Liu, Phys. Rev. C **107**, 054616 (2023).

Schematic view of the post-fission process



The maximal energy of a neutron emitted from a fragment (mother) can be obtained from the **energy conservation law**:

$$\epsilon_n^{\max} = M_M + E_M^* - M_D - M_n ,$$

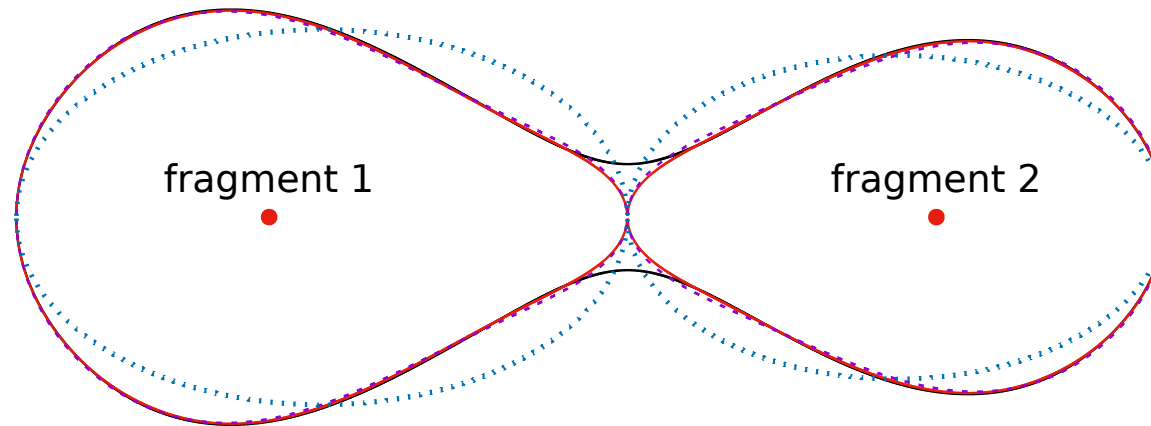
where M_M , M_D , M_n are respectively the **mass excesses** of mother and daughter nuclei, and the neutron. These data can be taken from a mass table.

The thermal excitation energy of the daughter nucleus is: $E_D^* = \epsilon_n^{\max} - \epsilon_n$.

Shapes of the mother and the fragment nuclei at scission

parent —
(c, a₃, a₄) —
(c, a₃, a₄=0) - - -
(c, a₃=0, a₄=0) ····

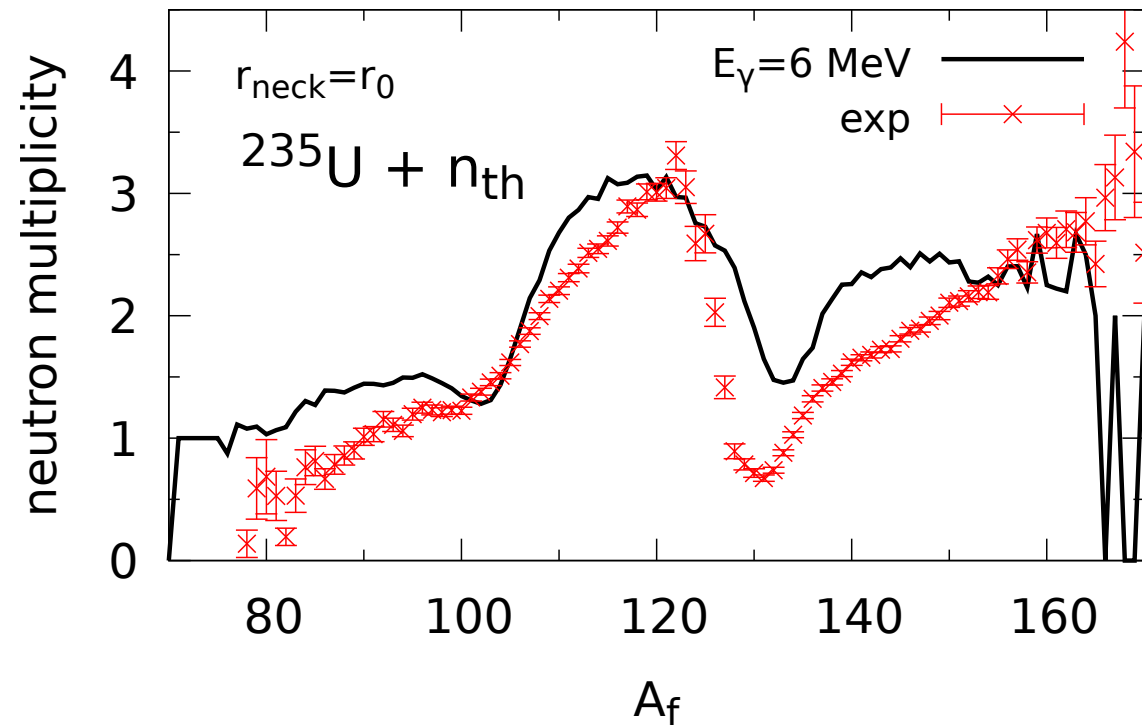
c=2.2, q₃=0.21, a₄=0.72



$c^{(1)}=1.384, a_3^{(1)}=-0.361, a_2^{(1)}=-0.021; c^{(2)}=1.403, a_3^{(2)}=0.312, a_4^{(2)}=-0.033$

The fission fragments have frequently **pear-like** shapes (red line). Omitting this degree of freedom in some parametrizations (e.g., in **the quadratic shapes of revolution** parametrization) may lead to significant **overestimation** of the Coulomb repulsion energy of fragments.

Number of neutrons emitted from the fragments:



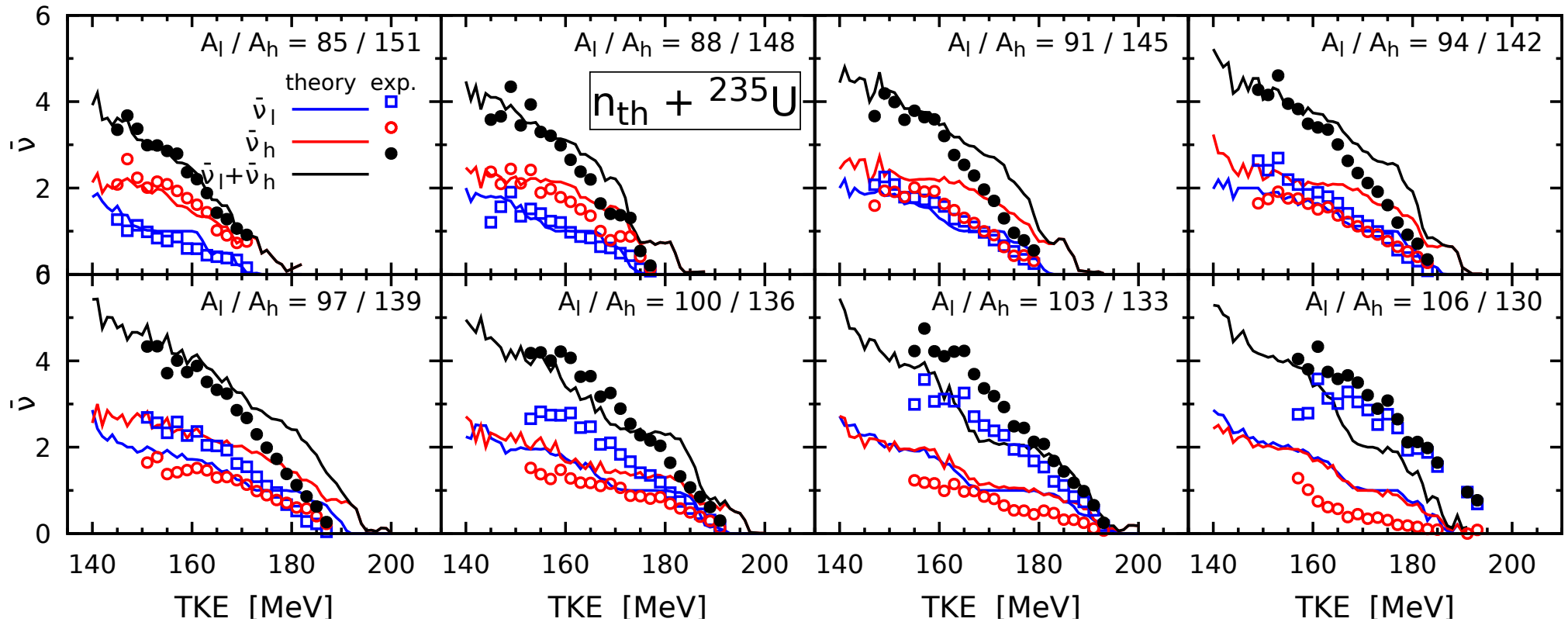
Experimental data: A. Al-Adili et al., PRC **102**, 064610 (2020).

Theory: K. P., B. Nerlo-Pomorska, C. Schmitt, Z.G. Xiao, Y.J. Chen, L.L. Liu, PRC **107**, 054616 (2023),

Our earlier works: Ch. Grégoire, H. Delagrange, K. P., K. Dietrich, Z. Phys. A **329**, 497 (1988),

K. P., B. Nerlo-Pomorska, A. Surowiec, M. Kowal, J. Bartel, K. Dietrich, J. Richert, C. Schmitt, B. Benoit, E. de Goes Brennand, L. Donadille, C. Badimon, Nucl. Phys. A **679**, 25 (2000), B. Nerlo-Pomorska, K. P., J. Bartel, K. Dietrich, Phys. Rev. C **67**, 051302 (2002).

Number of neutrons emitted from the fission fragments of $^{236}\text{U}_{\text{th}}$



Theory: K. P., B. Nerlo-Pomorska, C. Schmitt, Z.G. Xiao, Y.J. Chen, L.L. Liu, PRC **107**, 054616 (2023).

Exp. data: A. Göök, F.-J. Hamsch, S. Oberstedt, M. Vidali, PRC **98**, 044615 (2018).

On the charge equilibration at scission

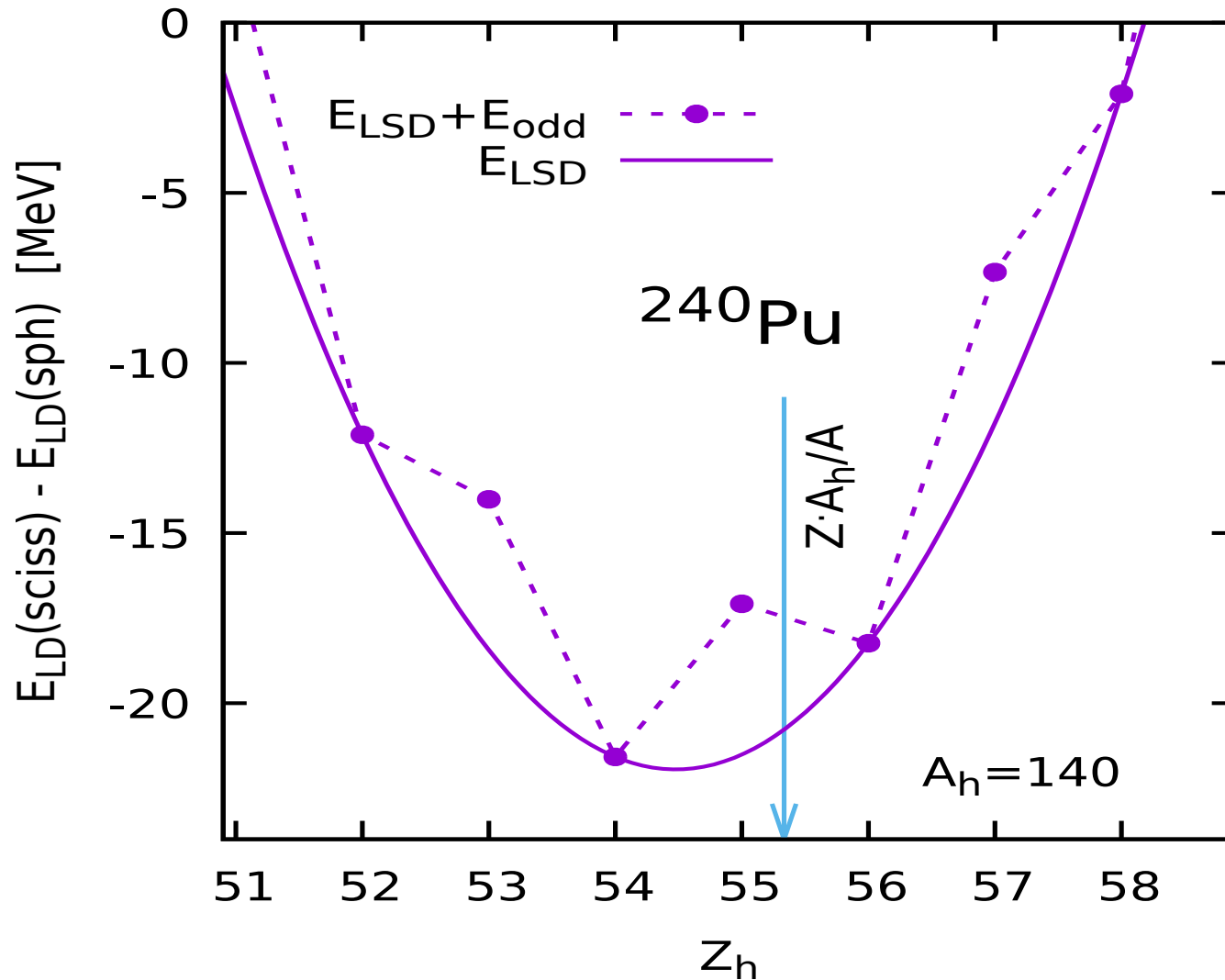
It is relatively easy to find the preferred charge for each fragment when knowing the fragment deformation at scission. Usually, one assumes that the isospin of a fragment is the same as the one of the fissioning nucleus. One obtains a better estimate by looking for the proton and neutron microscopic distribution.

A simple estimate of the proton-neutron equilibrium distribution at scission can also be made in the LD model. It is determined by the minimum with respect to Z_h of the following function:

$$\begin{aligned} E(Z, A, Z_h; B_f, \text{def}_h, \text{def}_l) &= E_{\text{LD}}(Z_h, AB_f; \text{def}_h) \\ &+ E_{\text{LD}}(Z - Z_h, A(1 - B_f); \text{def}_l) \\ &+ \frac{e^2 Z_h(Z - Z_h)}{R_{12}} - E_{\text{LD}}(Z, A; 0) , \end{aligned}$$

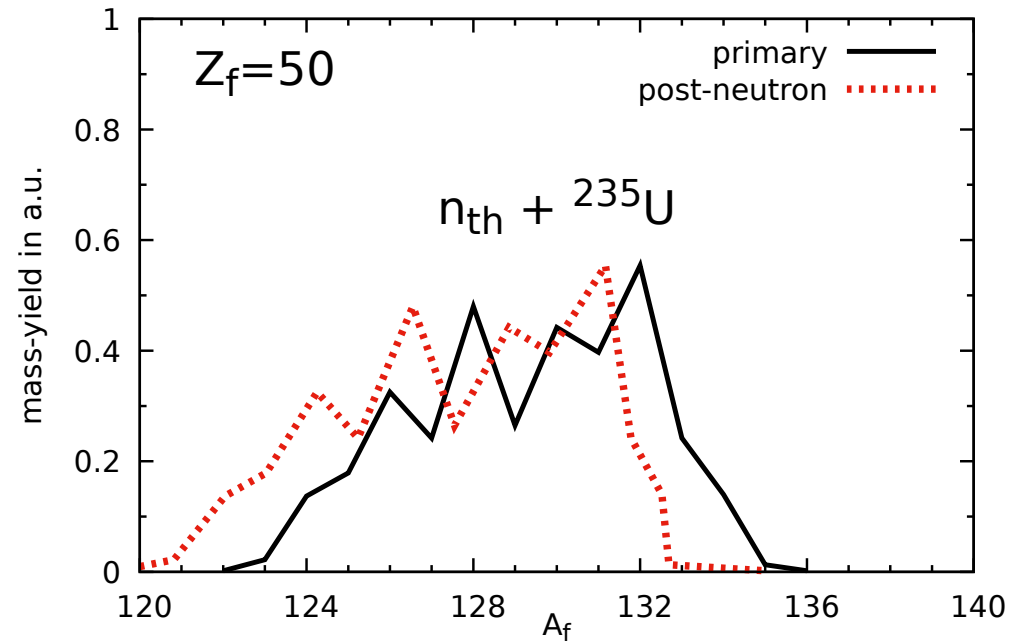
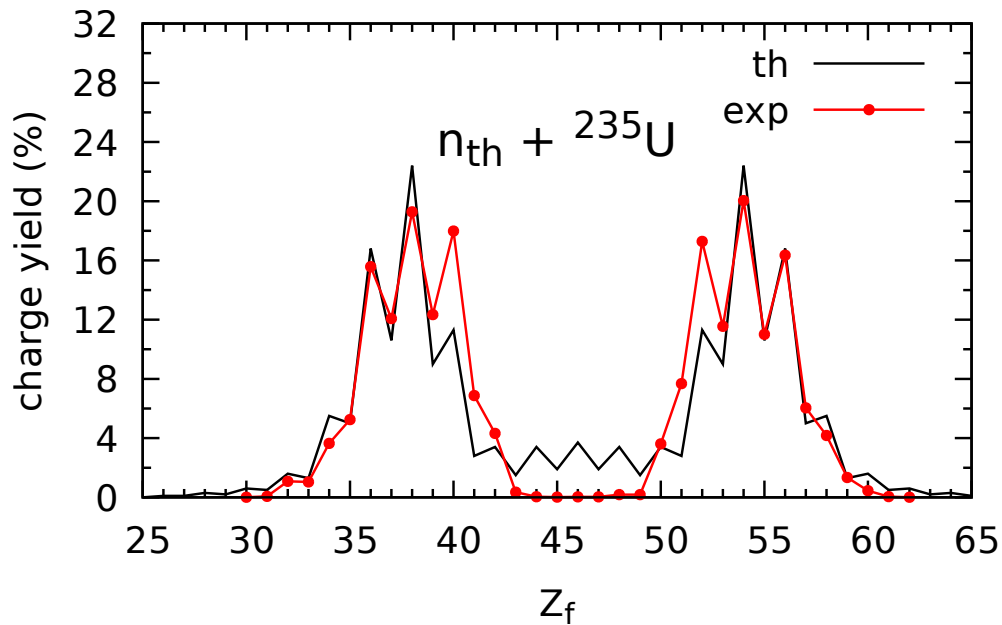
where Z, A and Z_h, A_h are the charge and mass numbers of the mother nucleus and the heavy fragment, respectively. The mass $A_h = A \cdot B_f(\text{def}_{\text{sc}})$ is fixed by the shape of the nucleus at scission, while def_h and def_l are the deformations of heavy and light fragment respectively and $B_f = \text{vol}(h)/\text{vol}(\text{total})$.

Total energy at scission as a function of the fragment charge number



The above effect has to be taken into account at the end of each Langevin trajectory, when one fixes the (**integer**) fragment mass and charge numbers.

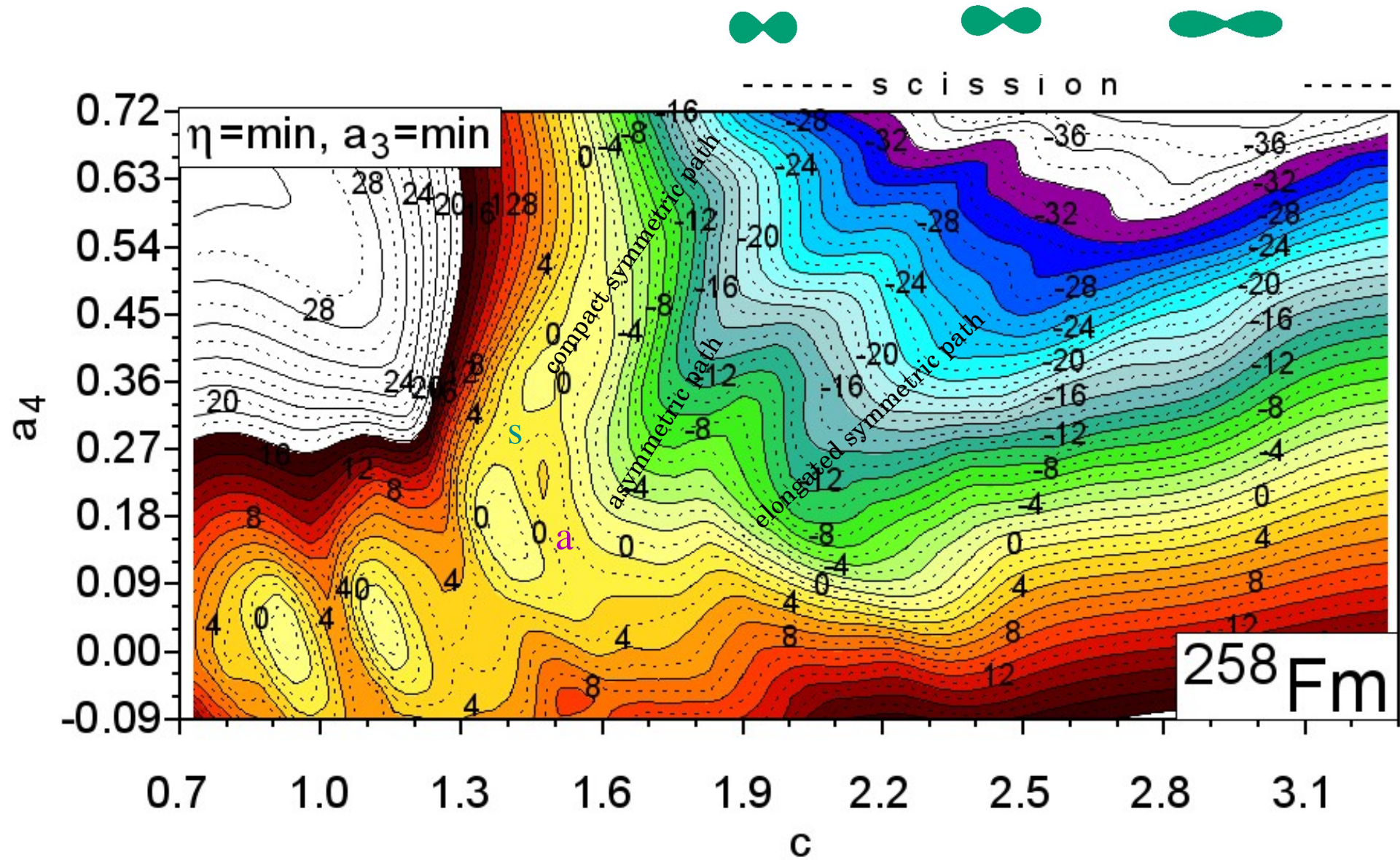
Charge and pre- post-neutron fragment yields of $^{236}\text{U}_{\text{th}}^*$



* K. P., B. Nerlo-Pomorska, C. Schmitt, Z.G. Xiao, Y.J. Chen, L.L. Liu, Phys. Rev. C **107**, 054616 (2023).

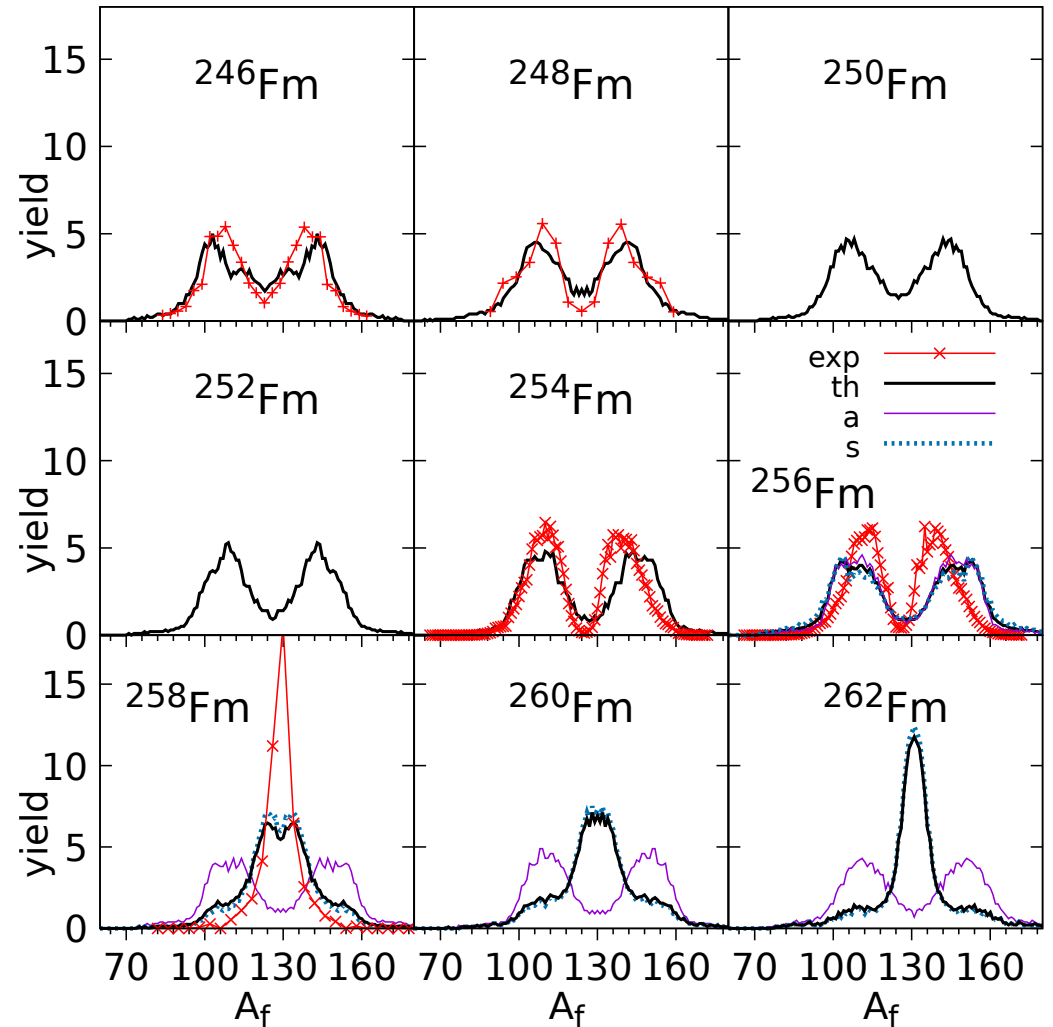
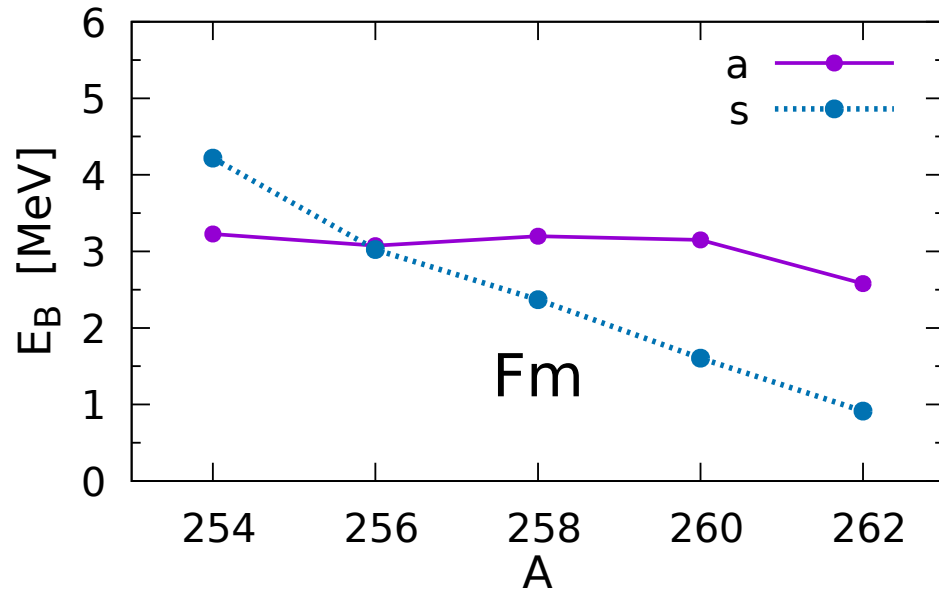
exp: JENDLLibrary, <http://wwwndc.jaea.go.jp/index.html>.

On bimodal fission of ^{258}Fm



K. P, A.Dobrowolski, B. Nerlo-Pomorska, M. Warda, A. Zdeb, J. Bartel, H. Molique, C. Schmitt, Z.G. Xiao, Y.J. Chen, L.L. Liu, Acta Phys. Polon. B **54** , 9-A2 (2023).

Barrier heights and mass-yields corresponding to the asymmetric and the compact-symmetric paths*



The **weighted mass-yield** Y_{th} is given by:

$$Y_{th}(A_f) = P_a \cdot Y_a(A_f) + P_s \cdot Y_s(A_f),$$

where $P_a + P_s = 1$ and

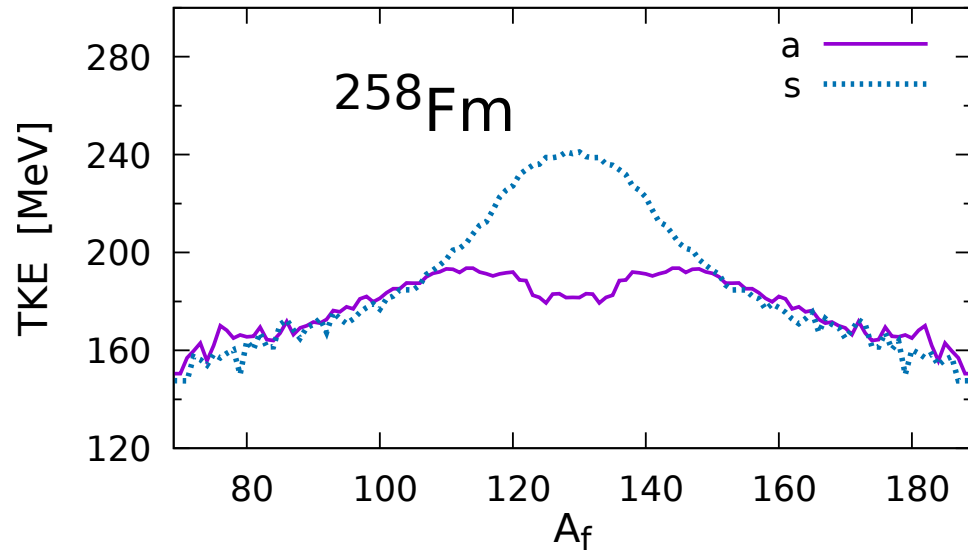
$$P_i = \exp(-S_i) / [\exp(-S_a) + \exp(-S_s)]$$

is the relative fission **barrier penetration probability** and S_i is the WKB action-integral[†] along the path i .

*K. P., B. Nerlo-Pomorska, C. Schmitt, Z.G. Xiao, Y.J. Chen, L.L. Liu, Phys. Rev. C **107**, 054616 (2023).

†K. P., A. Dobrowolski, B. Nerlo-Pomorska, M. Warda, J. Bartel, Z.G. Xiao, Y.J. Chen, L.L. Liu, J-L. Tian, X.Y. Diao, Eur. Phys. Journ. A **58**, 77 (2022).

Fission fragment total kinetic energy yield of $^{258}\text{Fm}_{sf}$

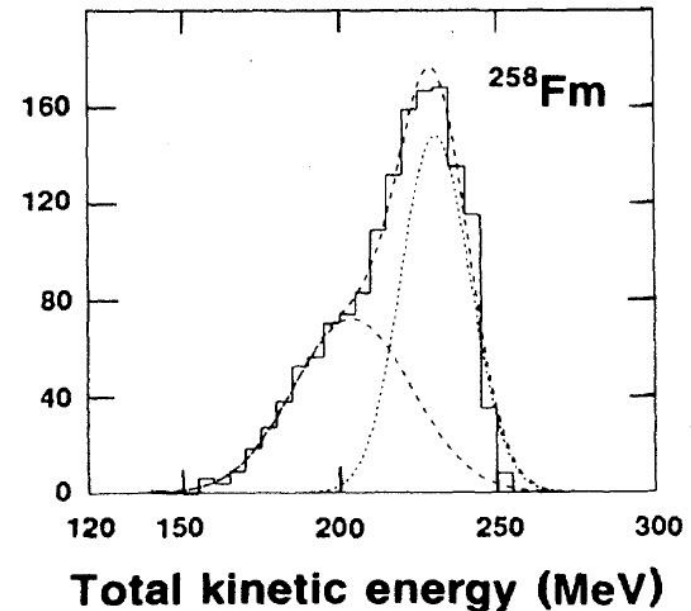
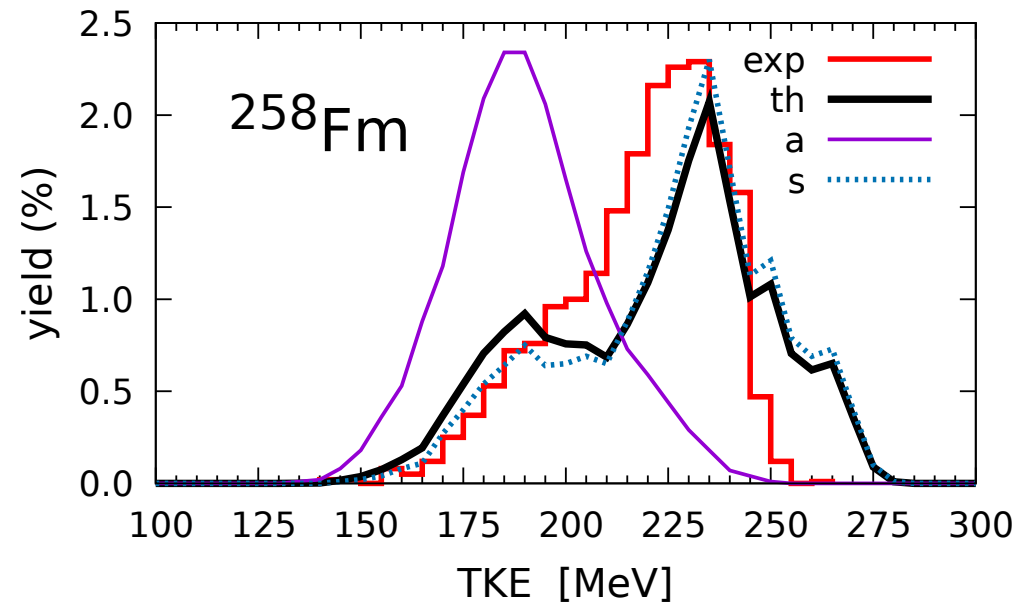


The TKE as function of the fragments mass A_f corresponds to the asymmetric (a) and the compact-symmetric (s) modes.

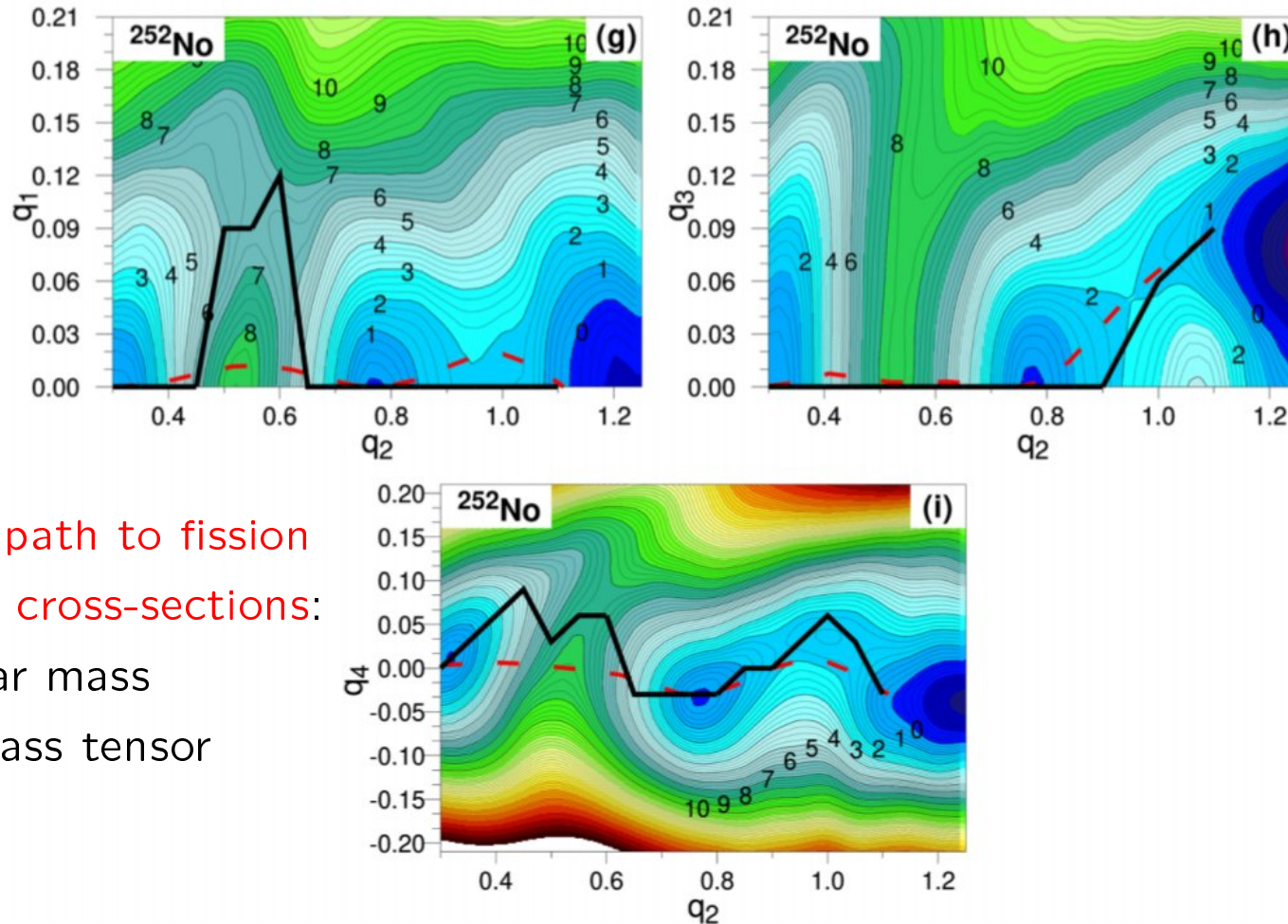
Experimental data by Hulet et al. \longrightarrow

E. K. Hulet et al. Phys. Rev. Lett. **56**, 313 (1986);

Phys. Rev. C **40**, 770 (1989).



Spontaneous fission lifetimes*

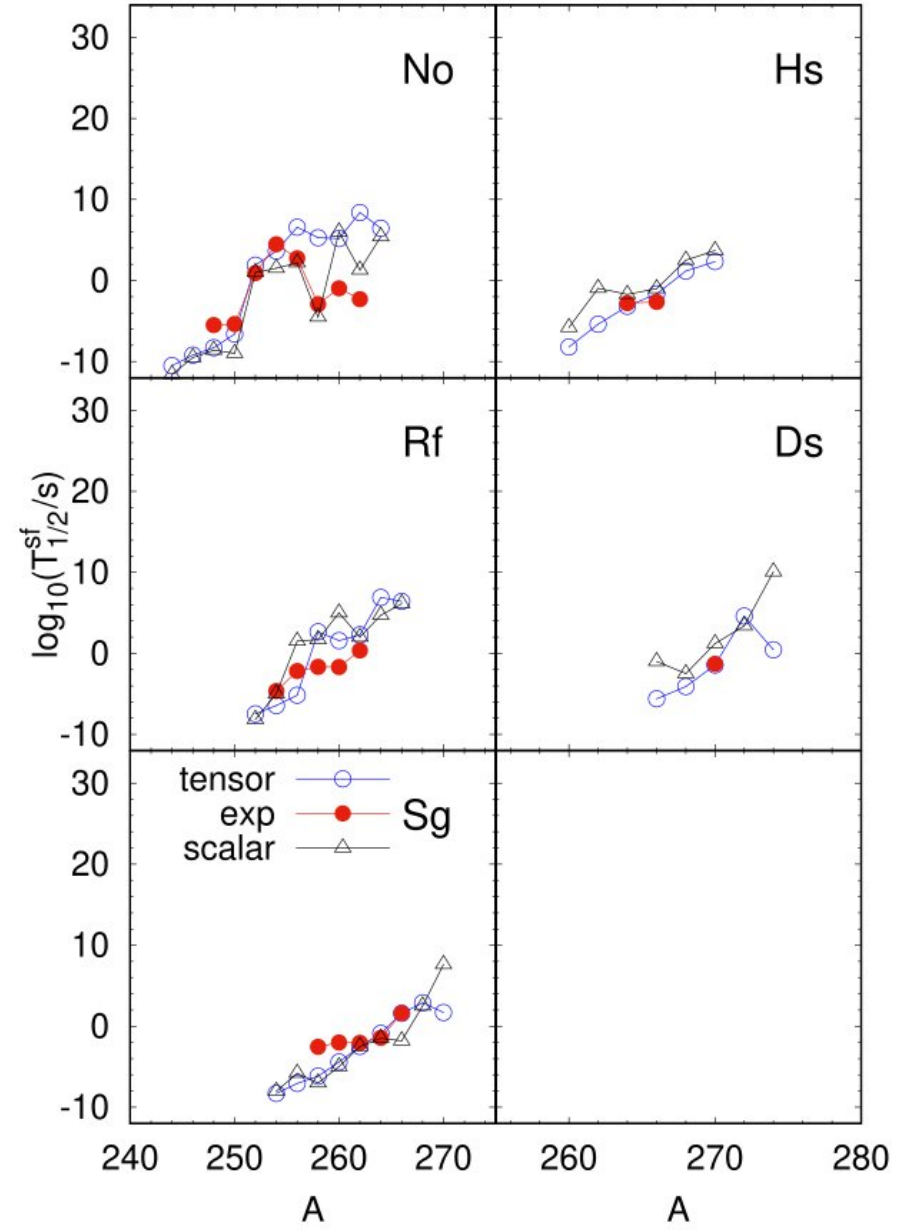
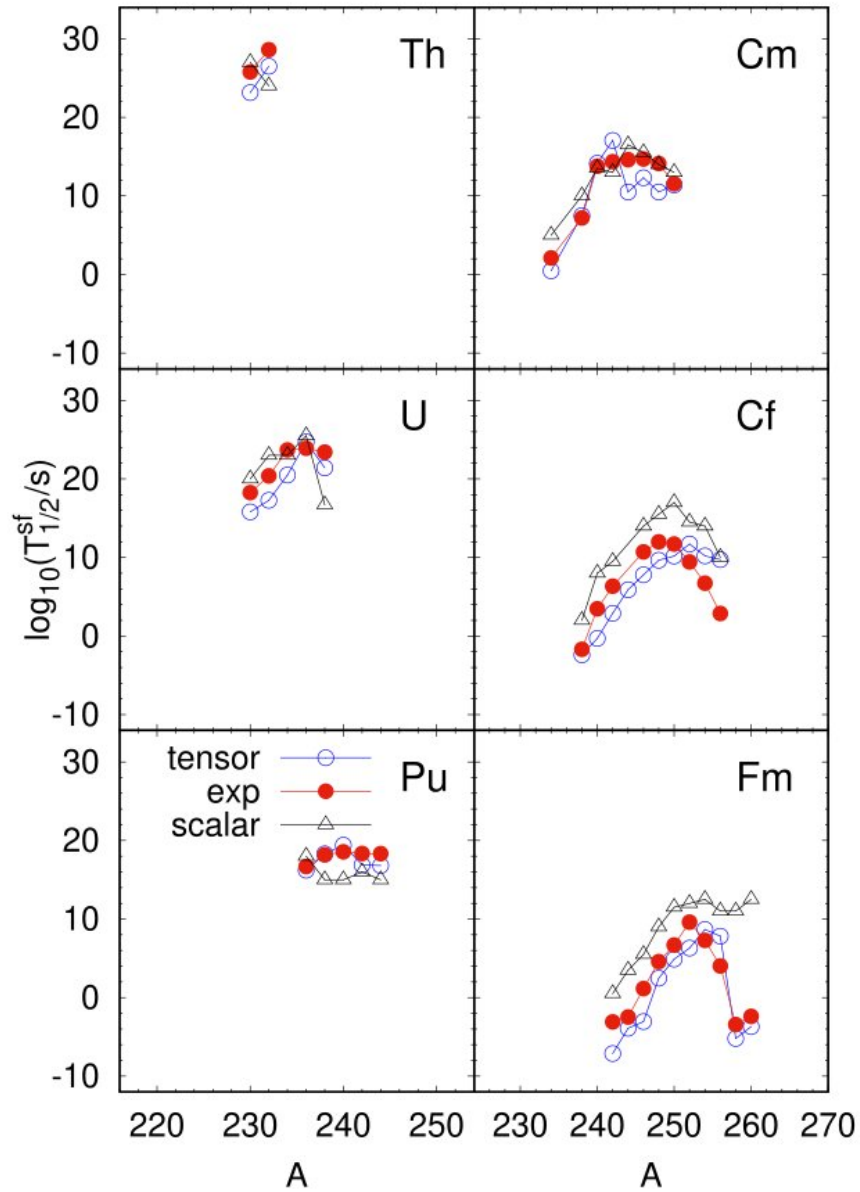


Minimal action path to fission
on various PES cross-sections:
solid line - scalar mass
dashed line - mass tensor

Minimum of the WKB action integral $S = \int_{\text{g.s.}}^{\text{exit}} dq_2 \sqrt{\frac{2}{\hbar^2} \sum_{i,j=1}^4 \beta B_{ij}(\{q_k\}) [\mathcal{E}(\{q_k\}) - E_{\text{g.s.}}] \frac{\partial q_i}{\partial q_2} \frac{\partial q_j}{\partial q_2}}$
determines the lifetime $T_{sf} = \frac{2\pi \ln 2}{\omega_0} \cdot (1 + \exp 2S)$

* J.M. Blanco, A. Dobrowolski, A. Zdeb, J. Bartel, Phys. Rev. C **108**, 044618 (2023).

Estimates of spontaneous fission lifetimes*



* J.M. Blanco, A. Dobrowolski, A. Zdeb, J. Bartel, Phys. Rev. C **108**, 044618 (2023).

Liste des articles publiés au cours des 5 dernières années:

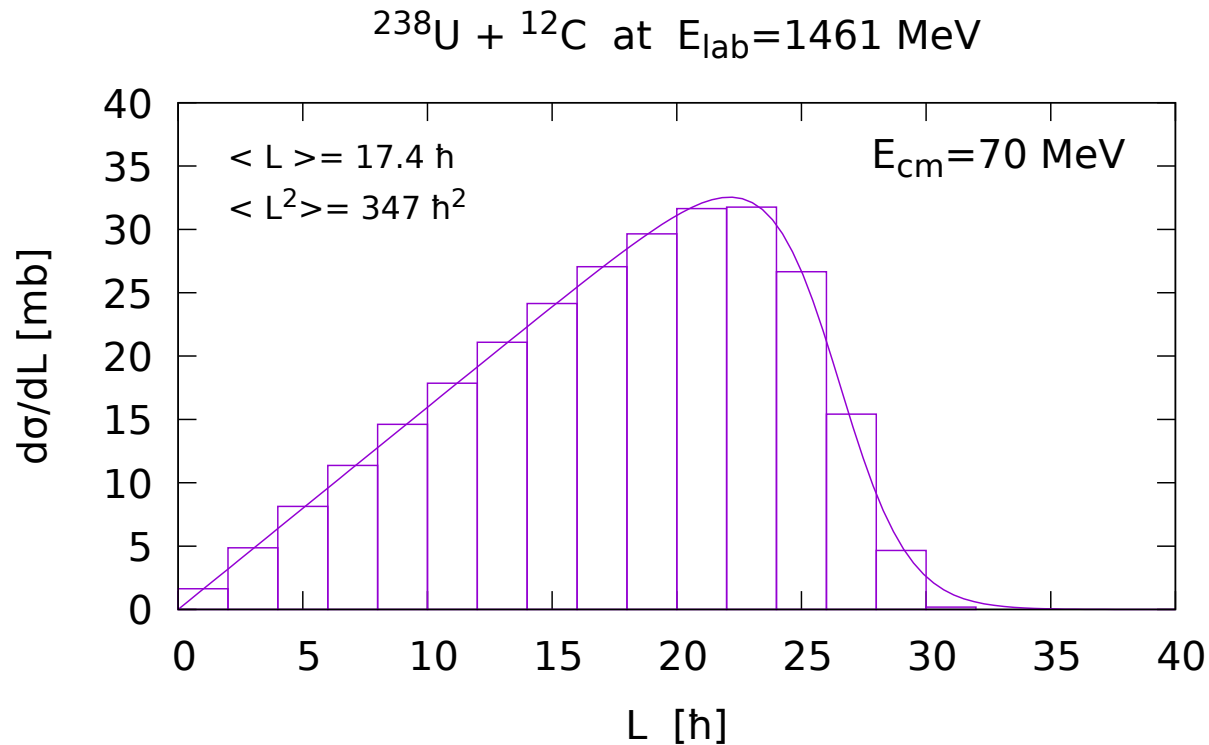
1. J.M. Blanco, A. Dobrowolski, A. Zdeb, J. Bartel, *Spontaneous fission half-lives of actinides and super-heavy elements*, Phys. Rev. C **108**, 044618 (2023).
2. K. Pomorski, A. Dobrowolski, B. Nerlo-Pomorska, M. Warda, A. Zdeb, J. Bartel, H. Molique, C. Schmitt, Z.G. Xiao, Y.J. Chen, L.L. Liu: *Fission fragment mass and kinetic energy yields of Fermium isotopes*, Acta Phys. Polon. **B54**, 9-A2 (2023).
3. K. Pomorski, B. Nerlo-Pomorska, C. Schmitt, Z.G. Xiao, Y.J. Chen, L.L. Liu: *Fourier-over-spheroid shape parametrization applied to nuclear fission dynamics*, Phys. Rev. C **107**, 054616 (2023).

4. K. Pomorski, A. Dobrowolski, B. Nerlo-Pomorska, M. Warda, J. Bartel, Z.G. Xiao, Y.J. Chen, L.L. Liu, J-L. Tian, X.Y. Diao: *On the Stability of Super-heavy Nuclei*, Eur. Phys. J. A **58**, 77 (2022).
5. K. Pomorski, B. Nerlo-Pomorska, J. Bartel, H. Molique: *Convergence study of the Fourier shape parametrization in the vicinity of the scission configuration*, Acta Phys. Pol. B Supl. **13**, 361 (2020).
6. B. Nerlo-Pomorska, K. Pomorski, J. Bartel, H. Molique: *On shape isomers of Pt-Pb isotopes in the 4D Fourier parametrisation*, Acta Phys. Pol. B Supl. **13**, 449 (2020).
7. K. Pomorski, B. Nerlo-Pomorska, A. Dobrowolski, J. Bartel, C. M. Petrache: *Shape isomers in Pt, Hg and Pb isotopes with $N < 126$* , Eur. Phys. J. **56**, 107 (2020).
8. K. Pomorski, B. Nerlo-Pomorska, J. Bartel, H. Molique: *On Shape Coexistence and Shape Isomerism in Even-Even Nuclei in the Vicinity of ^{208}Pb* , Bulg. Journ. Phys. **46**, 269 (2019) 269.
9. J. Bartel, K. Pomorski, B. Nerlo-Pomorska, A. Dobrowolski: *Transport coefficients within a Fourier shape parametrization*, Acta Phys. Polon. B Sup. **12**, 537 (2019).
10. B. Nerlo-Pomorska, K. Pomorski, J. Bartel: *Rotational bands in super-heavy nuclei within the LSD+YF model*, Acta Phys. Polon. B Sup. **12**, 665 (2019).
11. J. Bartel, B. Nerlo-Pomorska, K. Pomorski, A. Dobrowolski: *Transport coefficients in the Fourier shape parametrization*, Comp. Phys. Comm. **241**, 139 (2019).
12. K. Pomorski, B. Nerlo-Pomorska, J. Bartel, C. Schmitt: *On properties of super-heavy even-even nuclei around ^{294}Og* , Acta Phys. Polon. B **50**, 535 (2019).
13. A. Dobrowolski, J. Bartel, K. Pomorski: *Nuclear mass parameters and moments of inertia in a folded-Yukawa mean-field approach*, Comp. Phys. Comm. **237**, 253 (2019).
14. K. Pomorski, B. Nerlo-Pomorska, J. Bartel, C. Schmitt: *Stability of super-heavy nuclei*, Phys. Rev. C **97**, 034319 (2018).
15. K. Pomorski, B. Nerlo-Pomorska, J. Bartel, C. Schmitt: *Potential-energy surfaces of heavy and super-heavy nuclei*, Acta Phys. Polon. B Sup. **11**, 137 (2018).

Recherches en cours et prévues en 2024:

Fission of hot nuclei

Let us consider the partial fusion cross-section for synthesis of ^{250}Cf obtained in the following reaction*:



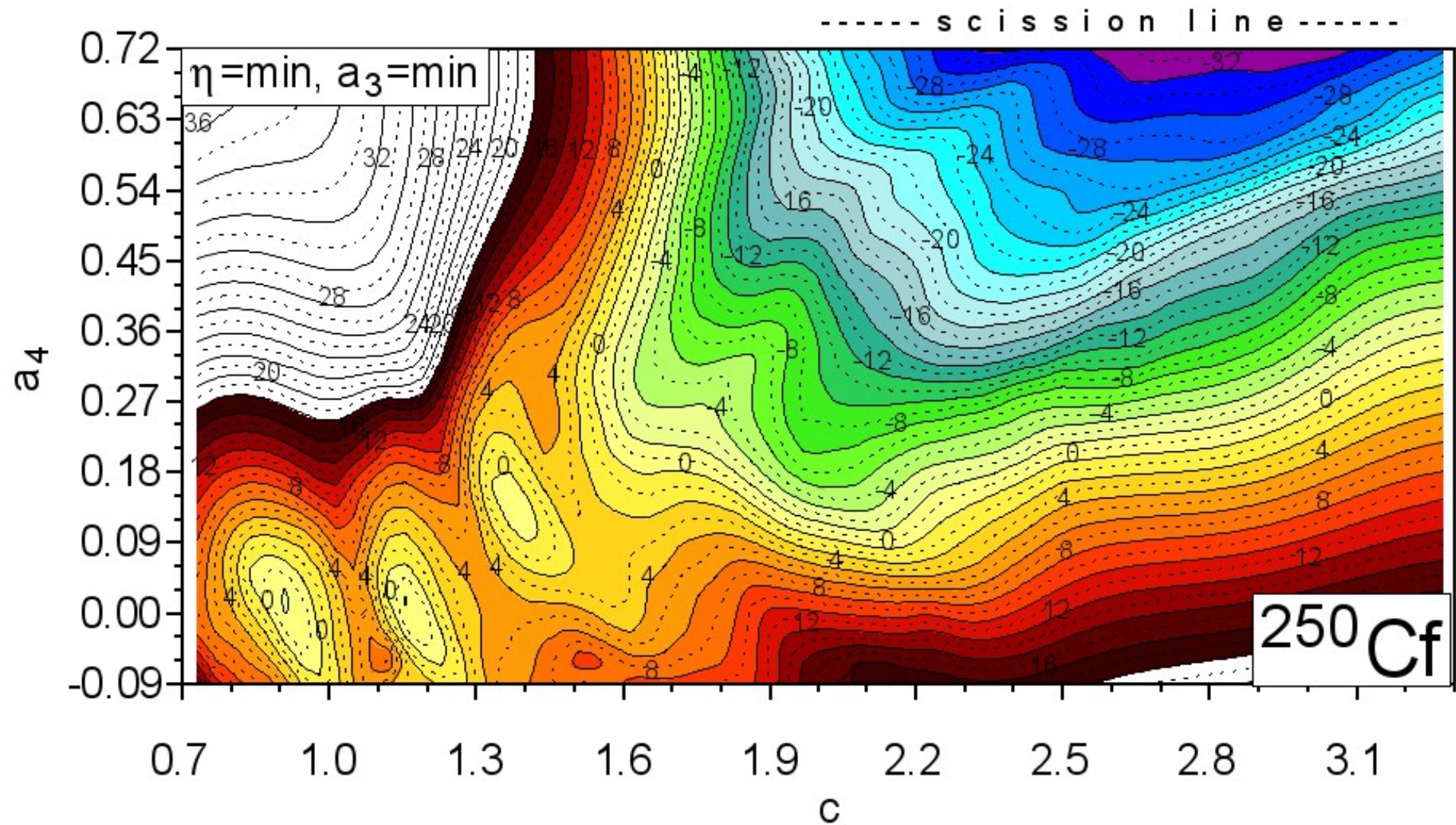
The above estimate was done using our old Langevin code for fusion:

K. P., W. Przystupa, J. Bartel, J. Richert, *Acta Phys. Polon. B* **30**, 809 (1999);

W. Przystupa, K. P., *Nucl. Phys. A* **572**, 153 (1994).

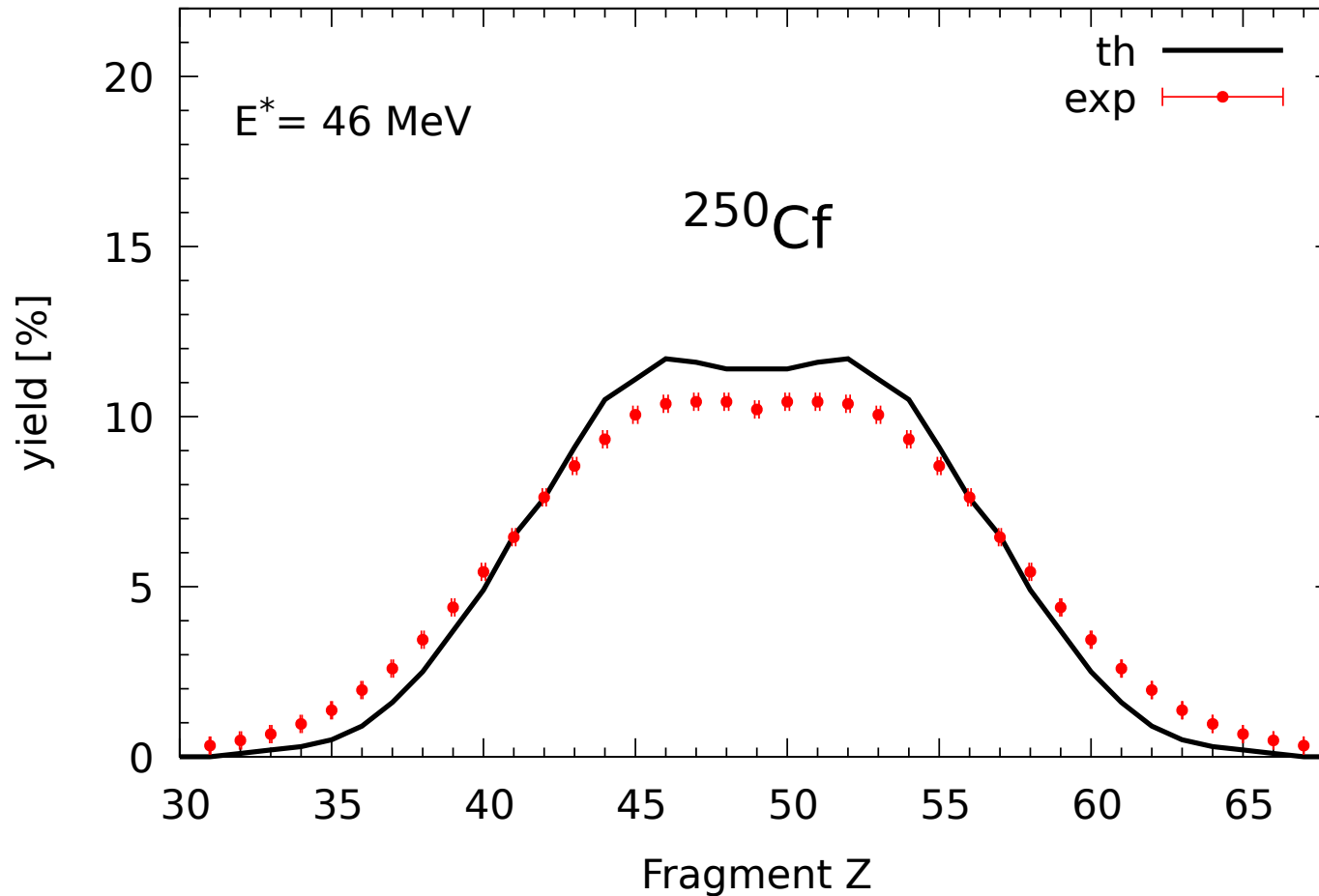
*D. Ramos et al. *Phys. Rev. C* **99**, 024615 (2019).

Cross-section (c, a_4) of the 4D PES of ^{250}Cf at $T=0$



The effect of temperature and rotation will be taken into account in our dynamical calculations.

Fission fragment mass yield of ^{250}Cf at $E^*=46$ MeV

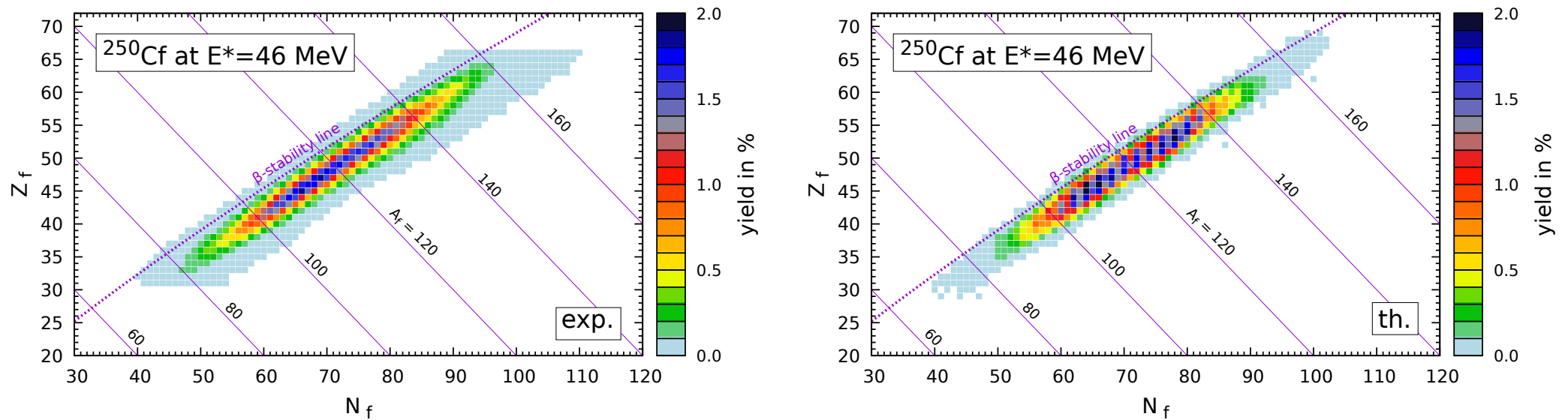


All parameters of the calculation are the same as those used to describe the fission of $^{236}\text{U}_{\text{th}}$ and $^{246-262}\text{Fm}_{\text{sf}}$ isotopes.

Exp. data (VAMOS GANIL): D. Ramos et al. Phys. Rev. c **99**, 024615 (2019).

Isotopic fission fragment yield of ^{250}Cf at $E^*=46$ MeV

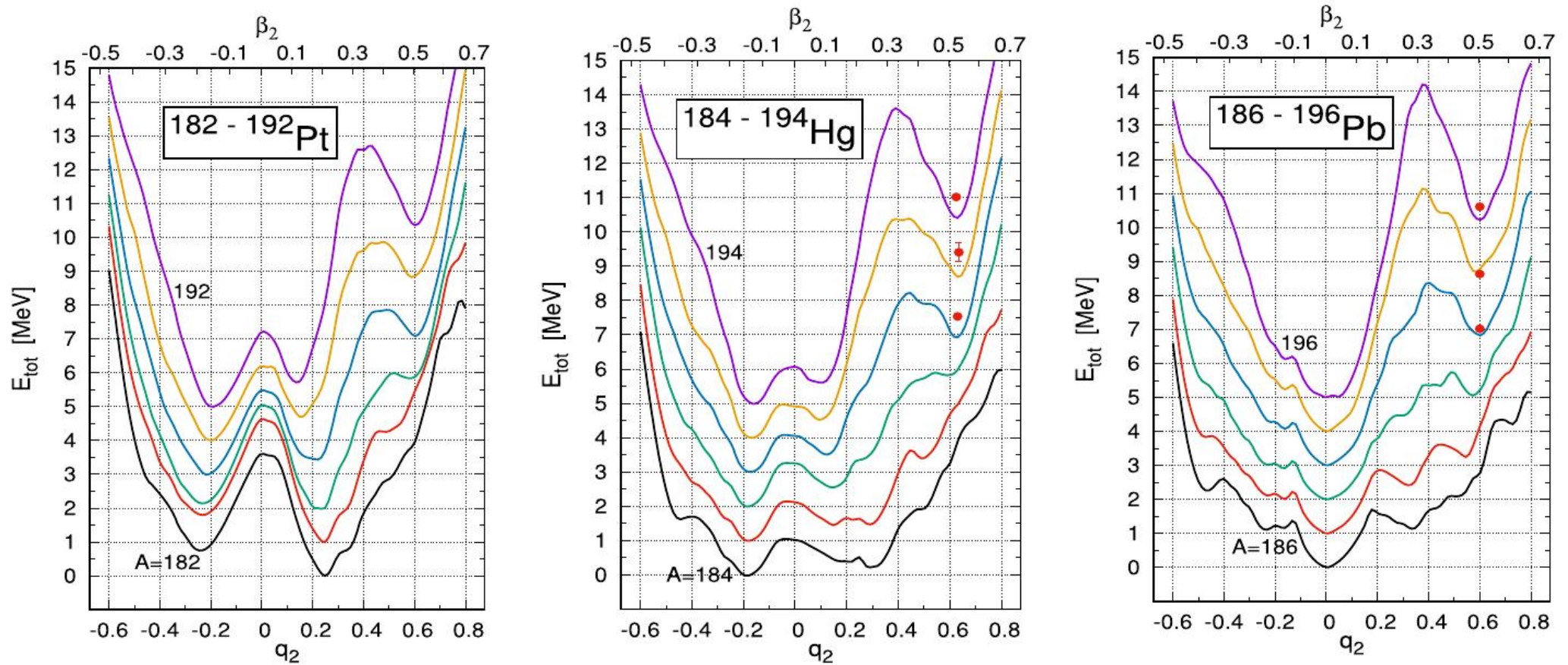
Preliminary results compared with the experimental data obtained in GANIL*:



The pre-fission neutrons are not taken into account in our estimates.
An appropriate numerical code is under construction.

Exp. data: D. Ramos et al. Phys. Rev. c **99**, 024615 (2019).

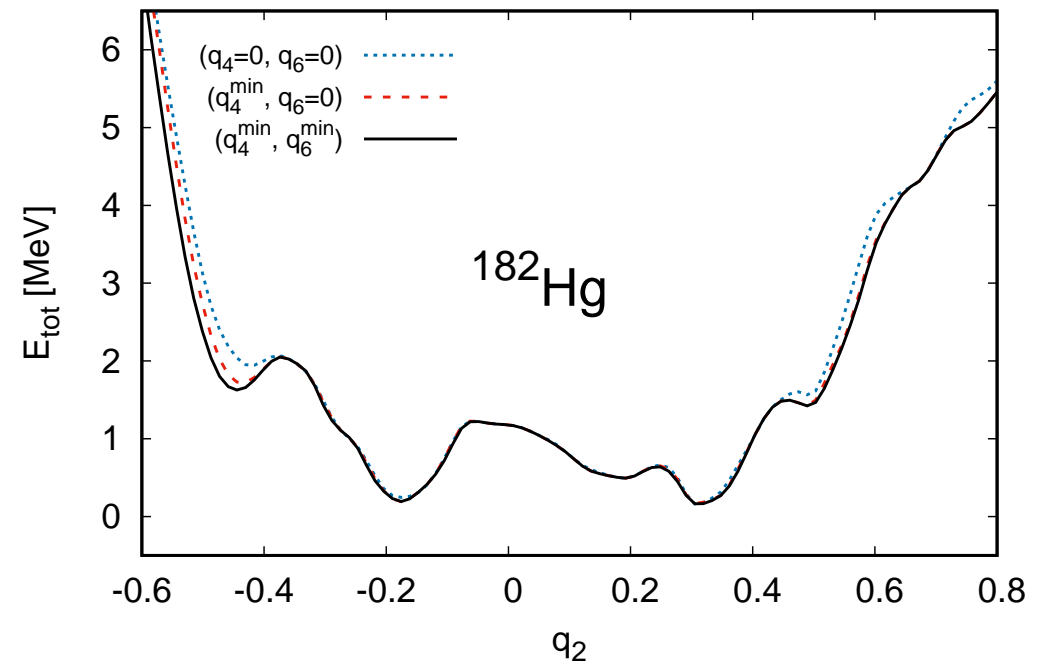
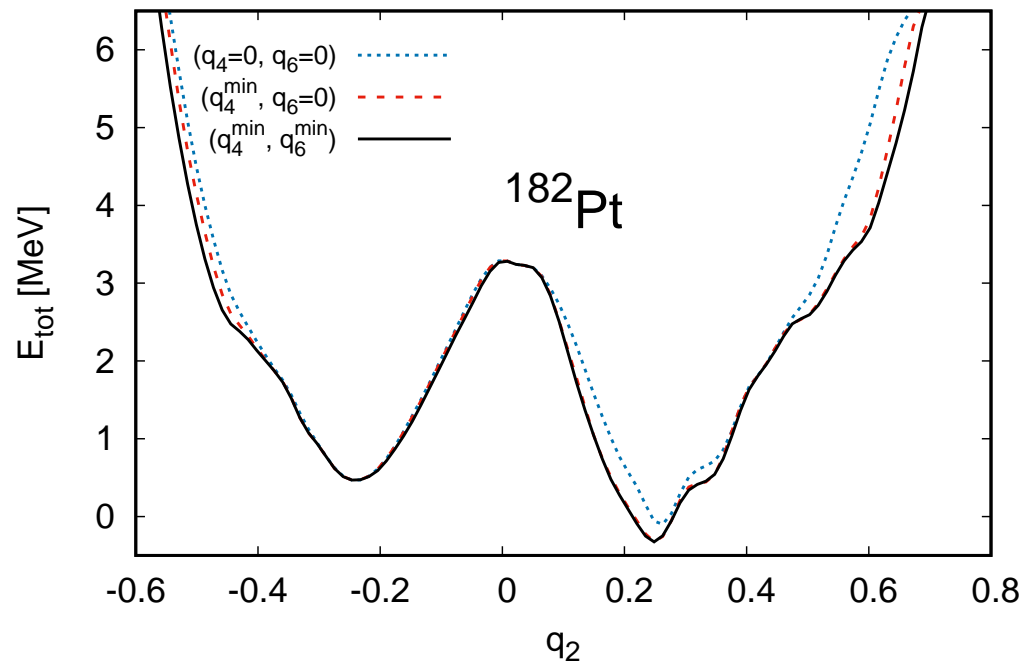
Searching for the shape-isomers in Pt, Hg, and Pb isotopes



We are going to continue our previous research made within the COPIN-IN2P3 collaboration, project No. 15-149 (Srebrny-Petrache):

K.P., B. Nerlo-Pomorska, A. Dobrowolski, J. Bartel, C. M. Petrache, *Eur. Phys. J. A* **56**, 107 (2020).

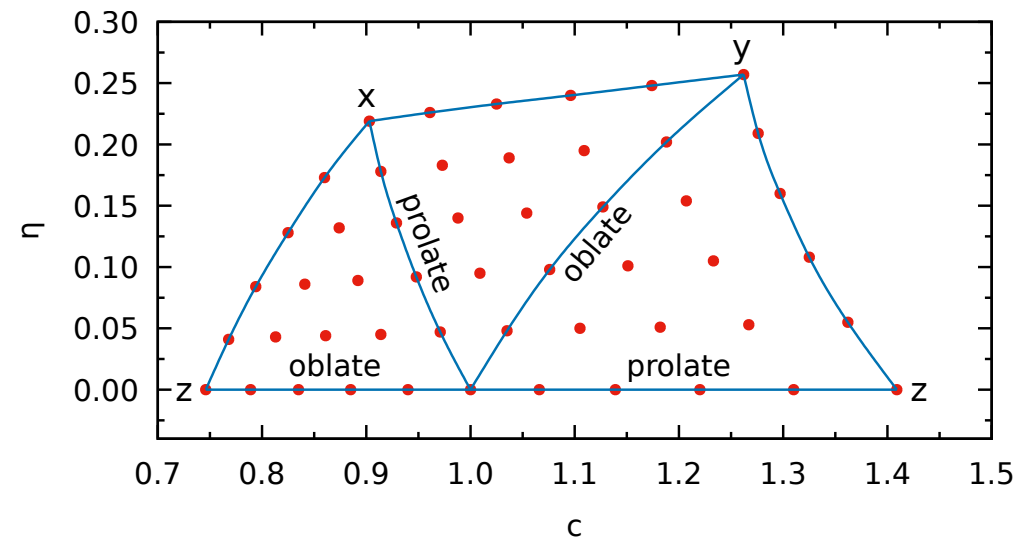
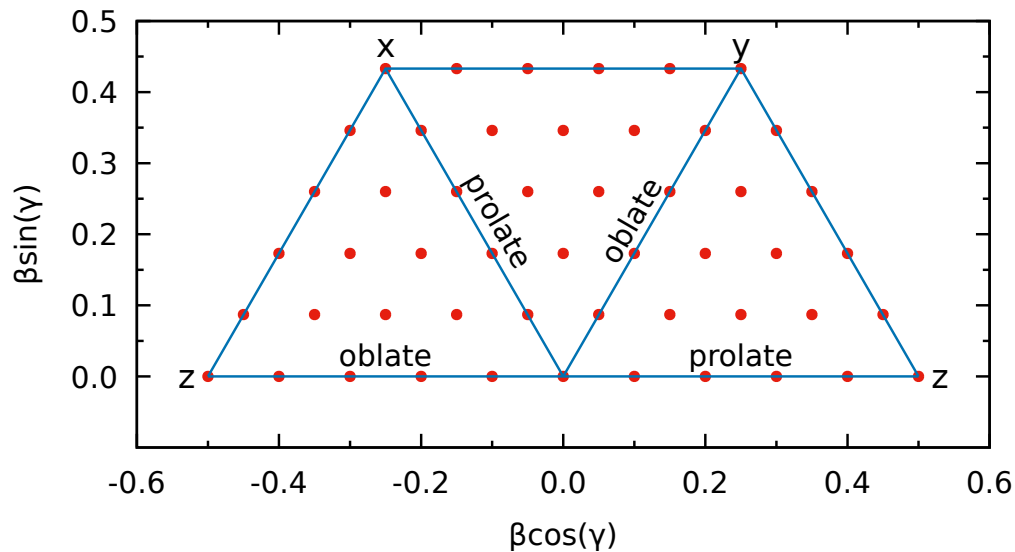
Effect of high-order deformations and of the pairing forces:



We are going to evaluate the PES of all considered nuclei in the **5D deformation parameters space**. In addition, apart from using the projected BCS formalism, we are planning together with our Chinese colleagues to use an **exact solution of the pairing eigenproblem***

*Xin Guan, Tian-Cong Wang, Wan-Qiu Jiang, Yang Su, Yong-Jing Chen, Krzysztof Pomorski, Phys. Rev. C **107**, 034307 (2023).

More detailed study of the role of nonaxial degrees of freedom



Grid in the (β, γ) plane and its projection on the (c, η) plan.

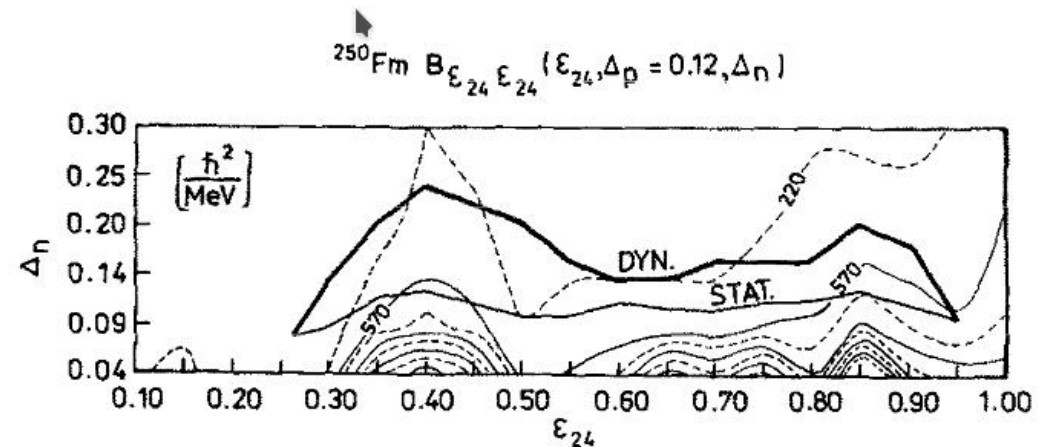
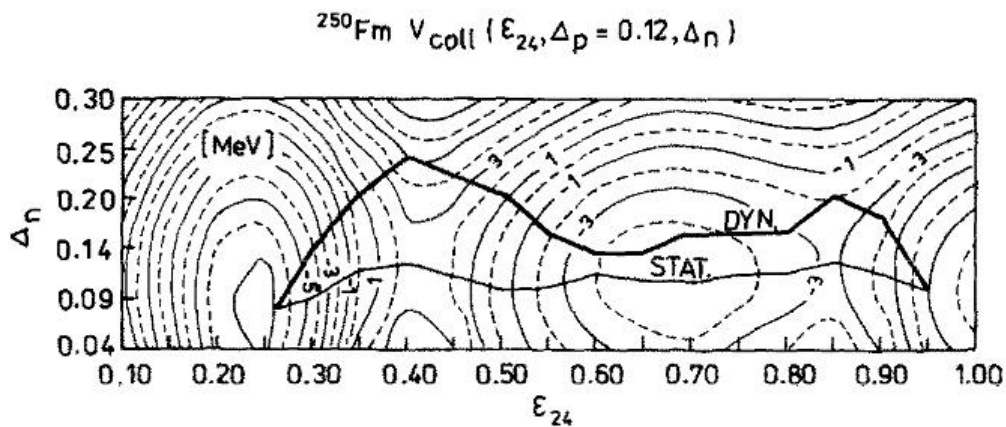
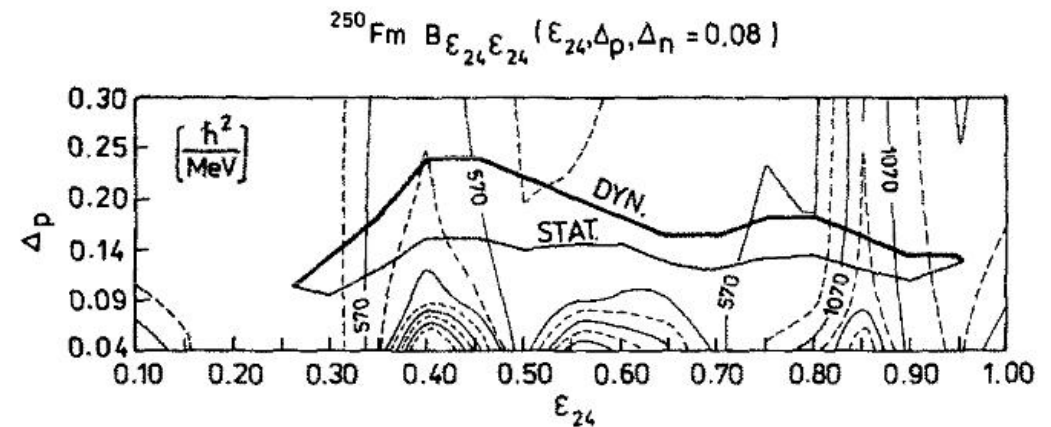
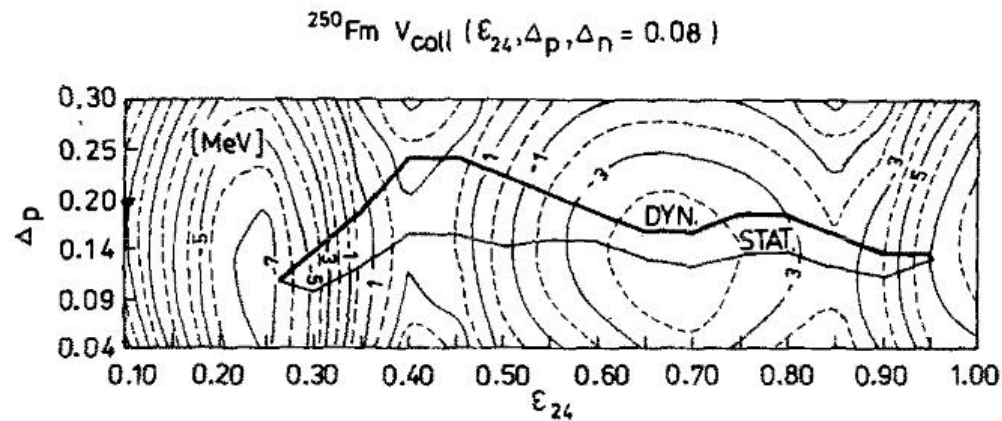
The potential energy in each 60° sector of a nucleus will be **minimized with respect to a_3 and a_4 deformations**. Then, the minimal value of the energy of each corresponding point in the three sectors will be selected. This procedure will ensure a proper energy surface in the $(0, 60^\circ)$ sector without double counting of the energies corresponding simply to **different orientations of a deformed nucleus in space**.

The proposed method is more general than the frequently used way of including higher-order deformations proposed by:

S. G. Rohoziński, A. Sobiczewski, Acta Phys. Polon. B **12**, 1001 (1981).

Dynamical treatment of the pairing correlations when evaluating T_{sf}

The **least action trajectories** corresponding to the BCS (static) and dynamical treatment of the pairing correlation*:



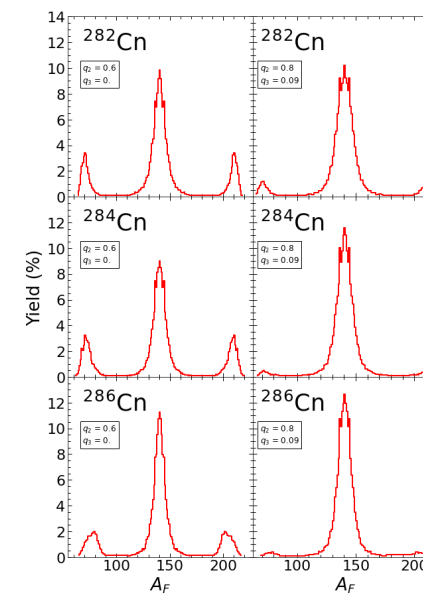
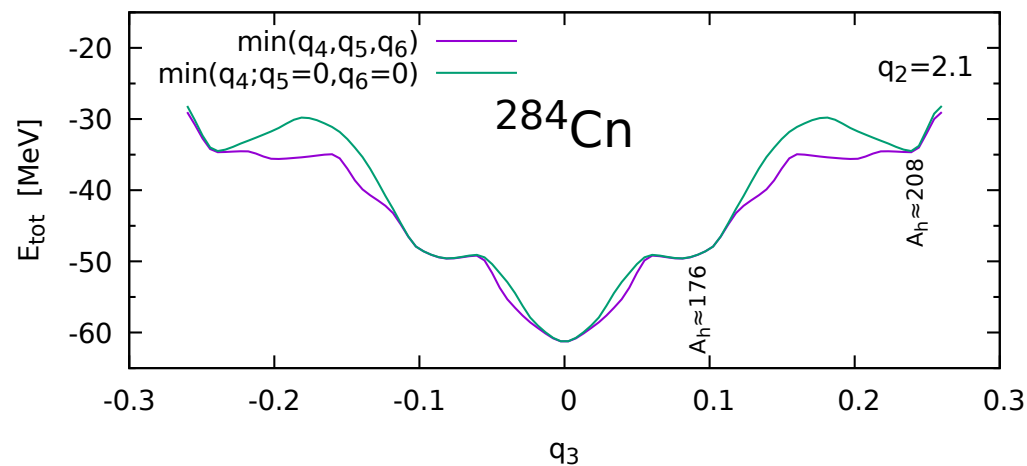
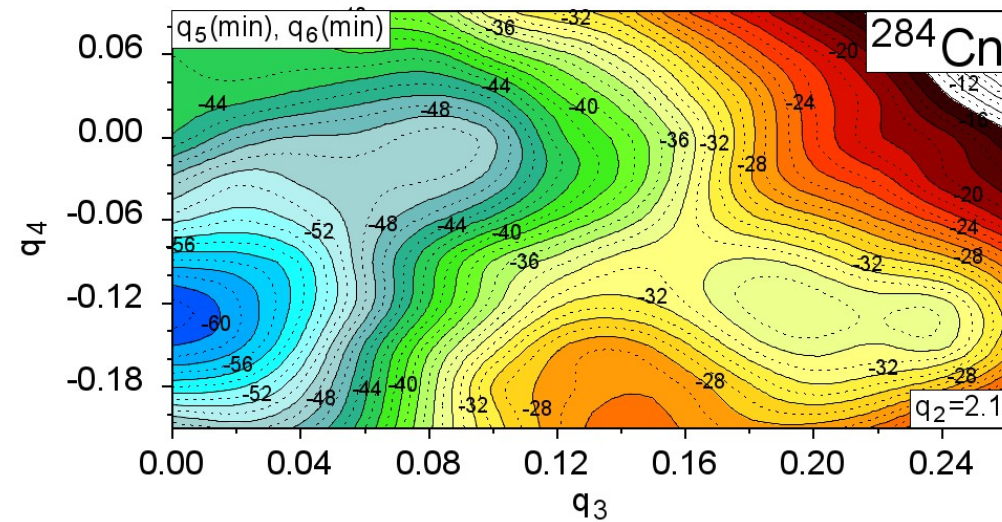
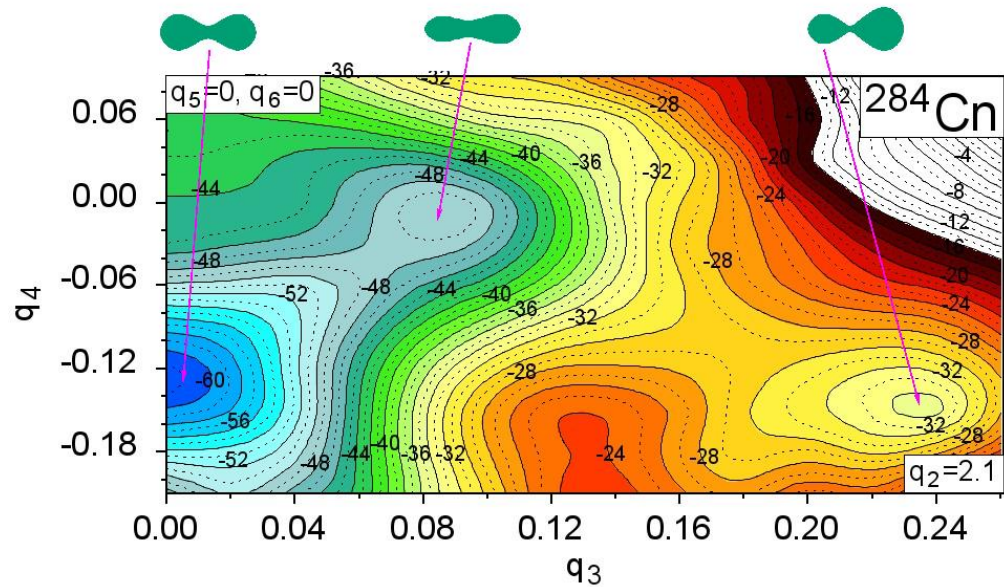
It was shown by Staszczak et al.* that the spontaneous fission lifetime evaluated along the dynamical path is a **few orders of magnitude shorter** than that corresponding to the static one.

We will perform a similar investigation but in the **6D** collective parameters space: $(c, a_3, a_4, \eta, \Delta_p, \Delta_n)$. The calculation will be done for **even-** and **odd-**A actinide nuclei.

*A. Staszczak, S. Piłat, K.P., Nucl. Phys. A **504**, 589 (1989).

Merci beaucoup pour votre attention!

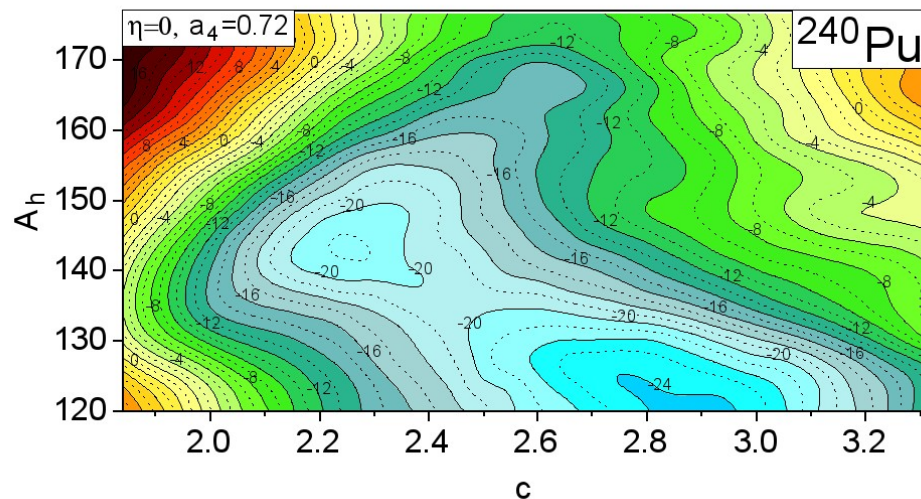
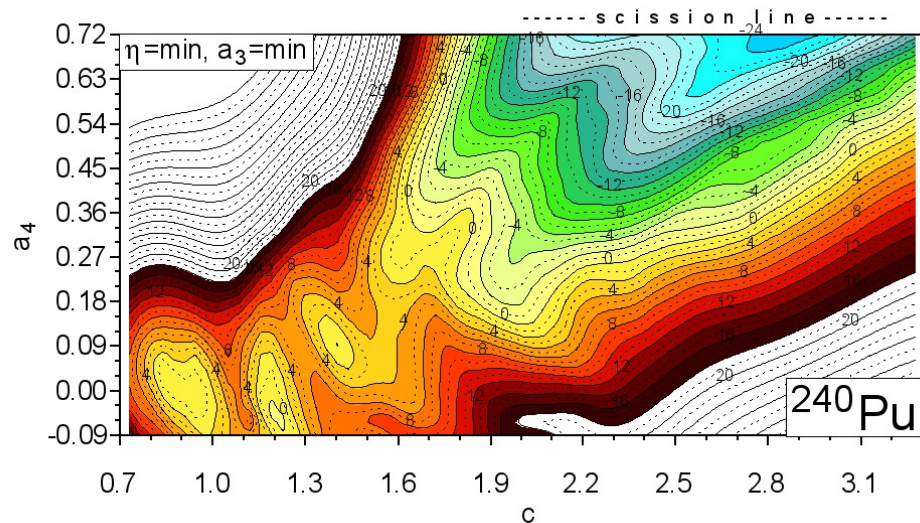
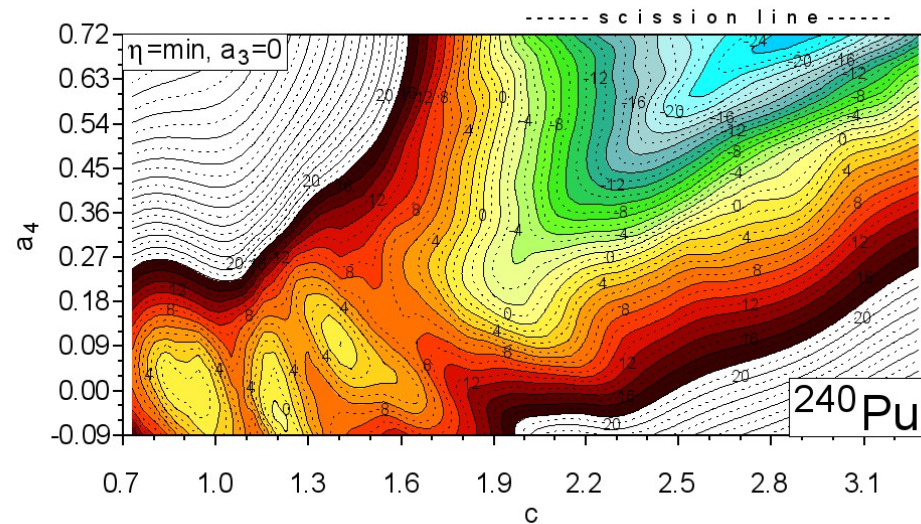
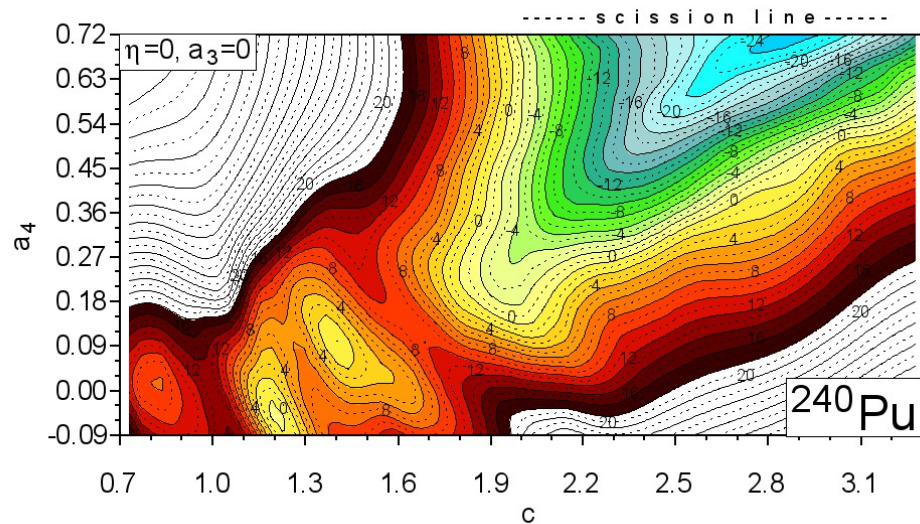
Effect of high-order deformations around the scission*



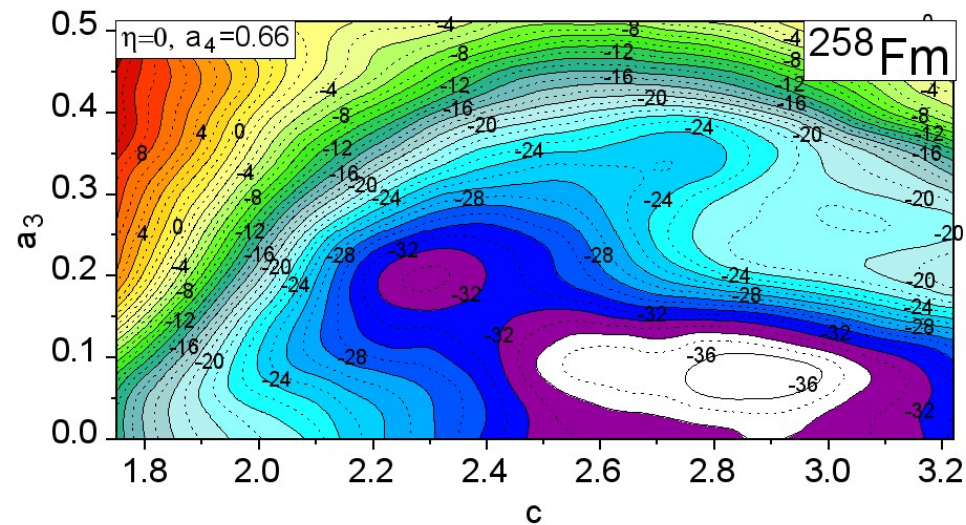
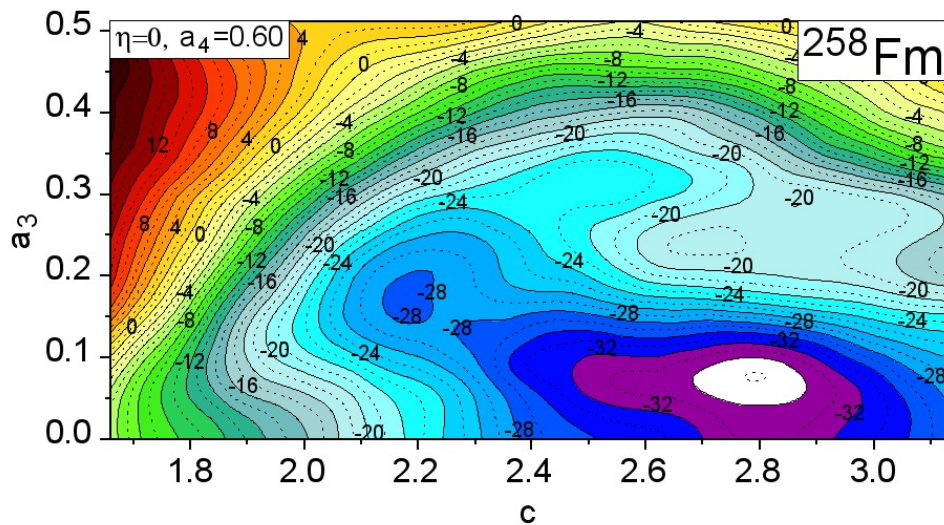
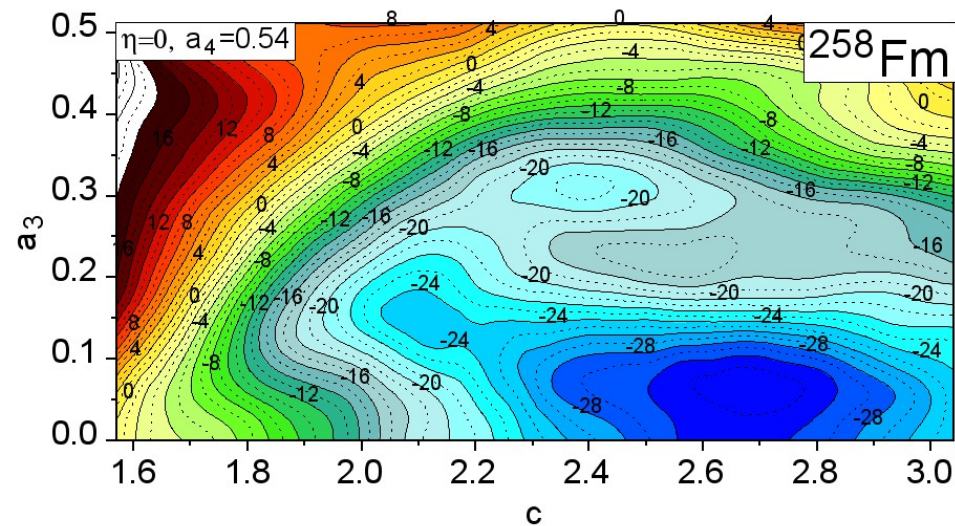
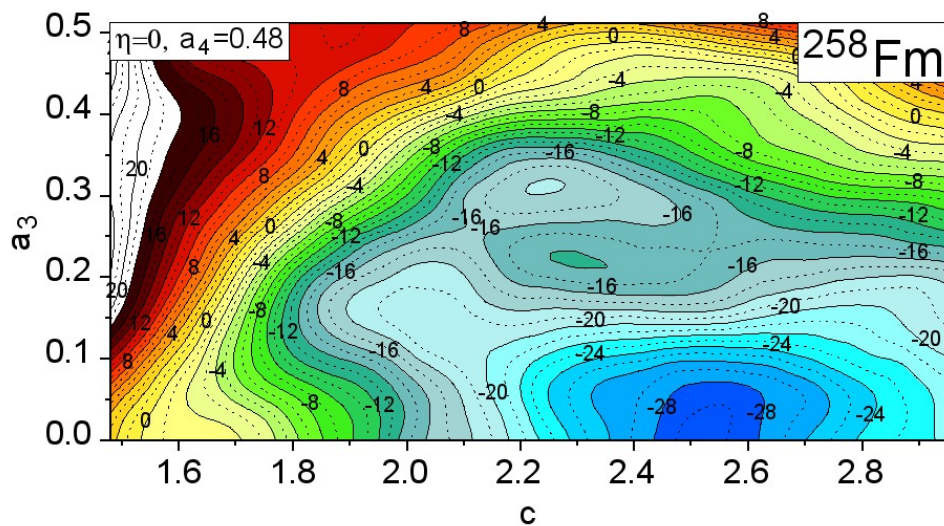
An asymmetric fission mode in some SHN with the heavy fragment mass $A \approx 208$ is predicted.

* P.V. Kostyukov, A. Dobrowolski, B. Nerlo-Pomorska, M. Warda, Z.G. Xiao, Y.J. Chen, L.L. Liu, J.L. Tian, K. P., Chin. Phys. C **45**, 124108 (2021).

Few cross-sections of the potential energy surface of ^{240}Pu



Few (c, a_3) cross-sections of the PES of ^{258}Fm

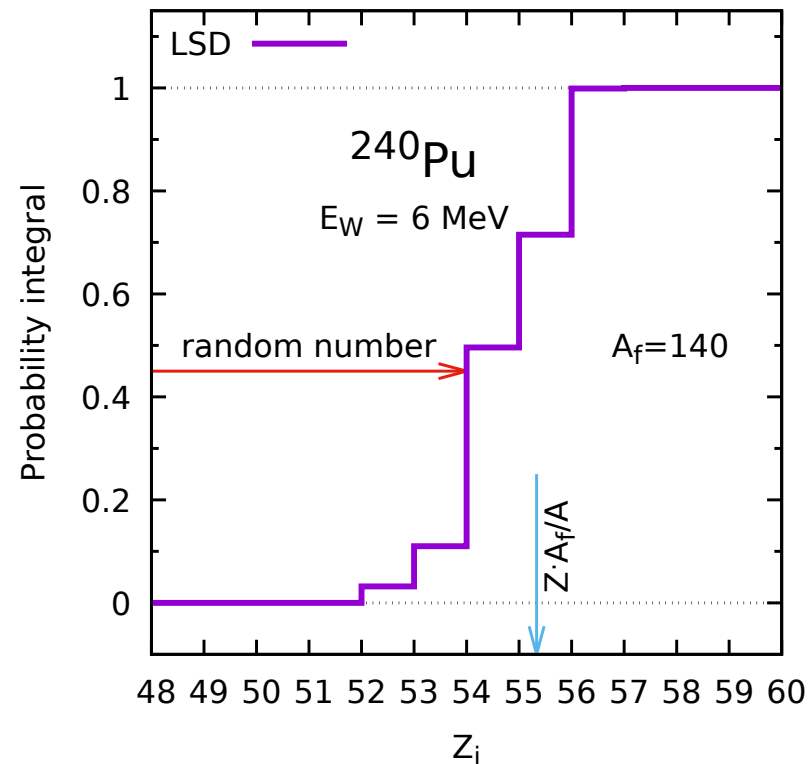
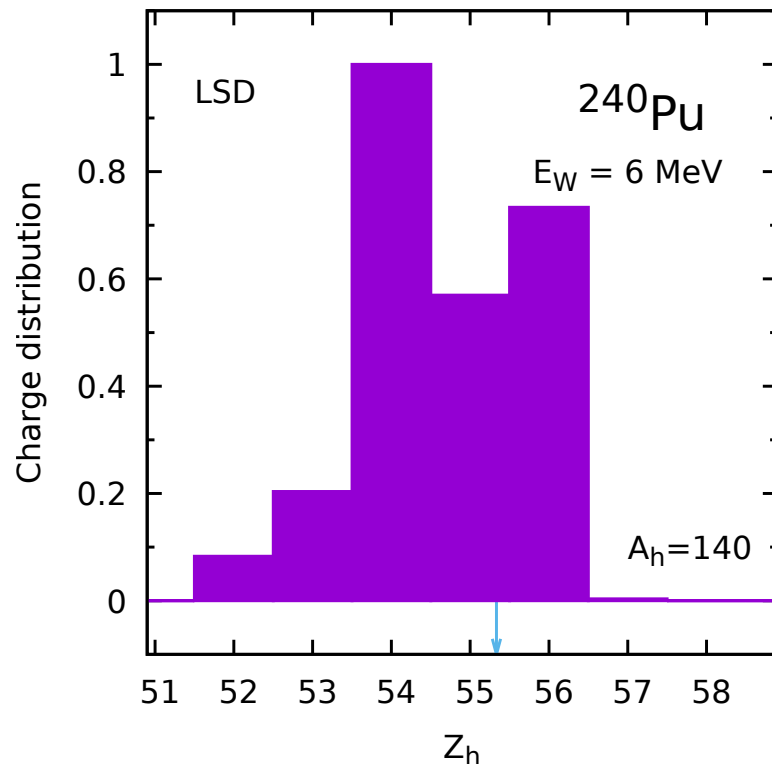


Distribution probability of the heavy-fragment charge number

The **Wigner function** corresponding to the thermal excitation E^* of the fissioning nucleus at the scission point:

$$W(Z_i) = e^{-\left(\frac{E_i - E_{\min}}{E_W}\right)^2},$$

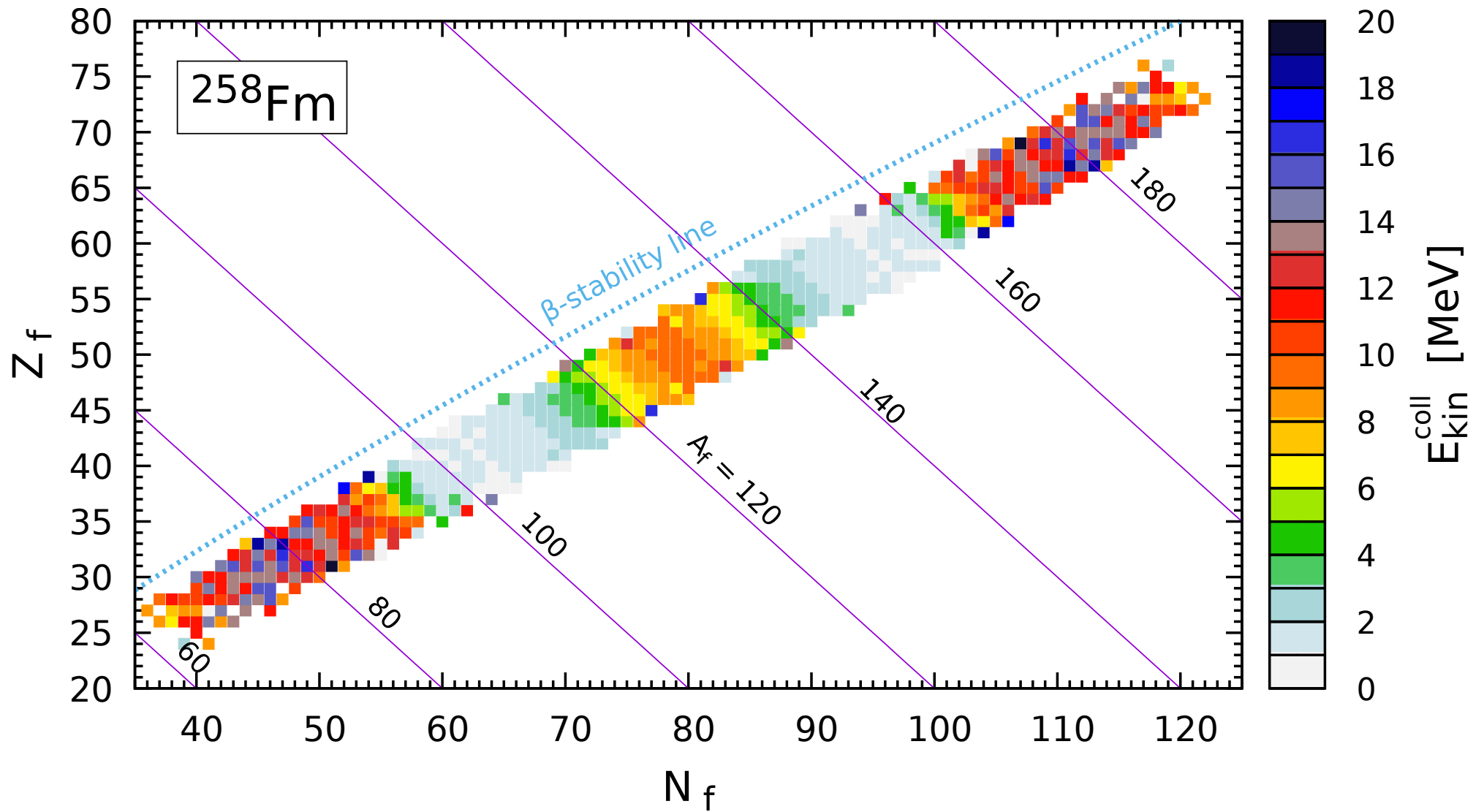
gives the **distribution probability** of the charge of the fragment:



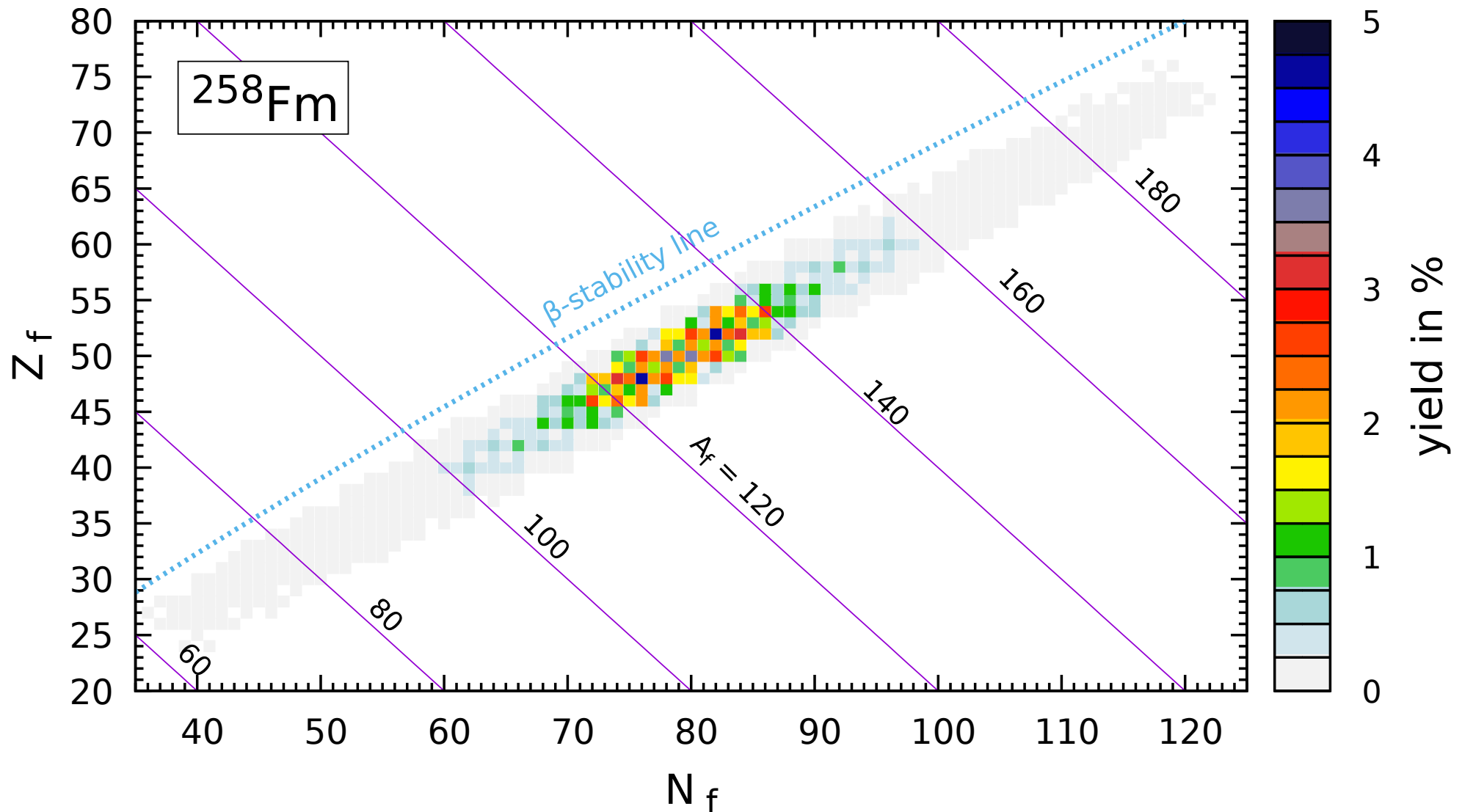
Here E_{\min} is the lowest **discrete** energy as function of Z_i and a subsequent random number decides about the charge number Z_h of the heavy fragment, with $Z_l = Z - Z_h$.

The parameter E_W is taken here around the $\hbar\omega_0$ value.

Pre-fission fragment kinetic energy of $^{258}\text{Fm}_{\text{sf}}$



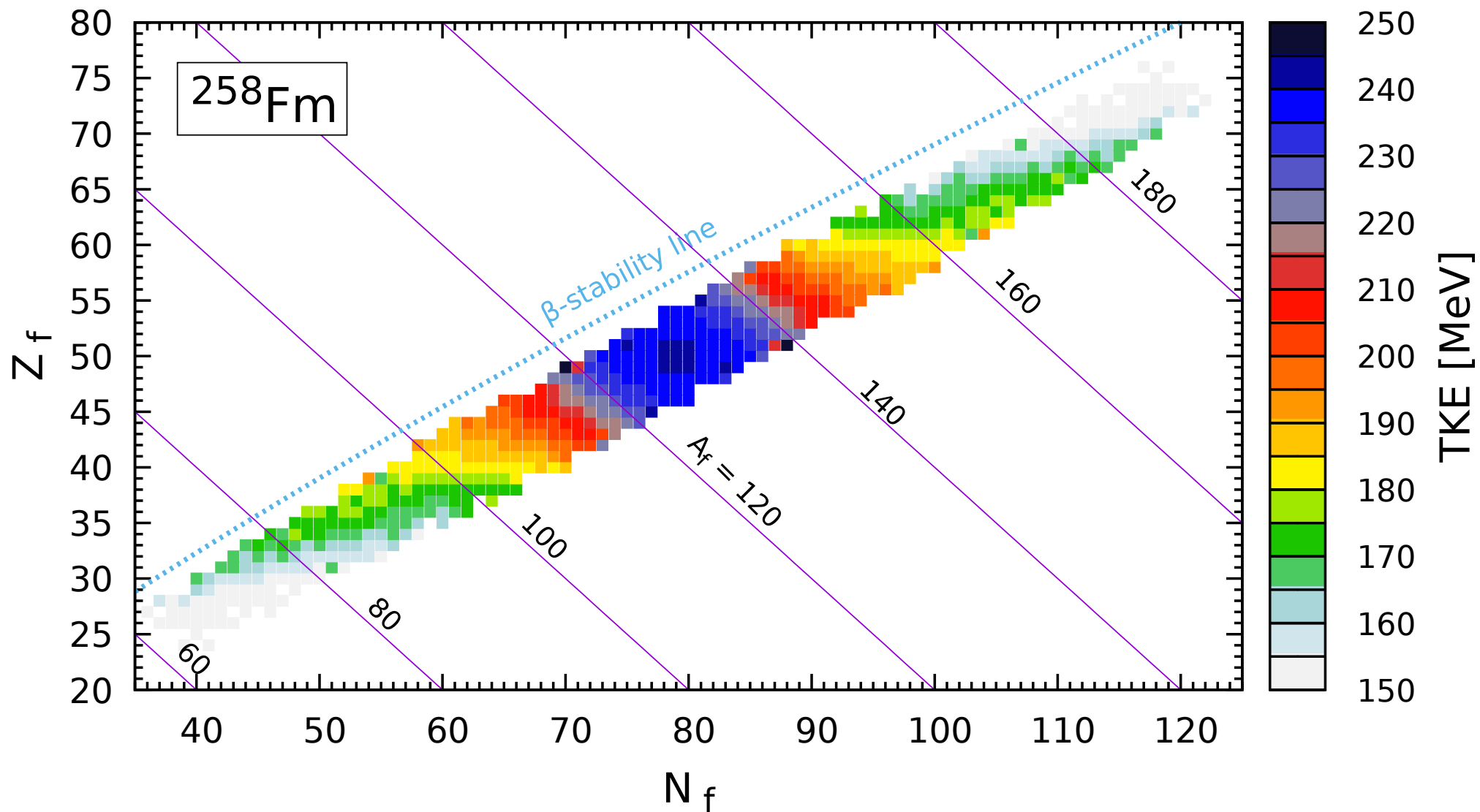
Fission fragment mass-yield of $^{258}\text{Fm}_{\text{sf}}$ *



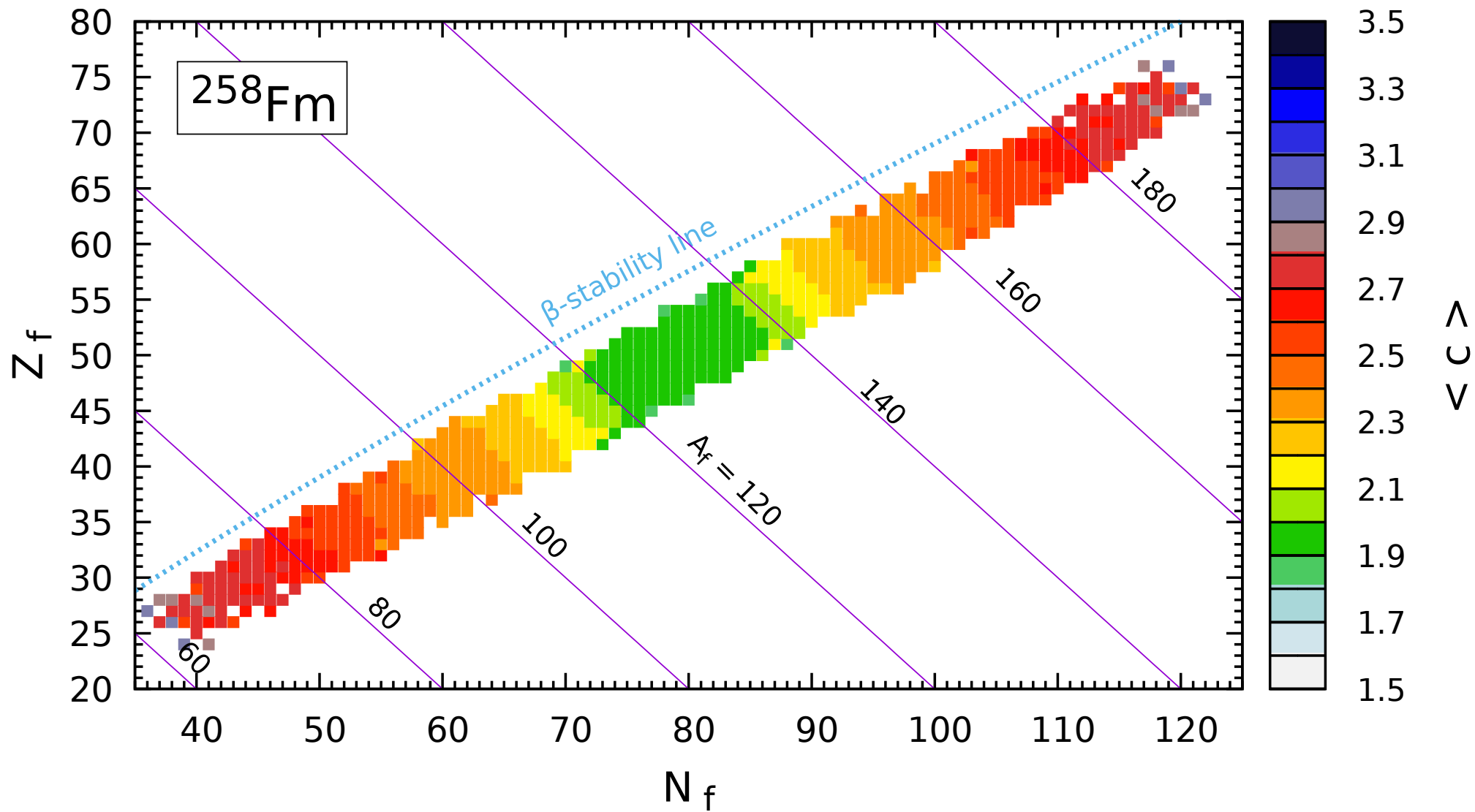
This and the following maps are made on the basis of 300k Langevin trajectories.

* K. P, A.Dobrowolski, B. Nerlo-Pomorska, M. Warda, A. Zdeb, J. Bartel, H. Molique, C. Schmitt, Z.G. Xiao, Y.J. Chen, L.L. Liu, Acta Phys. Polon. B **54** , 9-A2 (2023).

Fragment TKE of $^{258}\text{Fm}_{\text{sf}}$



Average elongation of $^{258}\text{Fm}_{\text{sf}}$ at scission



Post-fission neutron multiplicity of $^{258}\text{Fm}_{\text{sf}}$

