

Low energy nuclear fission dynamics within 3D Langevin model



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Results presented here are obtained in collaboration with:

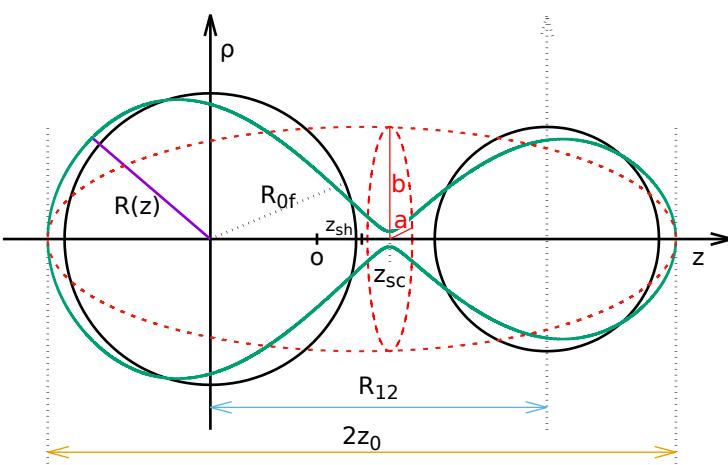
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J. Bartel, H. Molique, C. Schmitt .

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Program:

- Fourier over Spheroid parametrization of fissioning nuclei shapes,
- Choosing of an appropriate grid for the Potential Energy Surface calculation,
- Some examples of the 4D macroscopic-microscopic PES's,
- Mass and Total Kinetic Energy of fragments obtained within the 3D Langevin dissipative dynamics for $^{236}\text{U}_{\text{th}}$,
- Charge equilibration mode at scission configuration,
- Neutron emission from the fragments,
- Transition from the asymmetric to the compact-symmetric fission in Fermium isotopes,
- Fission yields of ^{250}Cf at $E^*=46$ MeV,
- On existence of a very asymmetric mode in fission of SH nuclei,
- Summary.

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 **reflectational 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

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

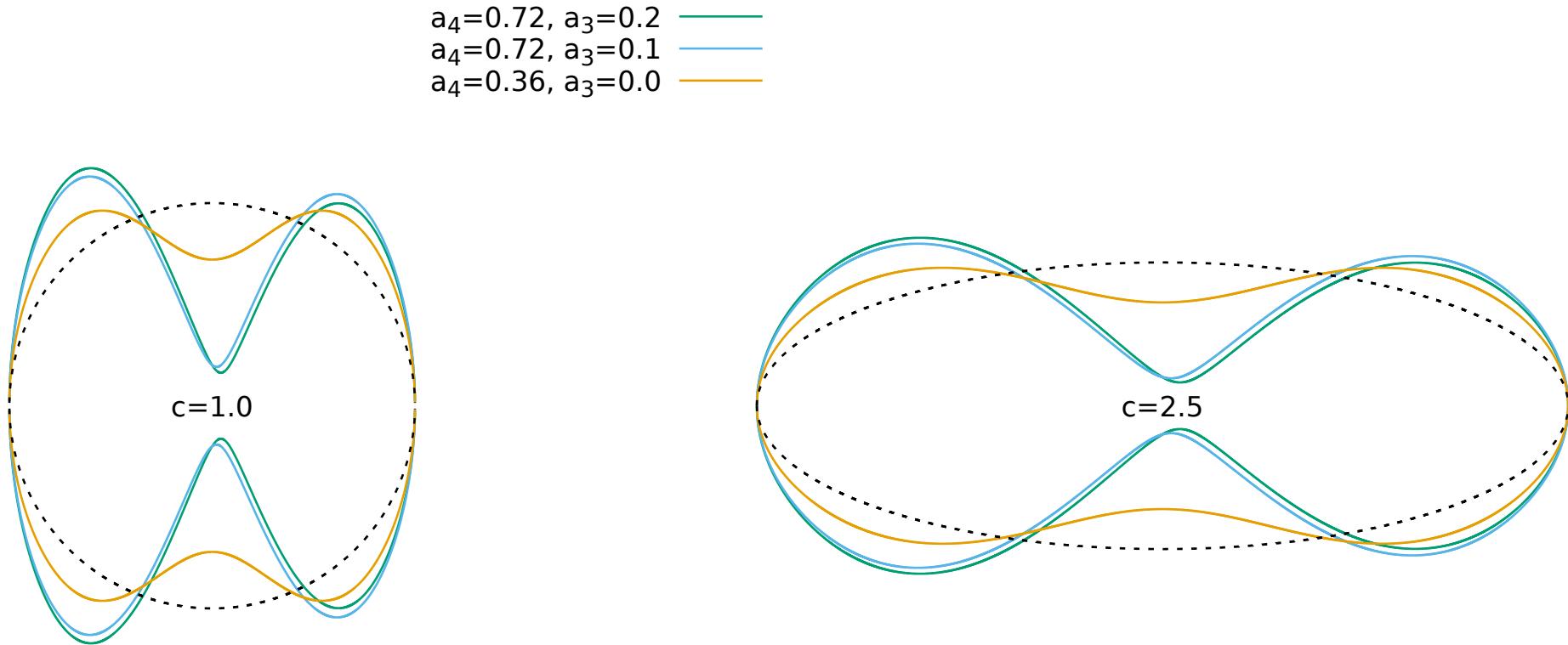
places the nuclear **center of mass** at the origin of the coordinate system.

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, Acta Phys. Pol. B Sup. **16**, 4-A21 (2023).

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

Effect of the stretching in z -direction

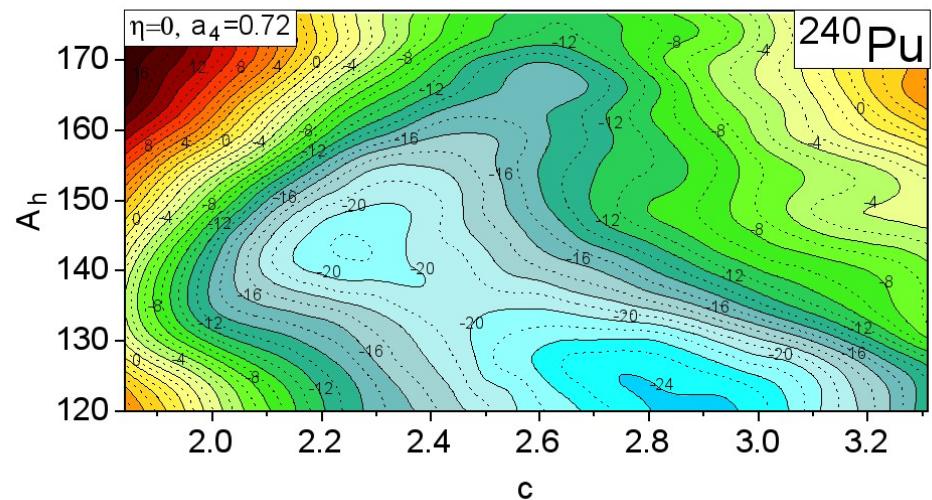
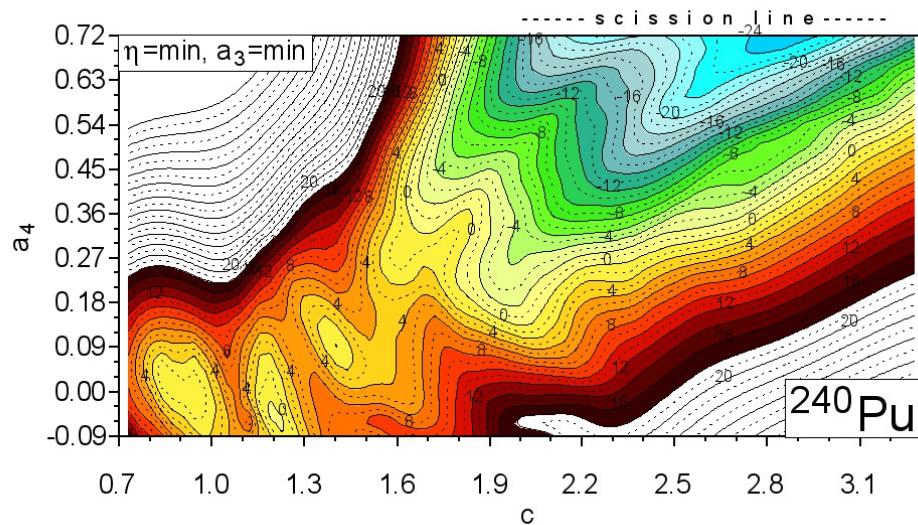
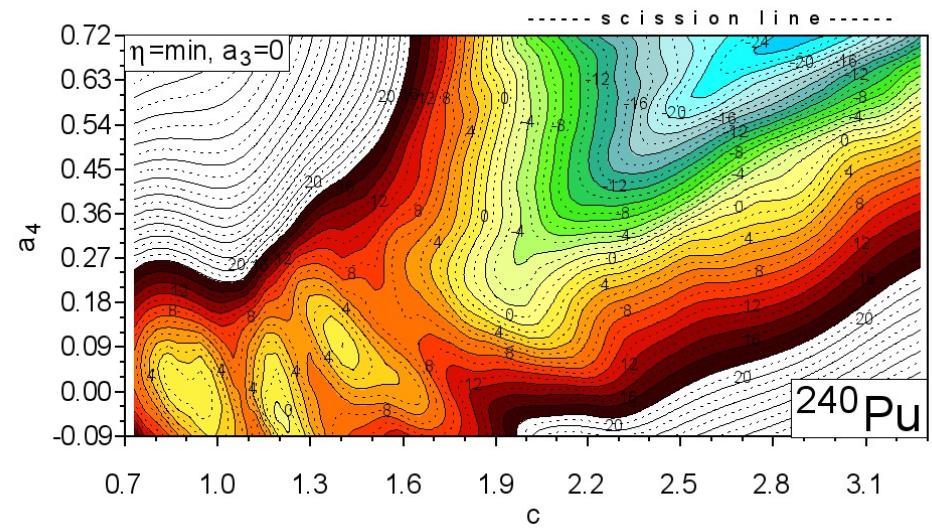
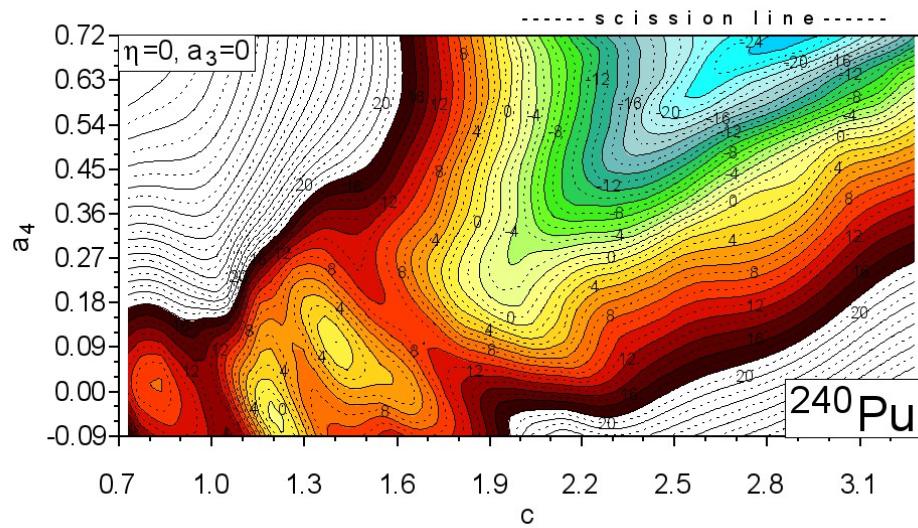


The both figures show the shapes obtained with the same Fourier expansion series but for two different elongations c .

Note: the expansion coefficients a_i are independent on the elongation c , what facilitates an appropriate grid construction in the deformation parameter space.

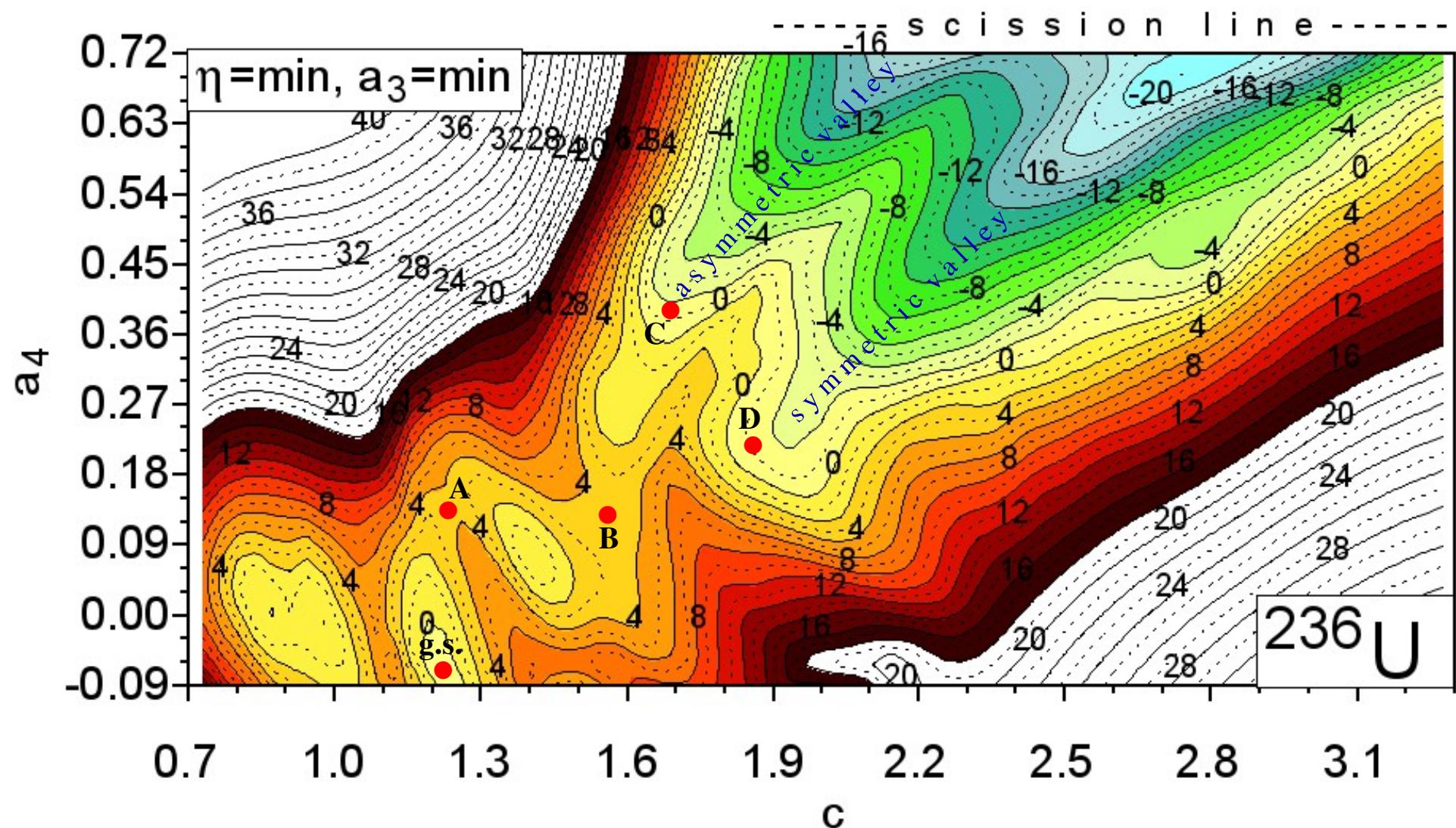
Extensive macroscopic-microscopic calculations of the PES's in the 4D space $\{\eta, c, a_3, a_4\}$ are performed for even-even nuclei with $90 \leq Z \leq 122$.

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



Potential energies of even-even actinide and SH nuclei are evaluated within the **macro-micro** method using the **LSD** formula for the macroscopic part of energy, while the microscopic one is obtained using the **Yukawa-folded** mean-field potential and the **Strutinsky** and the **BCS** methods. The mass of the heavy fragment is $A_h \approx \frac{A}{2}(1 + 1.01 a_3)$, independently on c value.

Potential energy surface of ^{236}U



Langevin and Master equations are used to 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:

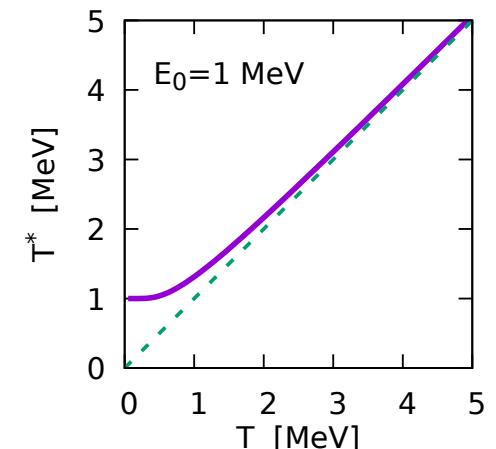
$$\begin{aligned}\frac{dq_i}{dt} &= \sum_j [\mathcal{M}^{-1}(\vec{q})]_{ij} p_j && \text{friction and random forces} \\ \frac{dp_i}{dt} &= -\frac{1}{2} \sum_{j,k} \frac{\partial[\mathcal{M}^{-1}(\vec{q})]_{jk}}{\partial q_i} p_j p_k - \frac{\partial V(\vec{q})}{\partial q_i} - \sum_{j,k} \gamma_{ij}(\vec{q}) [\mathcal{M}^{-1}(\vec{q})]_{jk} p_k + F_i(t) ,\end{aligned}$$

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**:

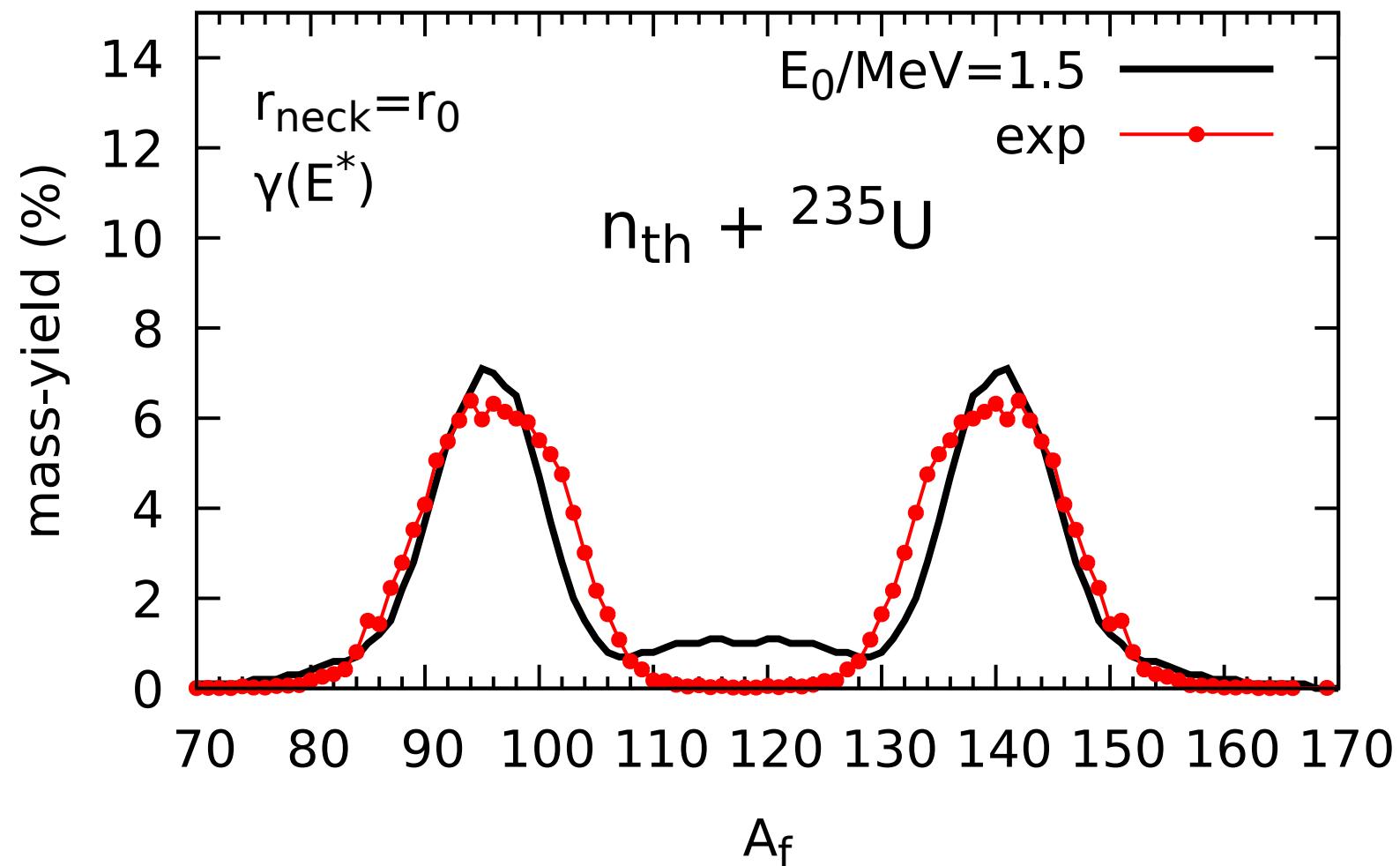
$$\mathcal{D}_{ij} = T^* \gamma_{ij} = \sum_k g_{ik} g_{jk} .$$



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-yield obtained by the 3D Langevin calculation*



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

Kinetic energy of the fission fragments

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}):

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

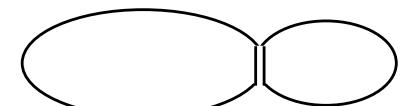
The Coulomb repulsion energy is equal to the difference between the total Coulomb energy of the nucleus at the scission configuration and the Coulomb energies of the both deformed fragments:

$$E_{\text{Coul}}^{\text{rep}} = \frac{3e^2}{5r_0} \left[\frac{Z^2}{A^{1/3}} B_{\text{Coul}}(\text{def}_{\text{sc}}) - \frac{Z_1^2}{A_1^{1/3}} B_{\text{Coul}}(\text{def}_1) - \frac{Z_2^2}{A_2^{1/3}} B_{\text{Coul}}(\text{def}_2) \right] .$$

It is a more accurate estimate of the Coulomb energy than the frequently used **point-to-point** (p-p) approximation: $E_{\text{Coul}}^{\text{p-p}} = e^2 Z_1 Z_2 / R_{12}$, where R_{12} is the distance between the fragment mass-centers, e the elementary charge, and r_0 the charge-radius constant.

The nuclear interaction energy between the fragments at the scission point is approximately equal to the change of the nuclear surface energy when the neck breaks:

$$V_{\text{nuc}}(q_{\text{sc}}) = -2 \times E_{\text{surf}}(\text{sph}) \frac{\pi r_n^2(\text{sc})}{4\pi R_0^2} = -\frac{1}{2} E_{\text{surf}}(\text{sph}) \left(\frac{r_n}{R_0} \right)^2 .$$



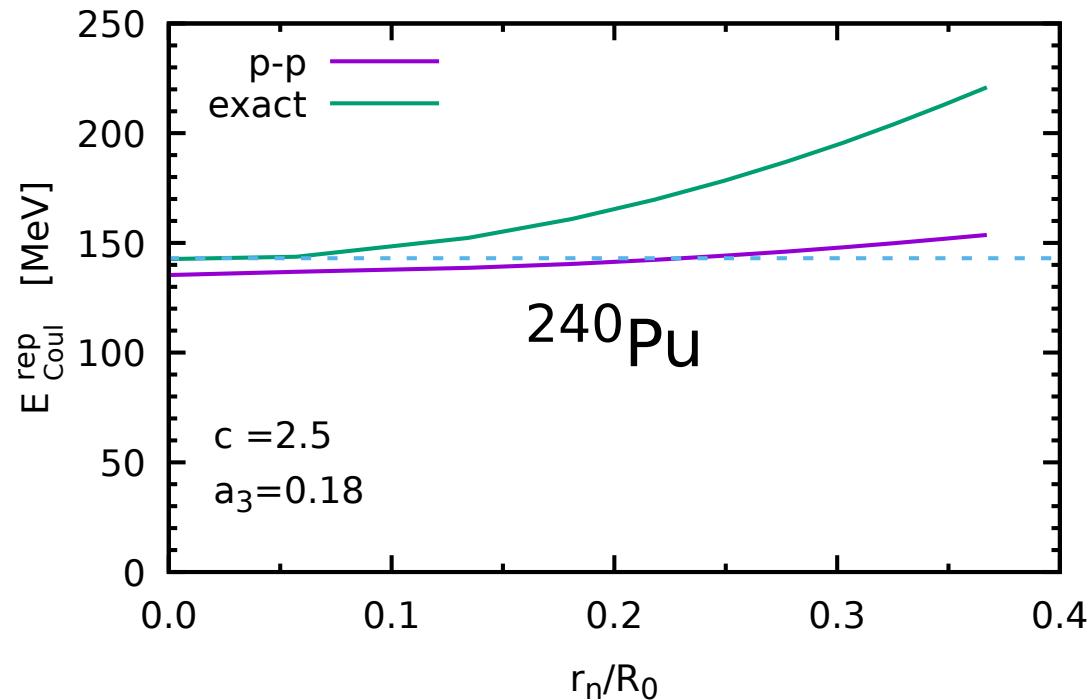
Here $E_{\text{surf}}(\text{sph}) = b_{\text{surf}} A^{2/3}$, where b_{surf} is the **surface tension** LD coefficient.

For the neck-radius $r_n = r_0$ and the nucleus radius $R_0 = r_0 A^{1/3}$ one obtains:

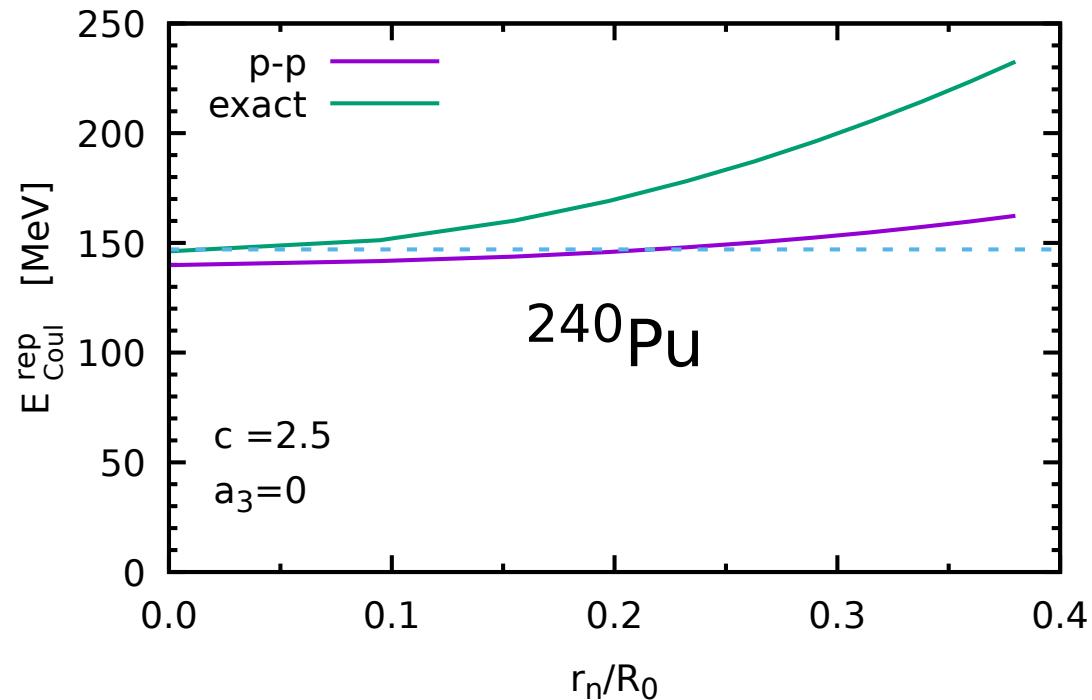
$$V_{\text{nuc}}(q_{\text{sc}}) = -\frac{1}{2} b_{\text{surf}} , \quad \text{i.e.,} \quad V_{\text{nuc}}(q_{\text{sc}}) \approx -9 \text{ MeV} .$$

Usually one evaluates this quantity by a folding integral of the nucleon-nucleon interaction with the density distribution of the both fragments, what is rather complicate.

Exact and p-p Coulomb repulsion energy at near scission configuration



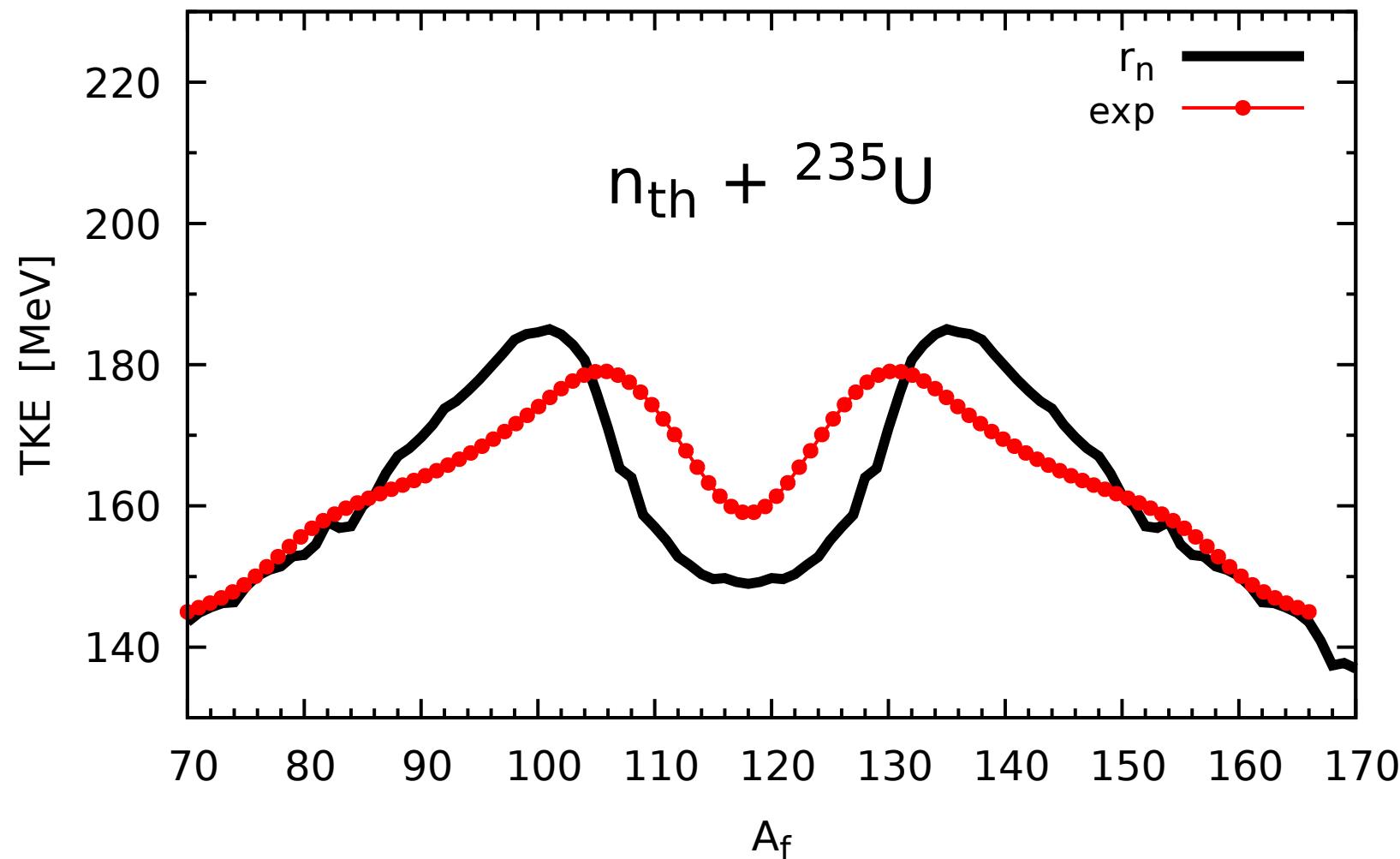
asymmetric fission



symmetric fission

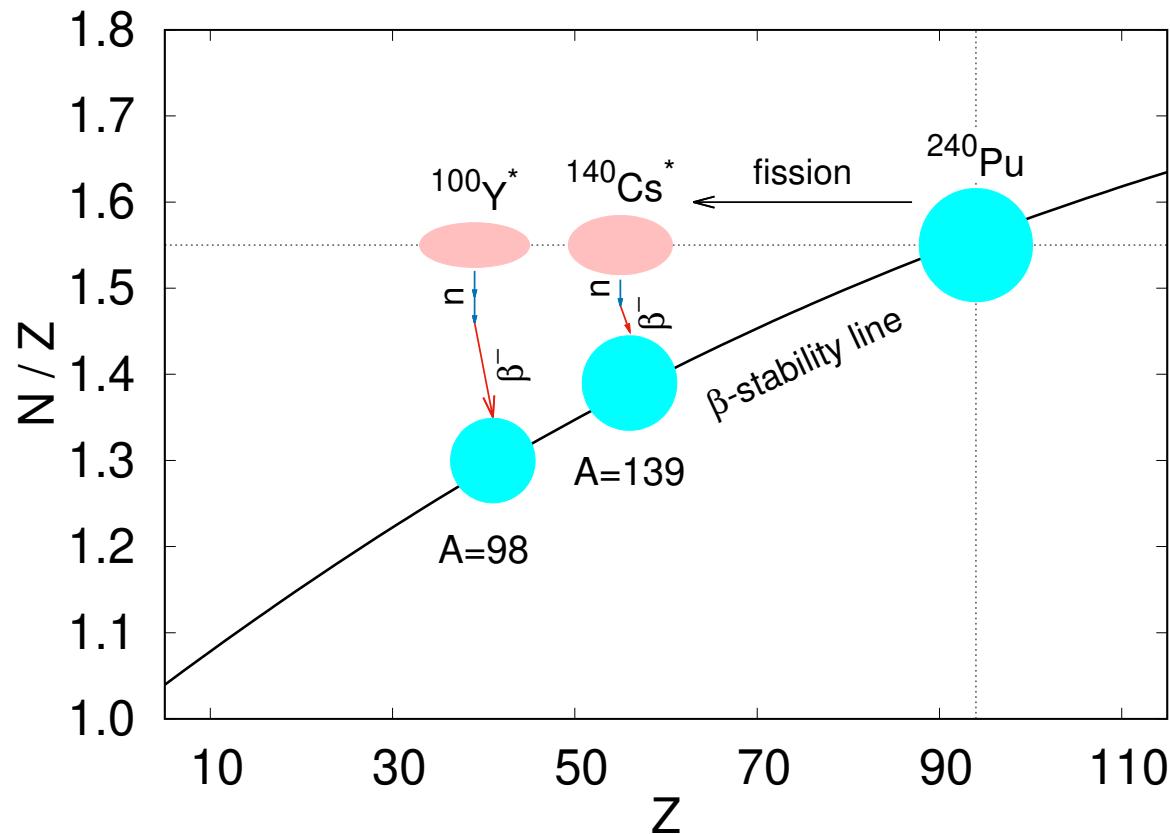
Note: the nuclear interaction energy $V_{\text{nuc}} \approx -9$ MeV for the neck radius equal to the nucleon radius $r_n \approx 0.16 R_0$ has to be subtracted from $E_{\text{Coul}}^{\text{rep}}$, while for the alpha-particle radius is $r_n = r_\alpha \approx 0.26 R_0$ this energy is around -23 MeV.

Example of TKE-yield obtained by the 3D Langevin calculation*



* 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

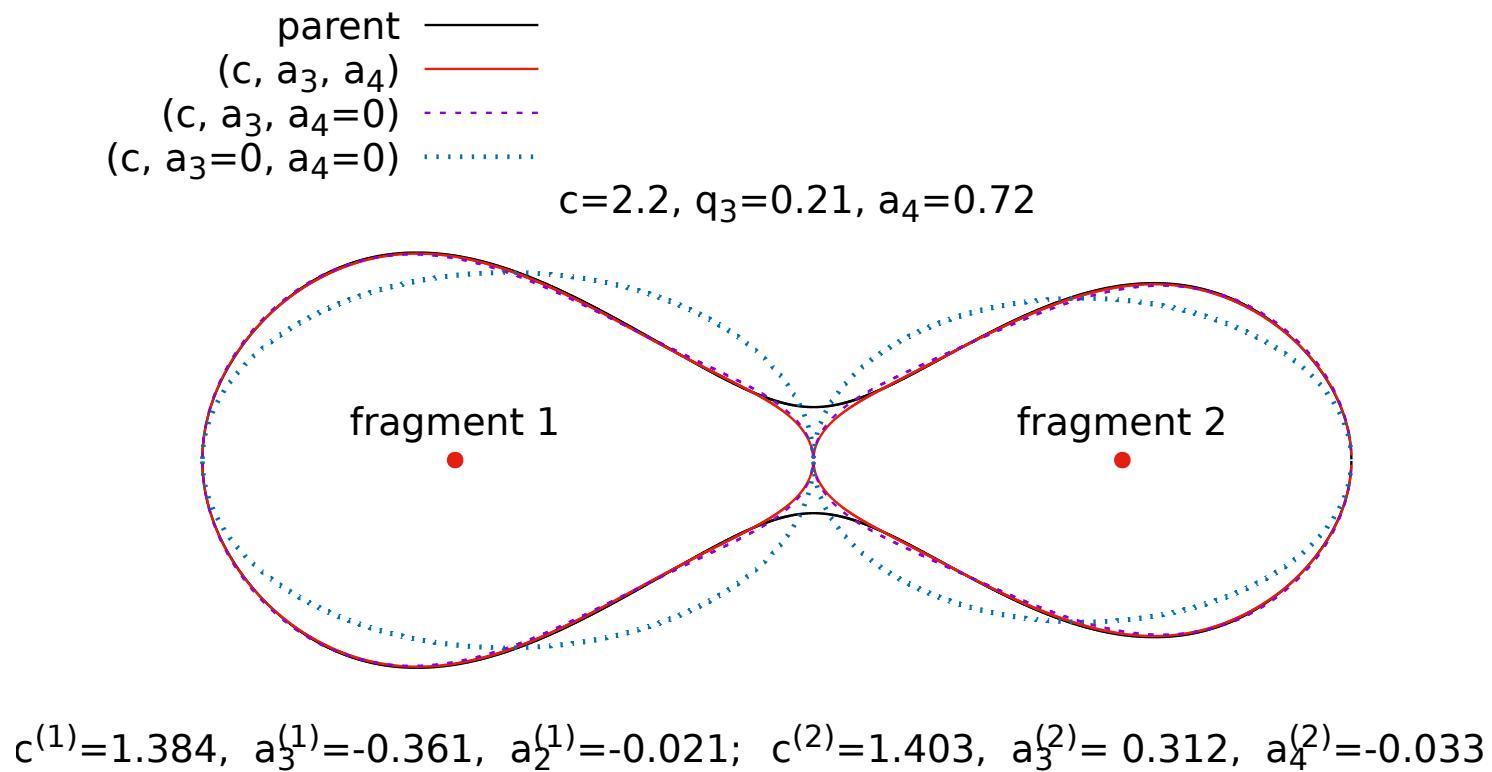


The maximal energy of a neutron emitted from a fragment (mother) can be obtained from the **energy conservation law**:

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

where M_M , M_D , M_n are respectively the **mass excesses** of mother and daughter nuclei, and of 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



The fission fragments have frequently a **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.

Neutron emission from the fission fragments

One assumes that the thermal energy of a fragment E_i^* in the scission point is proportional to its single-particle level density parameter $a(Z, A; \text{def})$:

$$\frac{E_1^*}{E_2^*} = \frac{a(Z_1, A_1; \text{def}_1)}{a(Z_2, A_2; \text{def}_2)} \quad \text{and} \quad E^* = a(Z, A; \text{def})T^2 = E_1^* + E_2^* .$$

The deformation energy of each fragment can be evaluated in the LD model:

$$E_{\text{def}}^{(i)} \approx E_{\text{LD}}(Z_i, A_i, \text{def}_i) - E_{\text{exp}}(Z_i, A_i, \text{g.s.}) .$$

The total excitation energy of fragment i is then the sum of its thermal and deformation energy:

$$E_{\text{exc}}^{(i)} = E_{\text{def}}^{(i)} + E_i^* .$$

This energy is converted into heat due to the presence of the friction force, which allows to evaluate the effective temperature T_i of each fragment:

$$E_{\text{exc}}^{(i)} = a(Z_i, A_i; \text{def}_i) T_i^2 ,$$

where i stays for light (l) or heavy (h) fragment. These estimates allow us to evaluate the number of neutrons emitted from each fragment.

Neutron emission width according to Weisskopf *

$$\Gamma_n(\epsilon_n) = \frac{2\mu}{\pi^2 \hbar^2 \rho_M(E_M^*)} \int_0^{\epsilon_n} \sigma_{inv}(\epsilon) \epsilon \rho_D(E_D^*) d\epsilon .$$

Here μ is the reduced mass of the neutron, σ_{inv} is the **neutron inverse cross-section**[†]:

$$\sigma_{inv}(\epsilon) = \left[0.76 + 1.93/A^{1/3} + \frac{1.66/A^{2/3} - 0.050}{\epsilon} \right] \pi (1.70A^{1/3})^2 ,$$

while ρ_M and ρ_D are respectively the **level densities** of mother and daughter nucleus:

$$\rho(E) = \frac{\sqrt{\pi}}{12a^{1/4}E^{5/4}} \exp(2\sqrt{aE}) ,$$

where a is the single-particle **level-density parameter**[‡]:

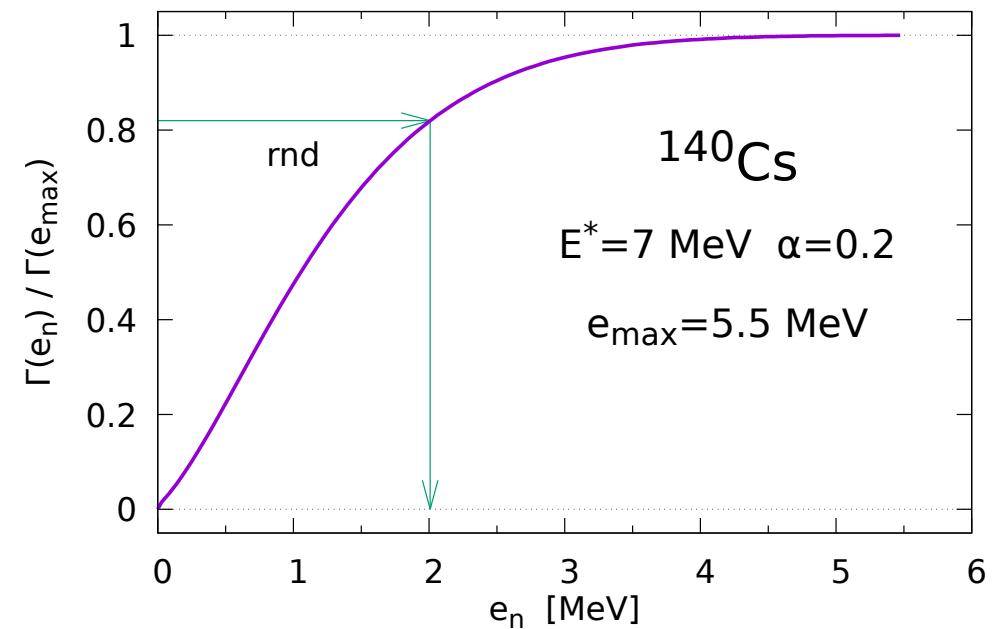
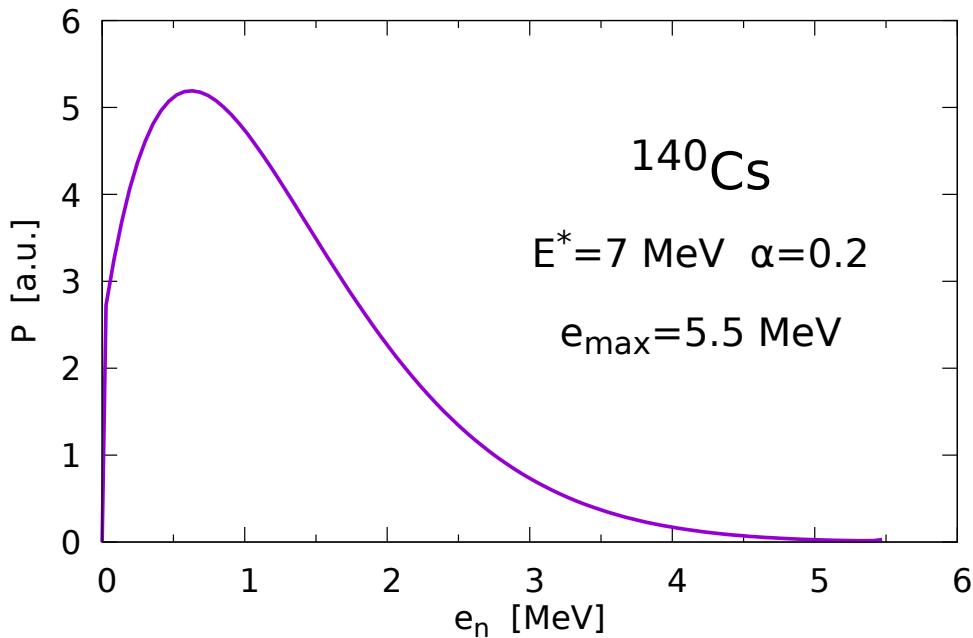
$$a(Z, A) \cdot \text{MeV} = 0.0126(1 - 6.275 I^2)A + 0.3804(1 - 1.101 I^2)A^{2/3} + 0.00014 \frac{Z^2}{A^{1/3}}$$

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

†I. Dostrovsky, Z. Fraenkel, G. Friedlander, Phys. Rev. C **21**, 1261 (1980).

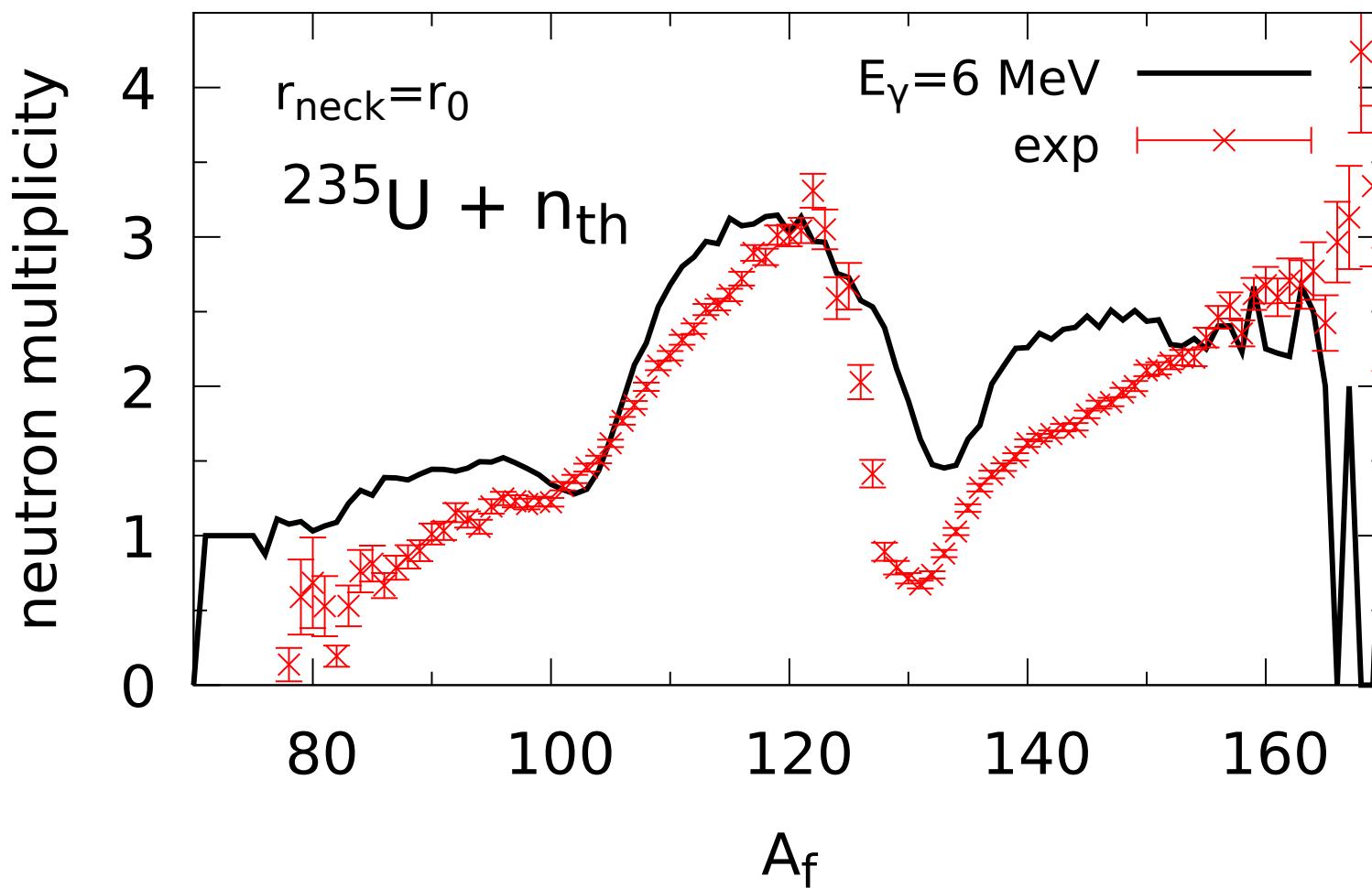
‡B. Nerlo-Pomorska, K. P., J. Bartel, K. Dietrich, Phys. Rev. C **67**, 051302 (2002).

Distribution probability of the neutron energy:



The **random number** (rnd) related to the distribution probability (l.h.s.) allows to chose the **kinetic energy** of the emitted neutron (r.h.s.).

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).

On the charge equilibration at scission

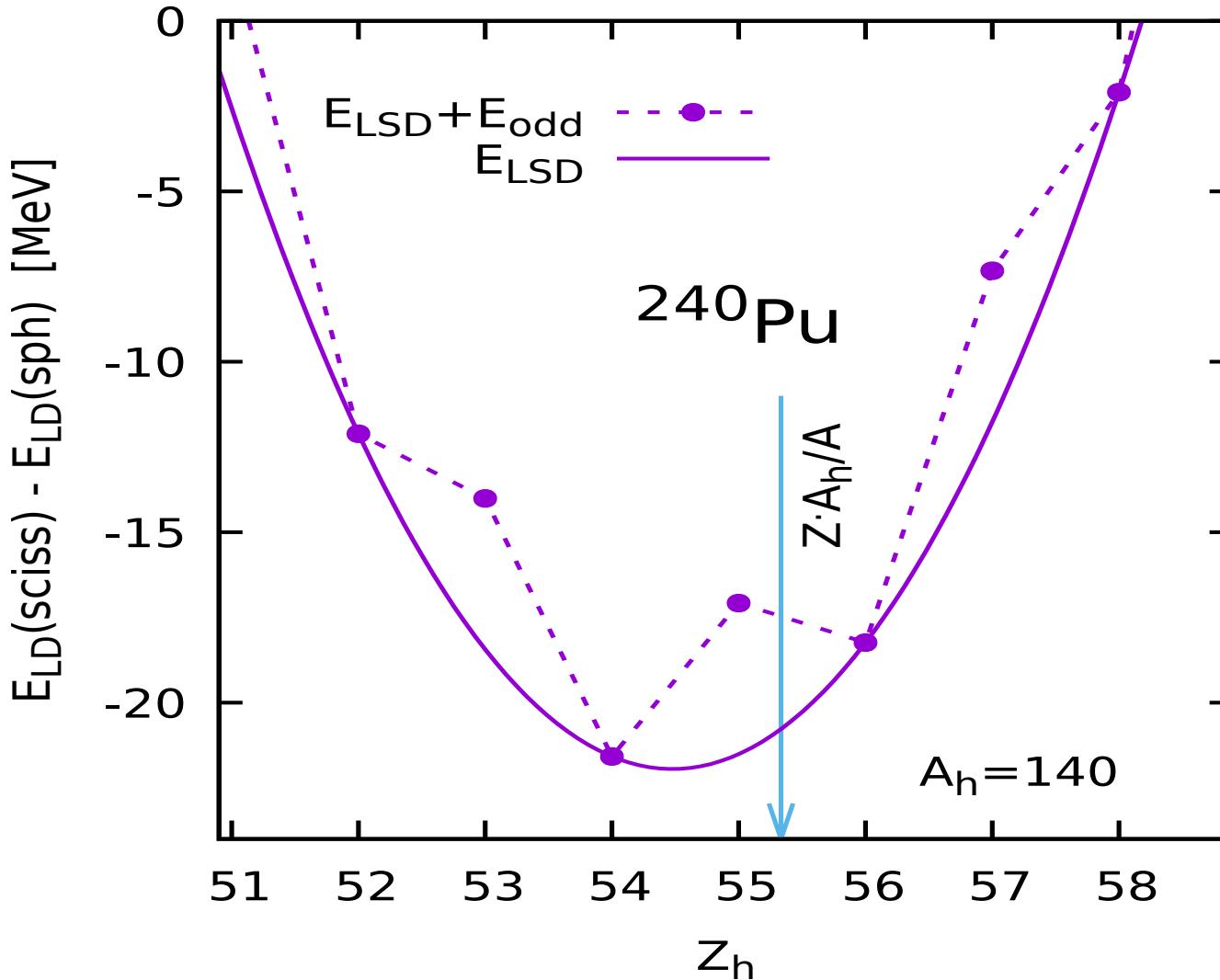
Knowing the fragment deformation at scission, it is relatively easy to find the preferred charge for each fragment. Usually one assumes that the isospin of a fragment is the same as the one of the fissioning nucleus. One obtains a better estimate looking for the proton and neutron microscopic distribution.

A simple estimate of the proton-neutron equilibrium 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:

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

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 $A_h = A \cdot B_f(\text{def}_{sc})$ 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 as a function of the fragment charge number



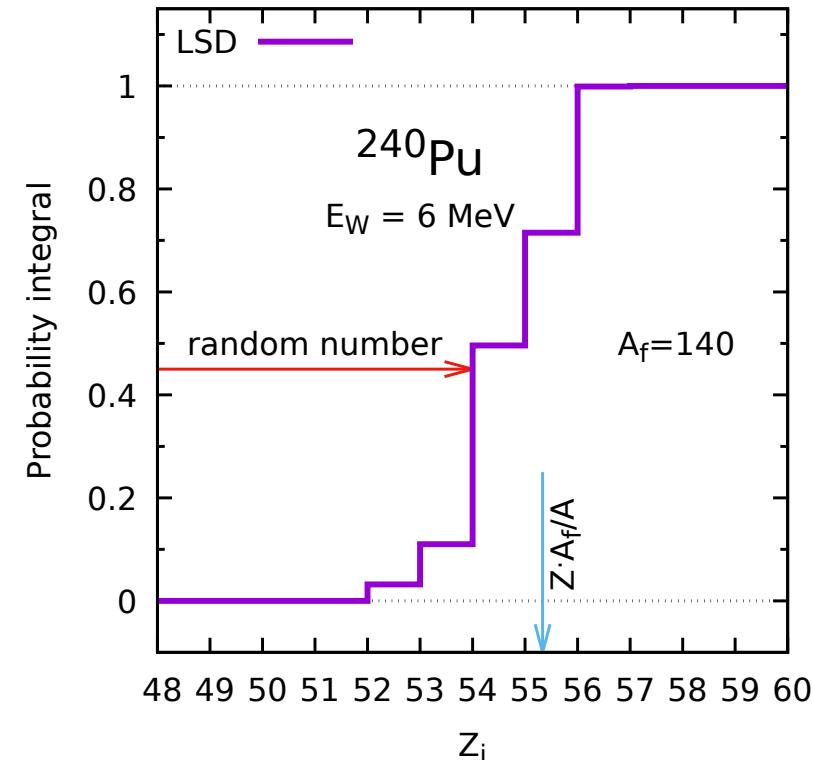
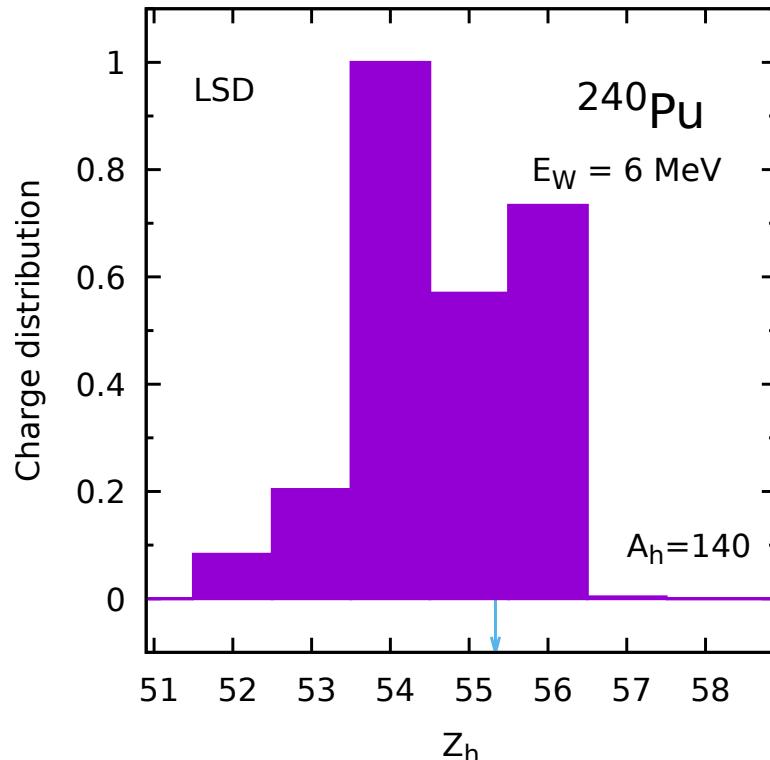
The above effect has to be taken into account at the end of each Langevin trajectory, when one fixes the (**integer**) fragment mass and charge numbers.

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:

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

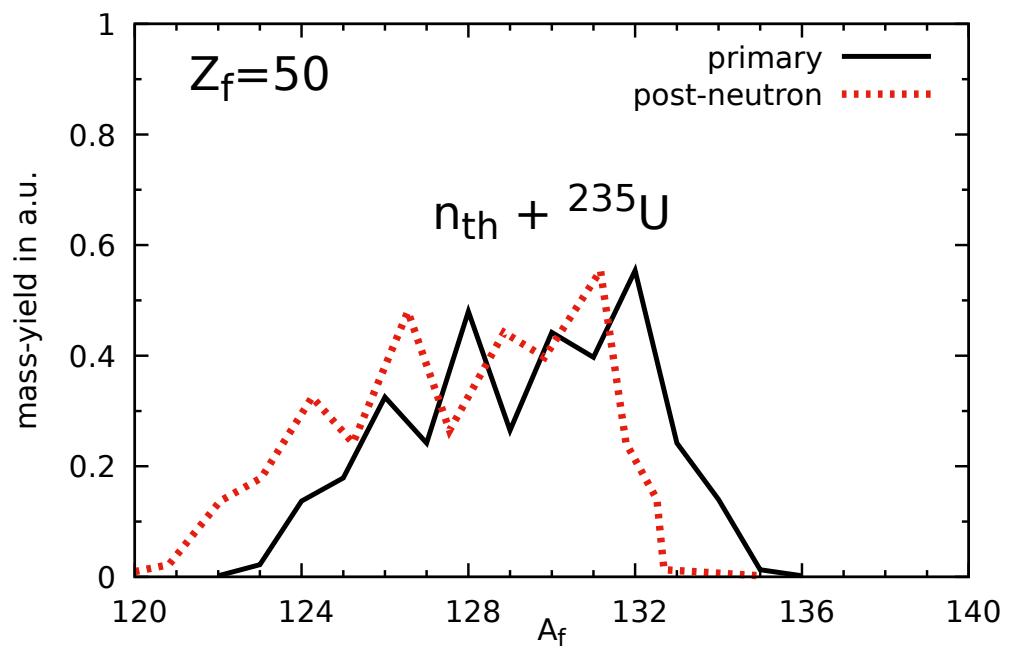
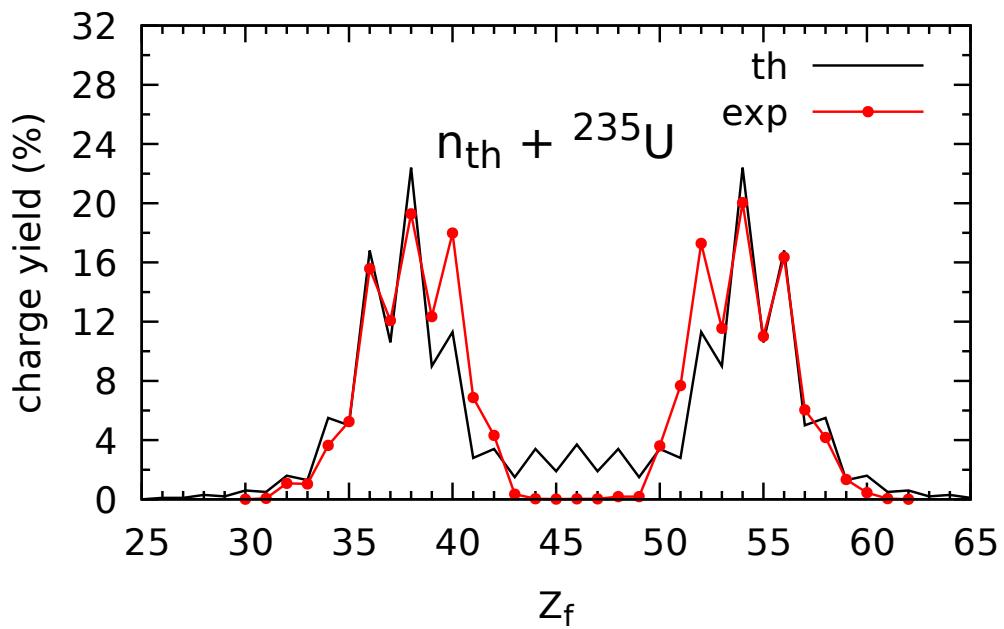
gives the distribution probability of the charge of the fragment:



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 $Z_1 = Z - Z_h$.

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

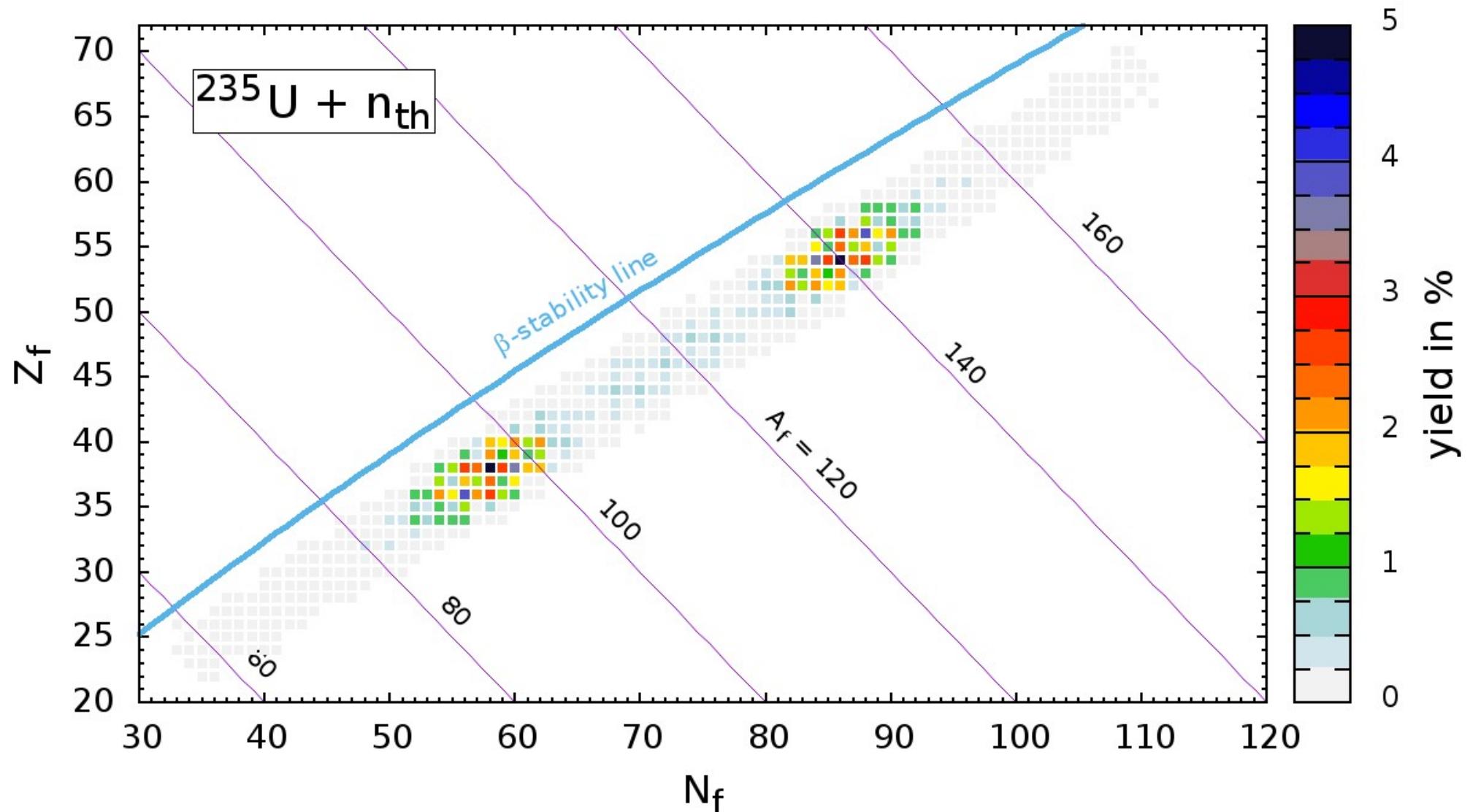
Effect of neutron evaporation on fission fragment yields of ^{235}U



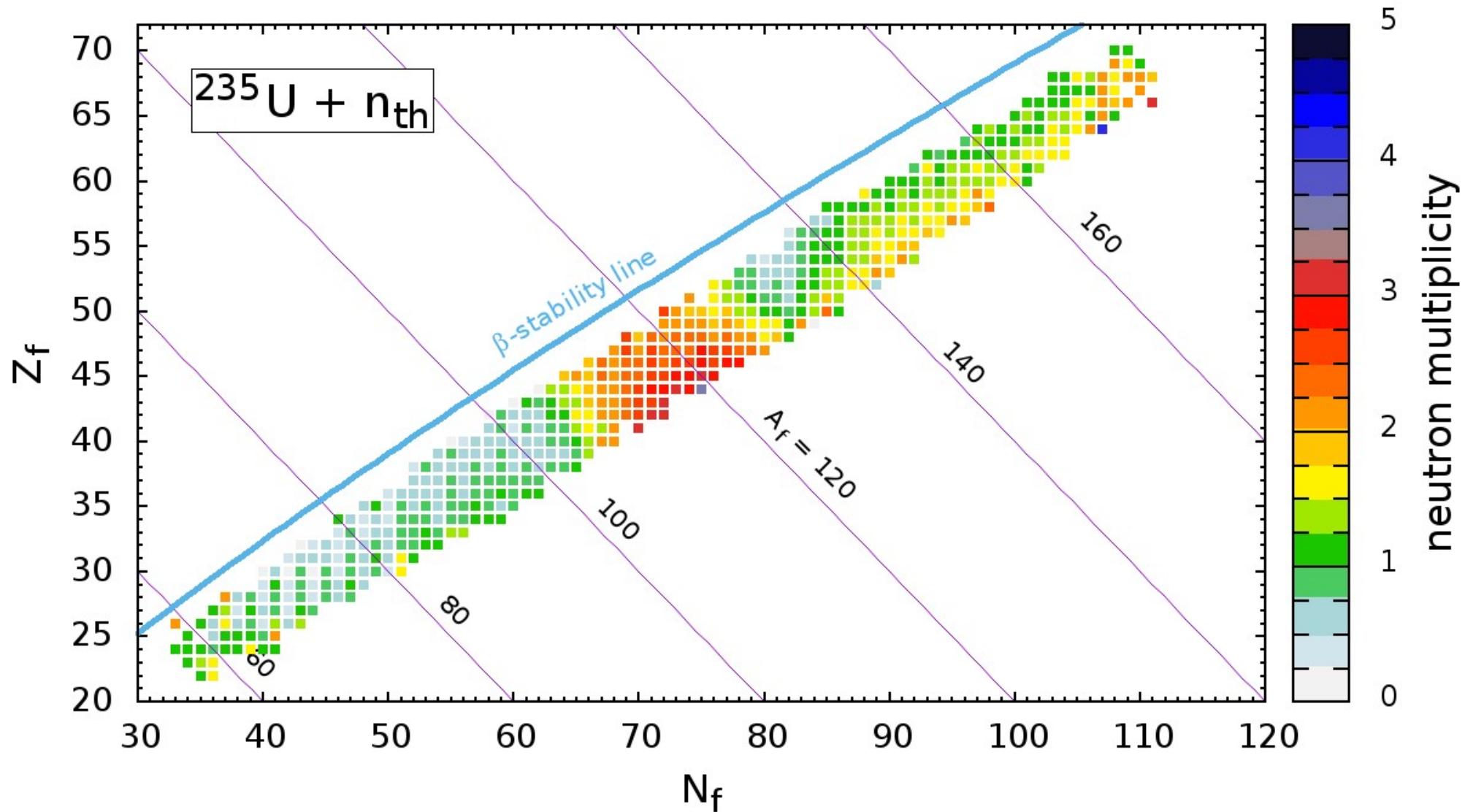
* K. P., B. Nerlo-Pomorska, C. Schmitt, Z.G. Xiao, Y.J. Chen, L.L. Liu, Phys. Rev. C **107**, 054616 (2023).

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

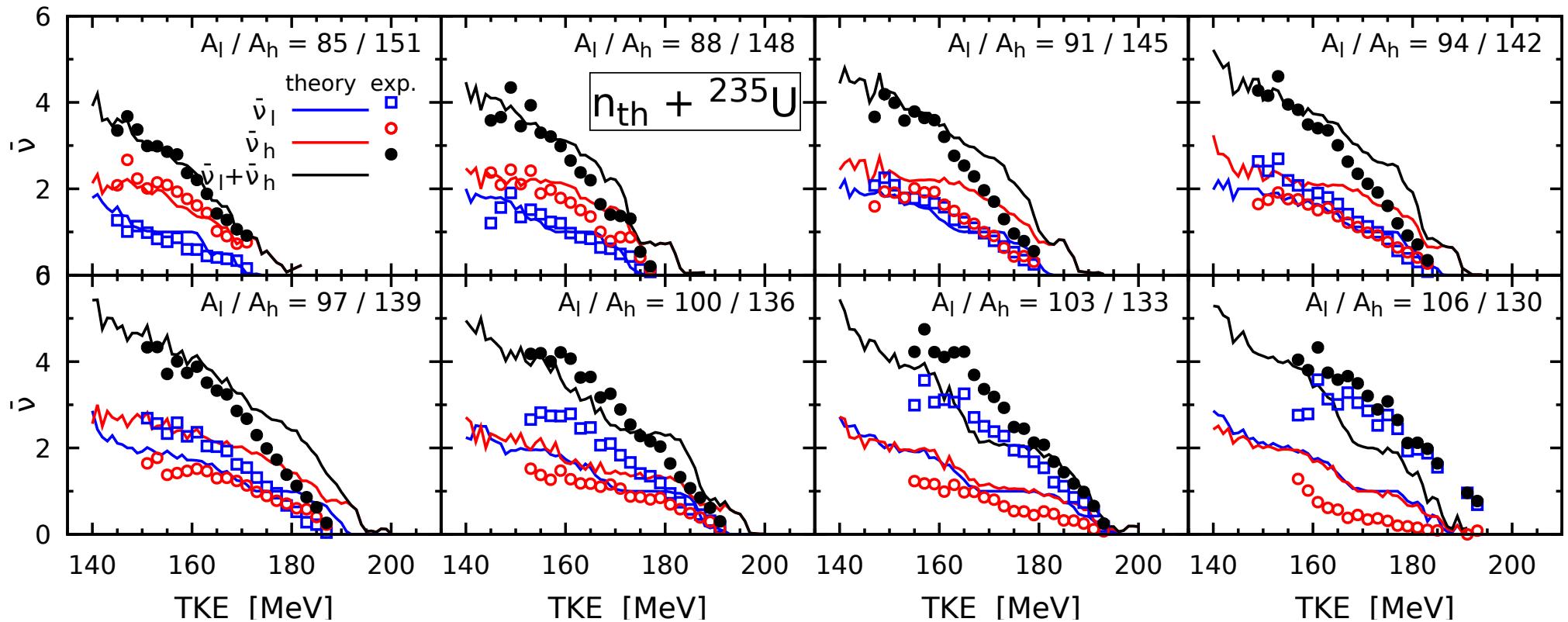
Map of isotopes produced in the fission of $^{236}\text{U}_{\text{th}}$



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



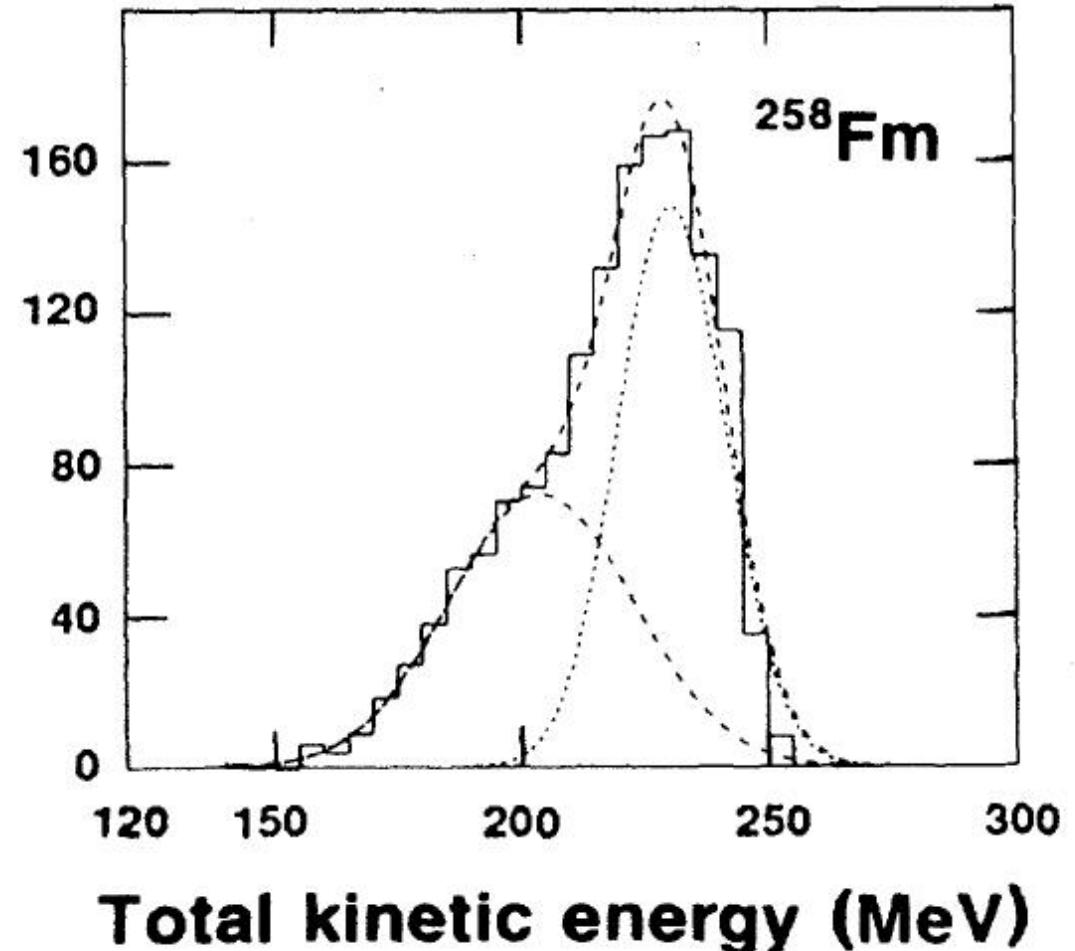
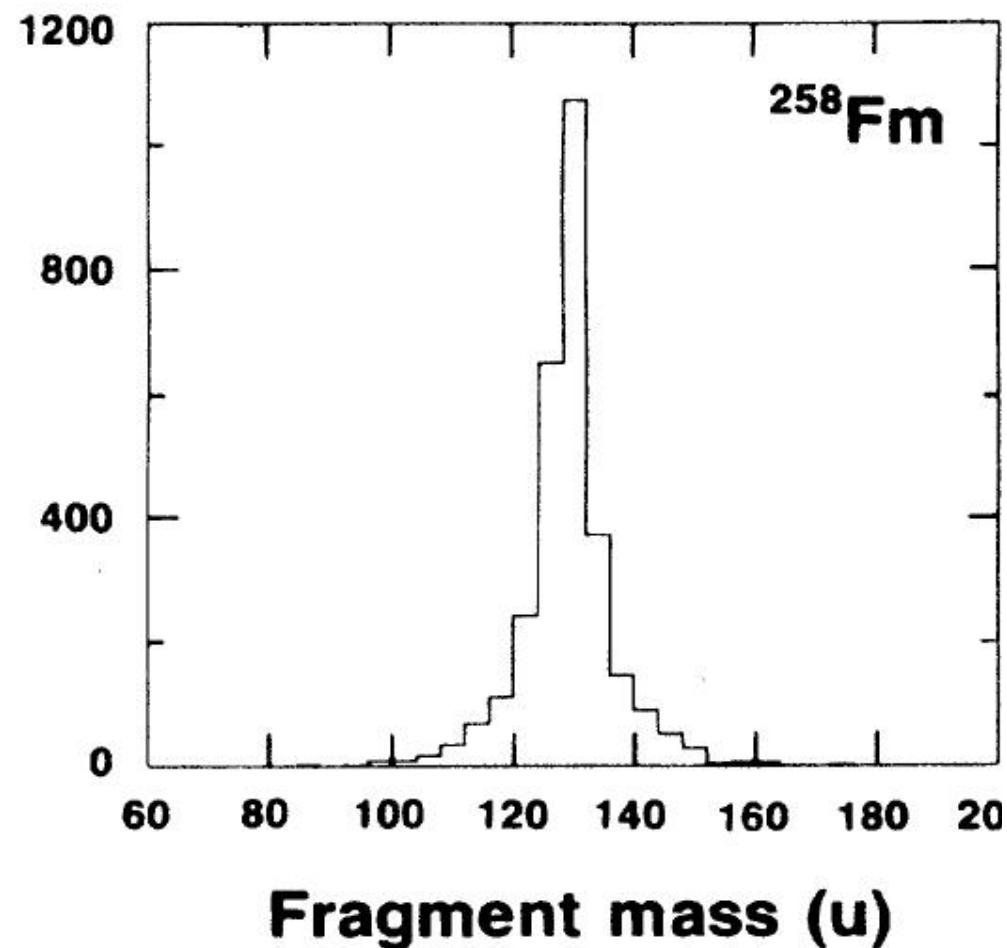
Number of neutrons emitted by the fission fragments of $^{236}\text{U}_{\text{th}}$



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

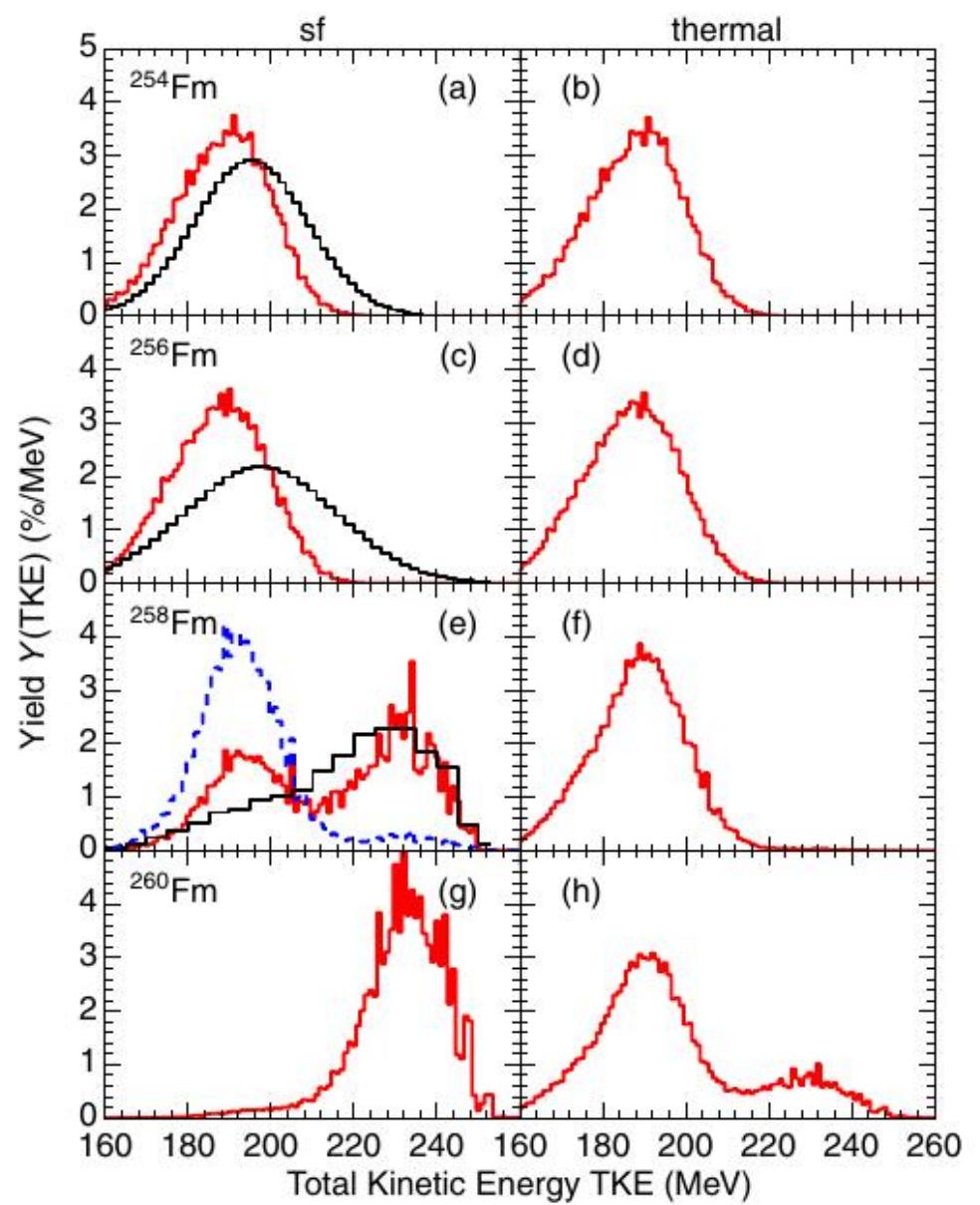
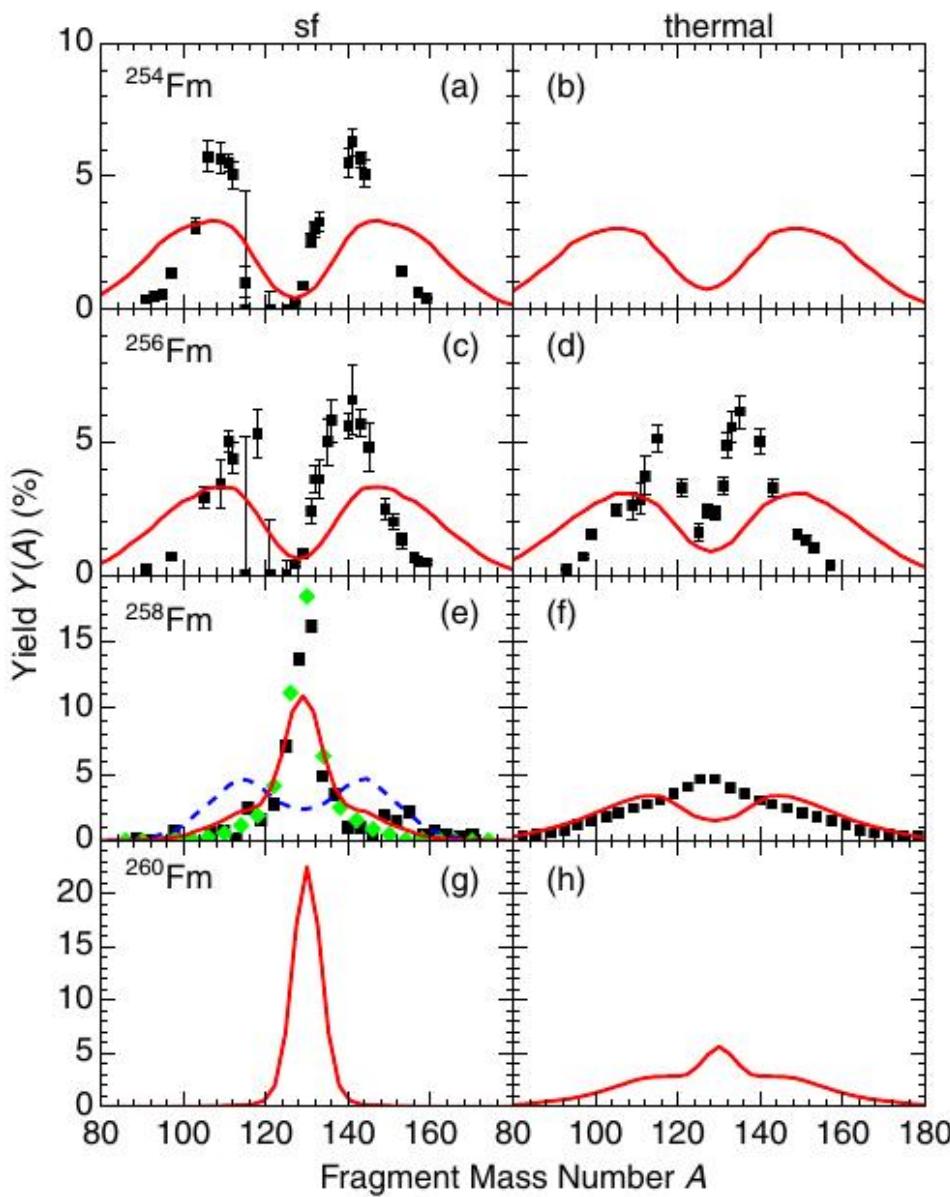
Exp. data: A. Göök, F.-J. Hambach, S. Oberstedt, M. Vidali, PRC **98**, 044615 (2018).

First observation of two modes in the spontaneous fission of $^{258}\text{Fm}^*$



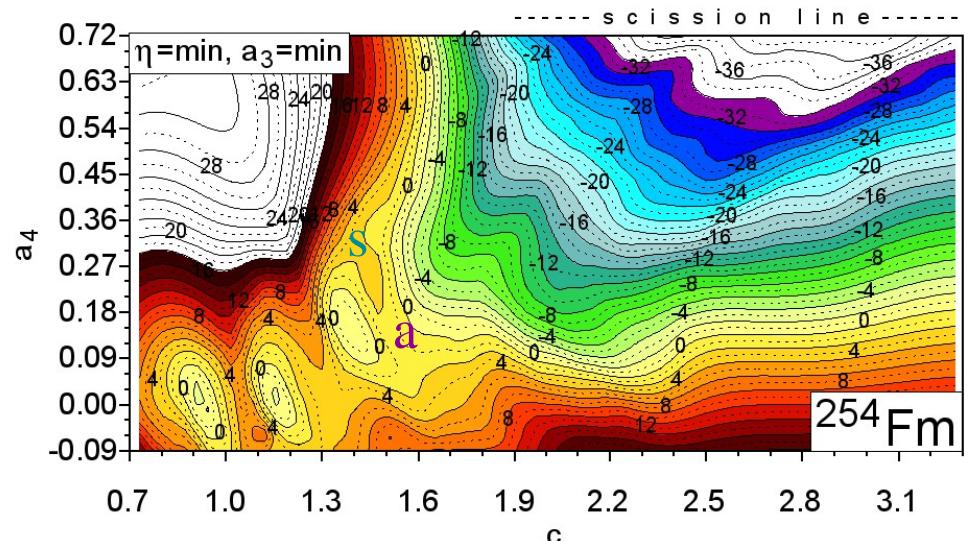
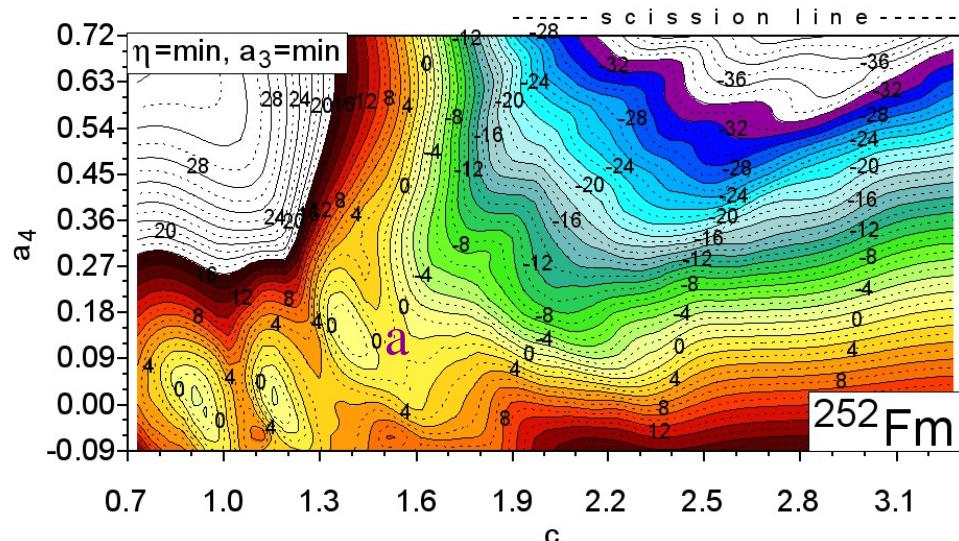
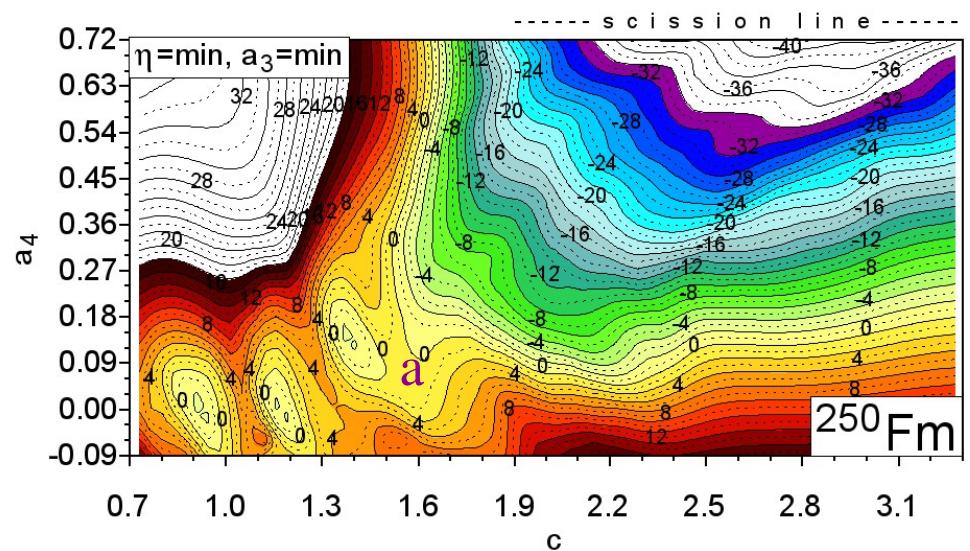
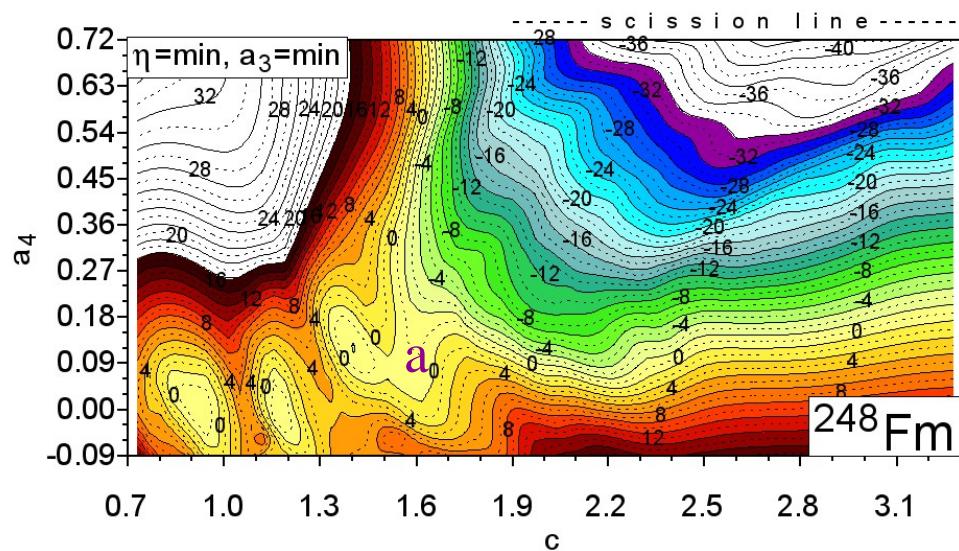
* E. K. Hulet et al. Phys. Rev. Lett. **56**, 313 (1986); Phys. Rev. C **40**, 770 (1989).

Estimates within the Lund-Kopenhagen-Berkeley-Honolulu 5D model*



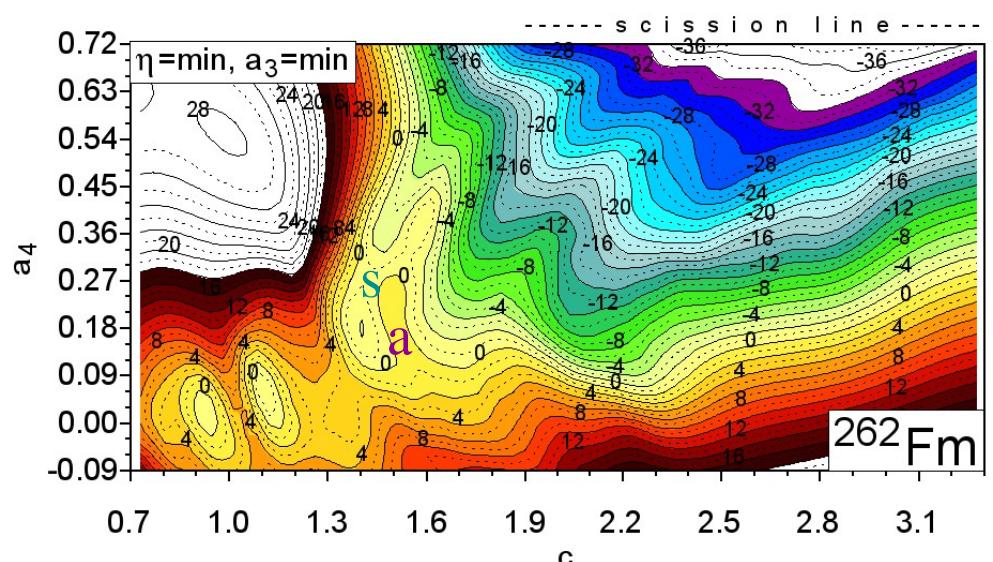
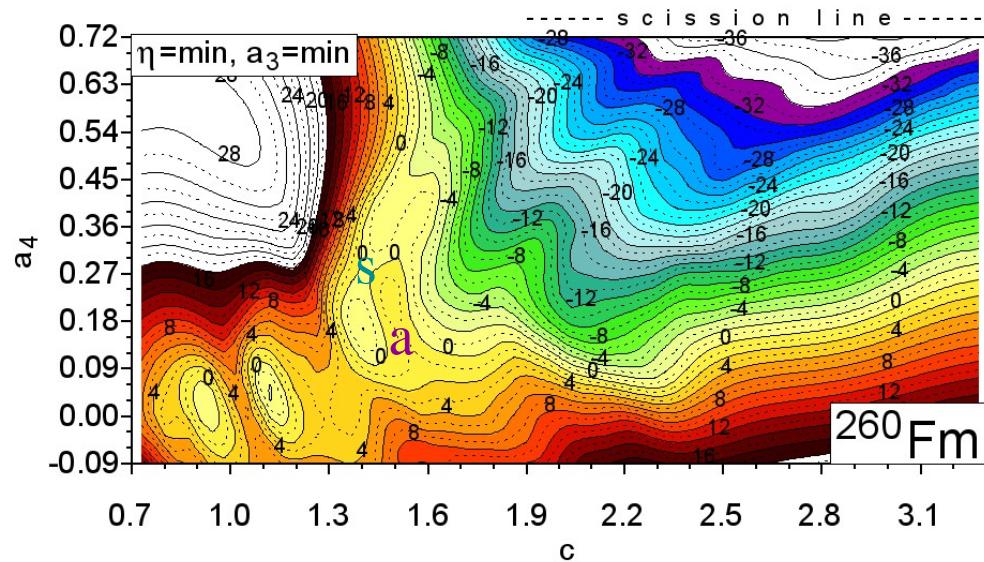
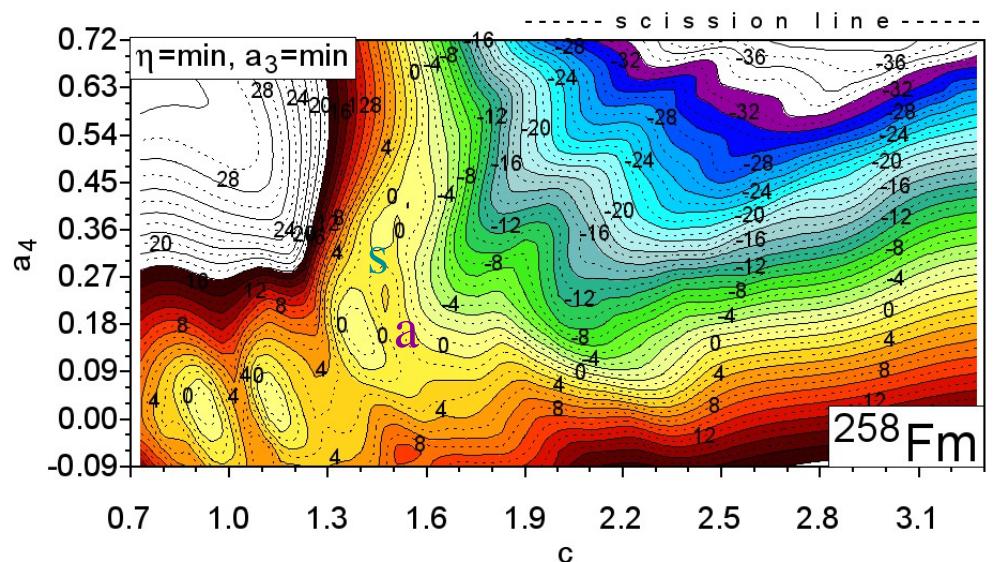
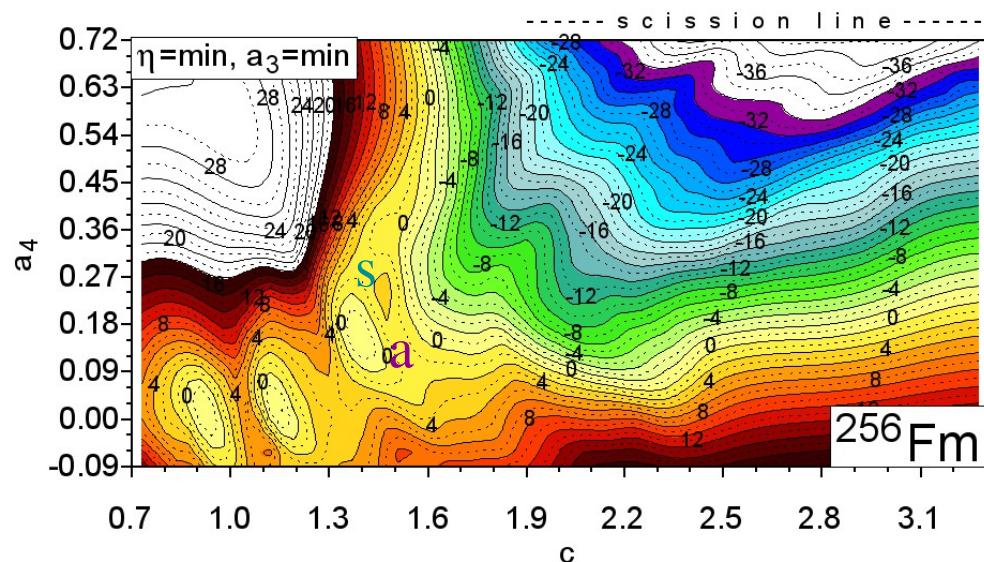
* M. Albertsson, B.G. Carlsson, T. Dossing, P. Möller, J. Randrup, S. Åberg, PRC **104**, 064616 (2021).

Potential energy surfaces of $^{248-254}\text{Fm}$



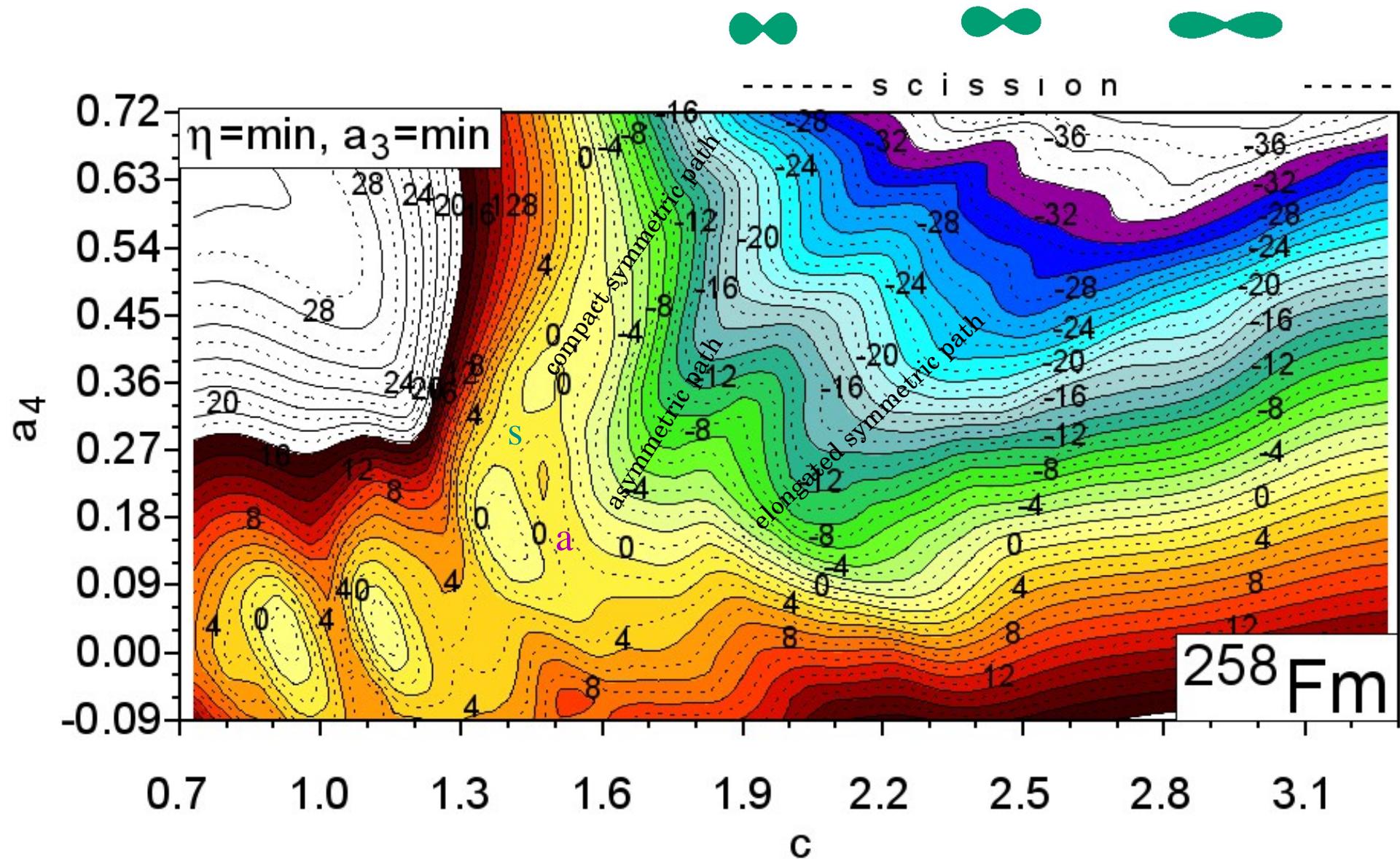
Our model with the same parameter-set as for ^{236}U is used to describe fission of Fermium isotopes. Only a **single 2nd saddle** is visible in each of the $^{248-254}\text{Fm}$ isotopes.

Potential energy surfaces of $^{256-262}\text{Fm}$

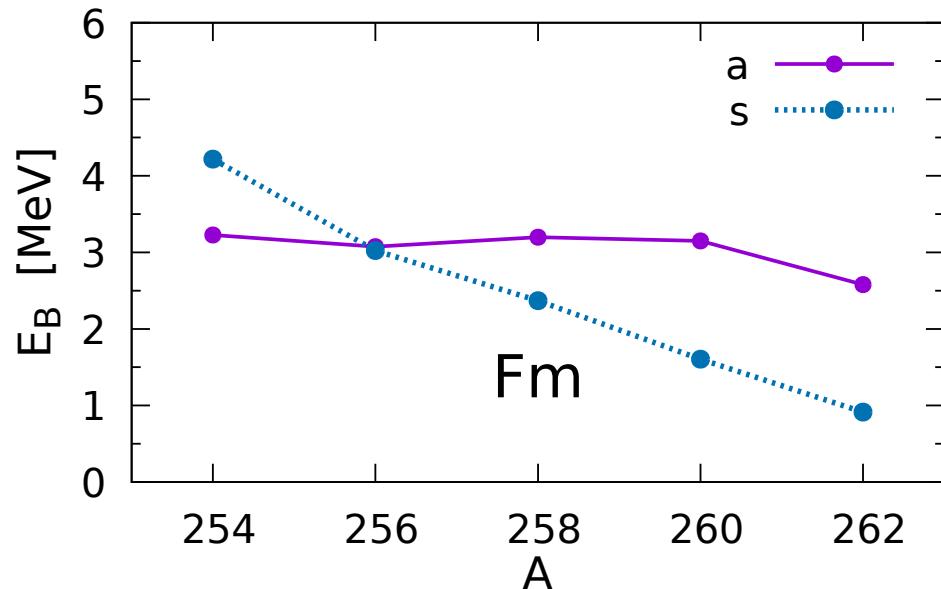


Double 2nd saddles and two saddle-points: ***a*** (asymmetric) and ***s*** (compact-symmetric) in the fission barrier are visible in the PES for $^{256-258}\text{Fm}$ isotopes.

Different paths to fission in the PES of ^{258}Fm



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



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

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

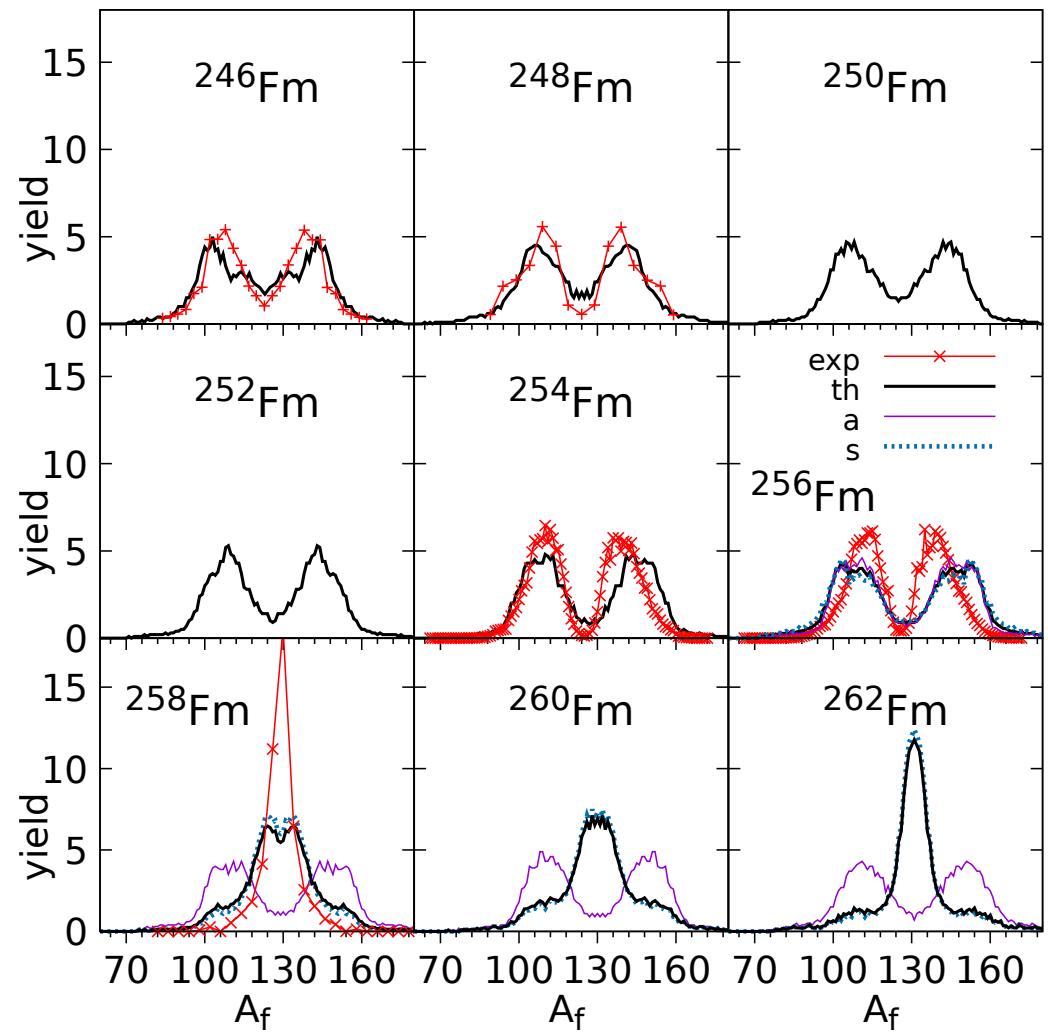
where $P_a + P_s = 1$ and

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

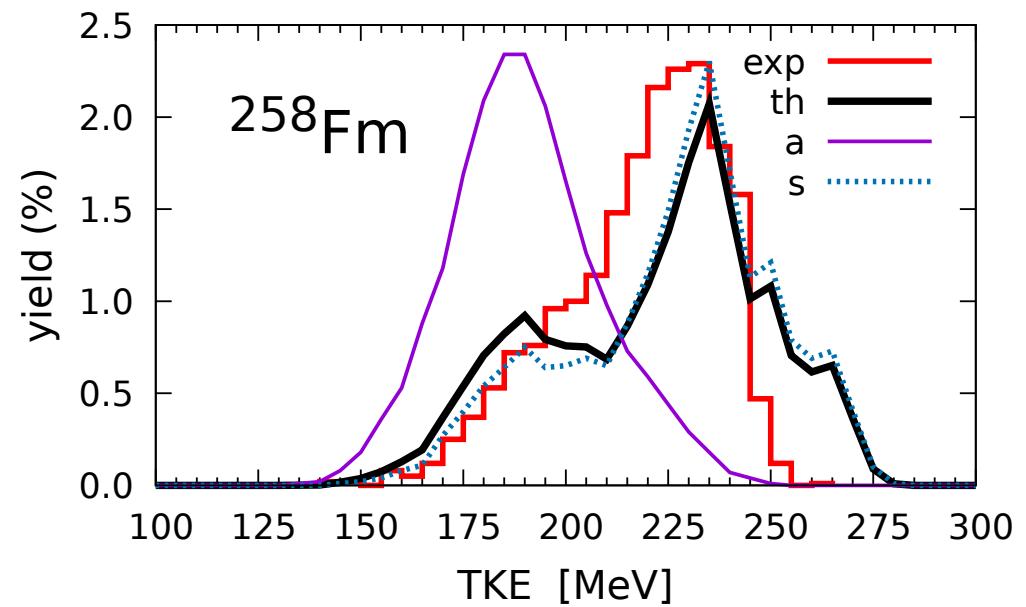
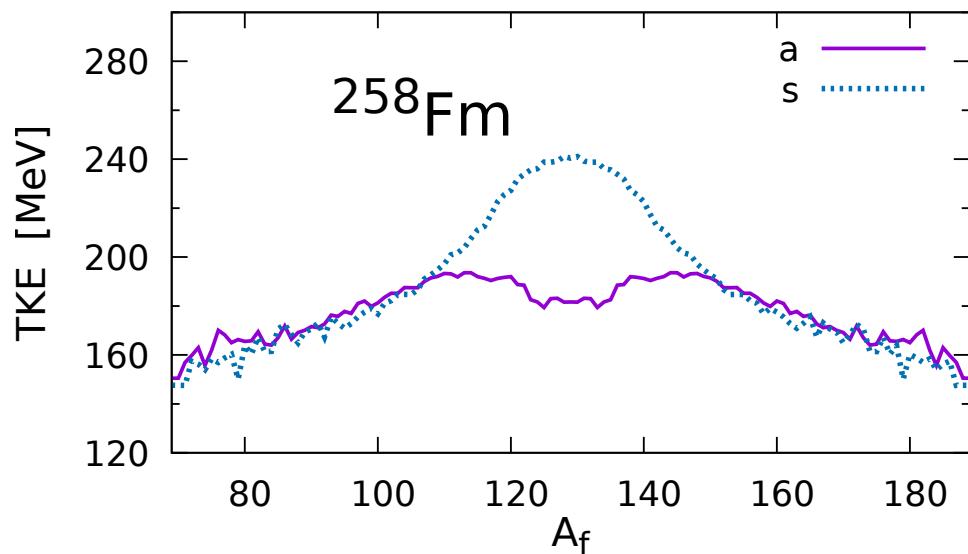
is the relative fission barrier penetration probability and S_i is the WKB action-integral[†] along the path i .

*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).

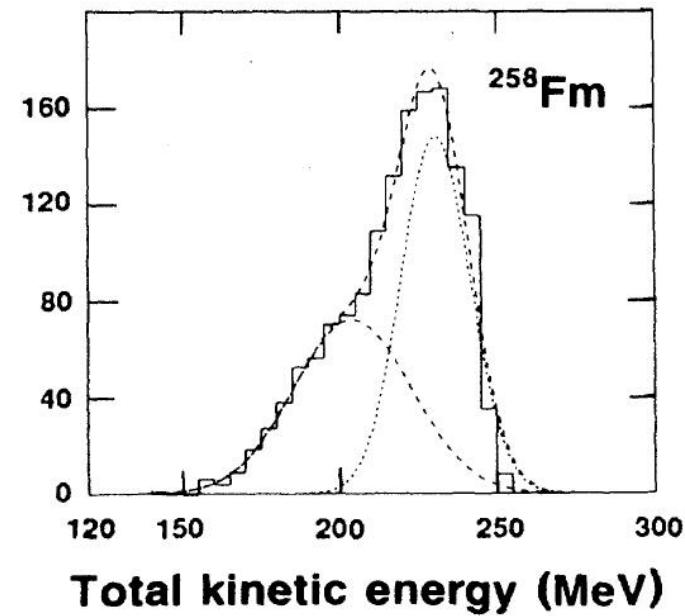


Fission fragment total kinetic energy yield of $^{258}\text{Fm}_{\text{sf}}$



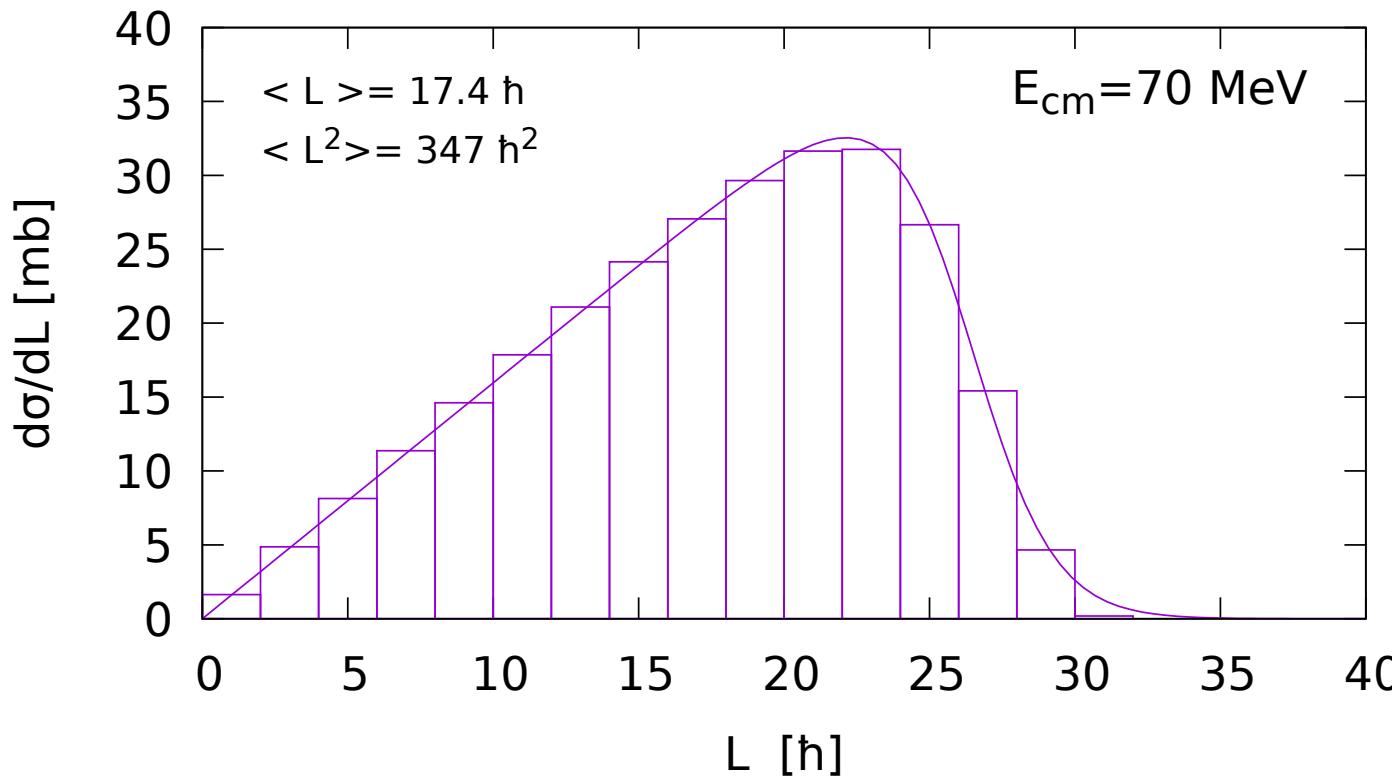
The TKE as a function of the fragments mass A_f corresponding to the asymmetric (a) and the compact-symmetric (s) modes.

Experimental data by Hulet et al. →



Fission of ^{250}Cf nucleus at $E^*=46$ MeV and $L=20\hbar$

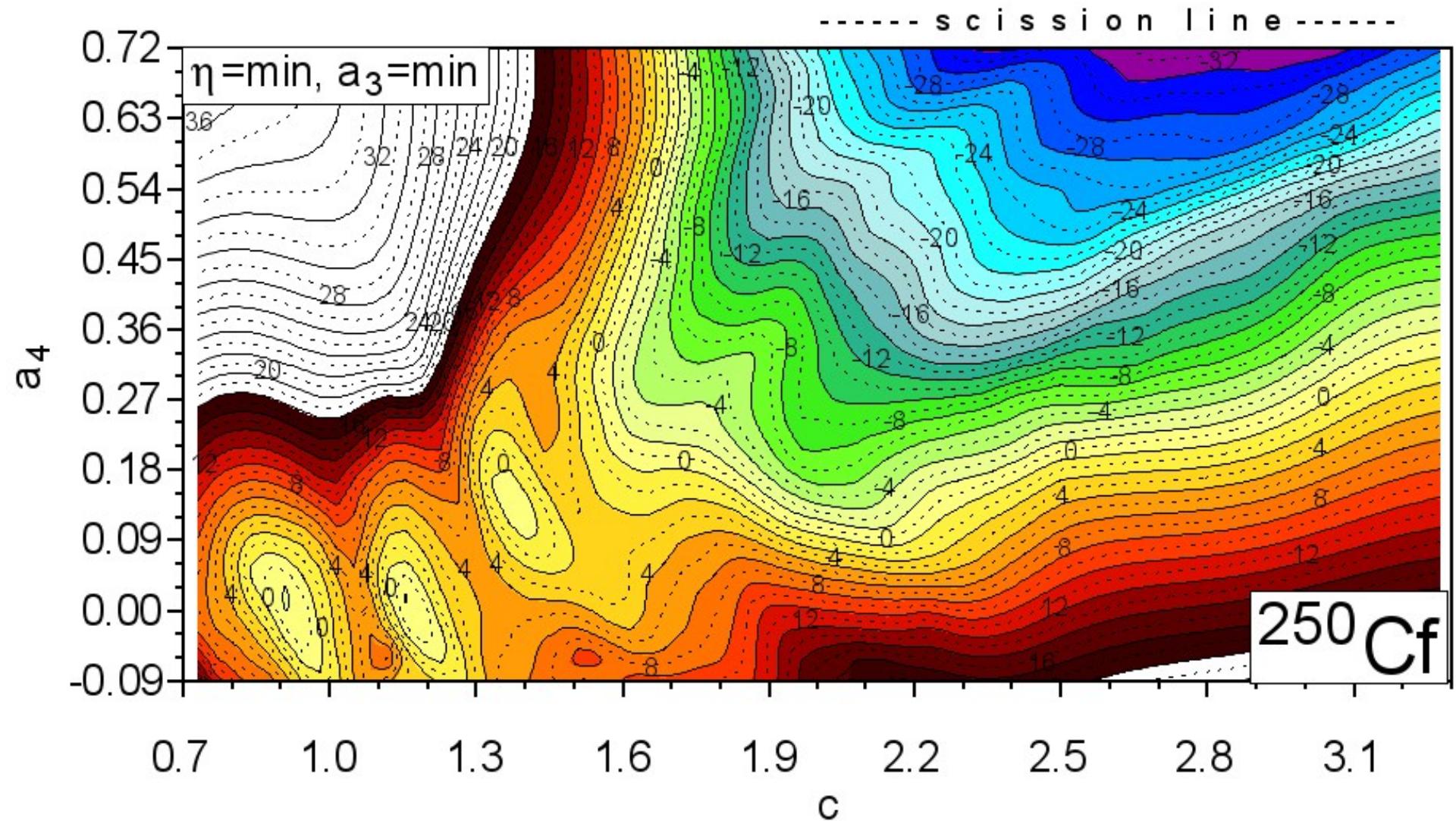
Partial fusion cross-section for synthesis of ^{250}Cf :



The above estimate was done using the 1D Langevin code for fusion of Peter Fröbrich*.

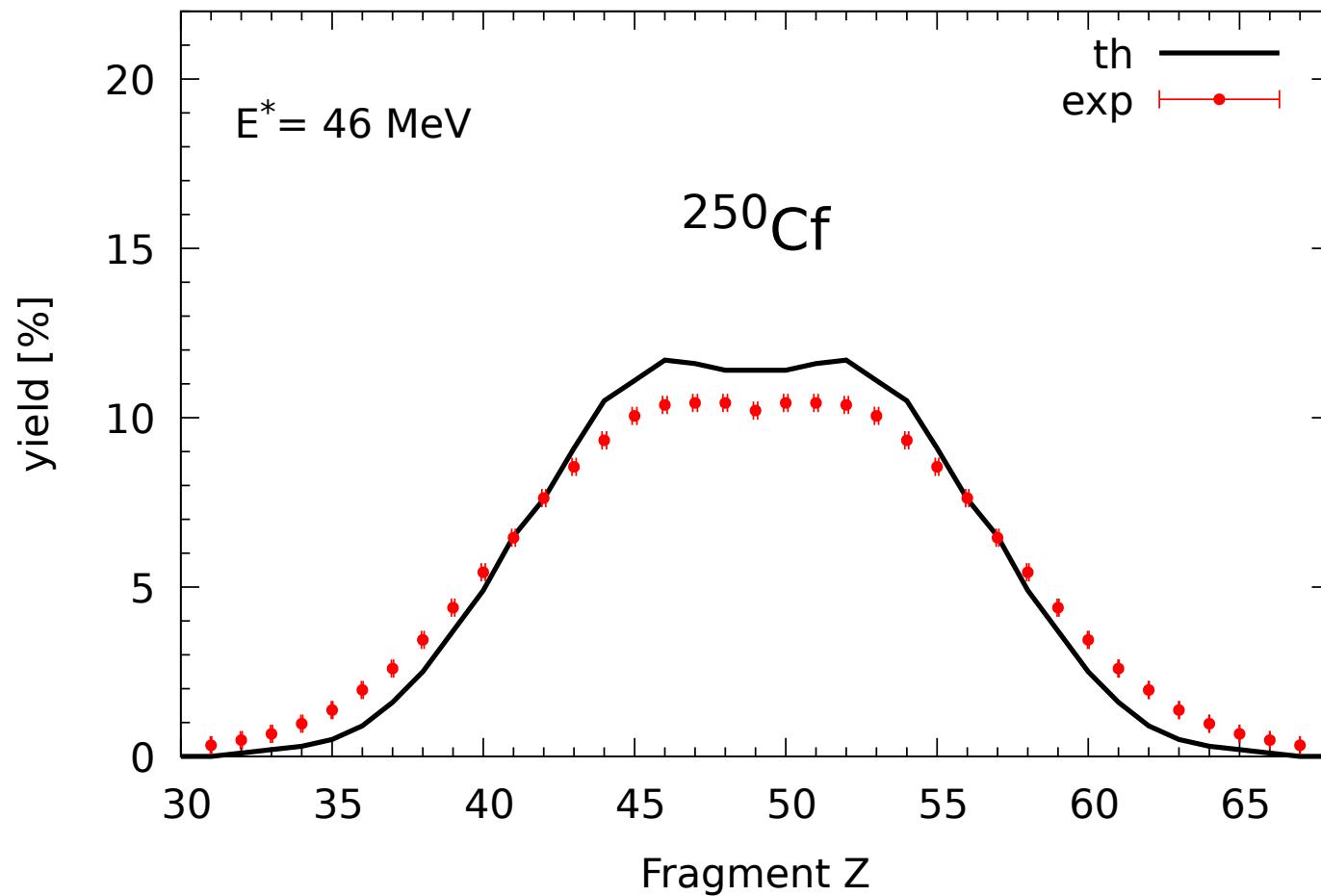
* See, e.g., P. Fröbrich, Nucl. Phys. **A545** (1992) 87c.

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



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

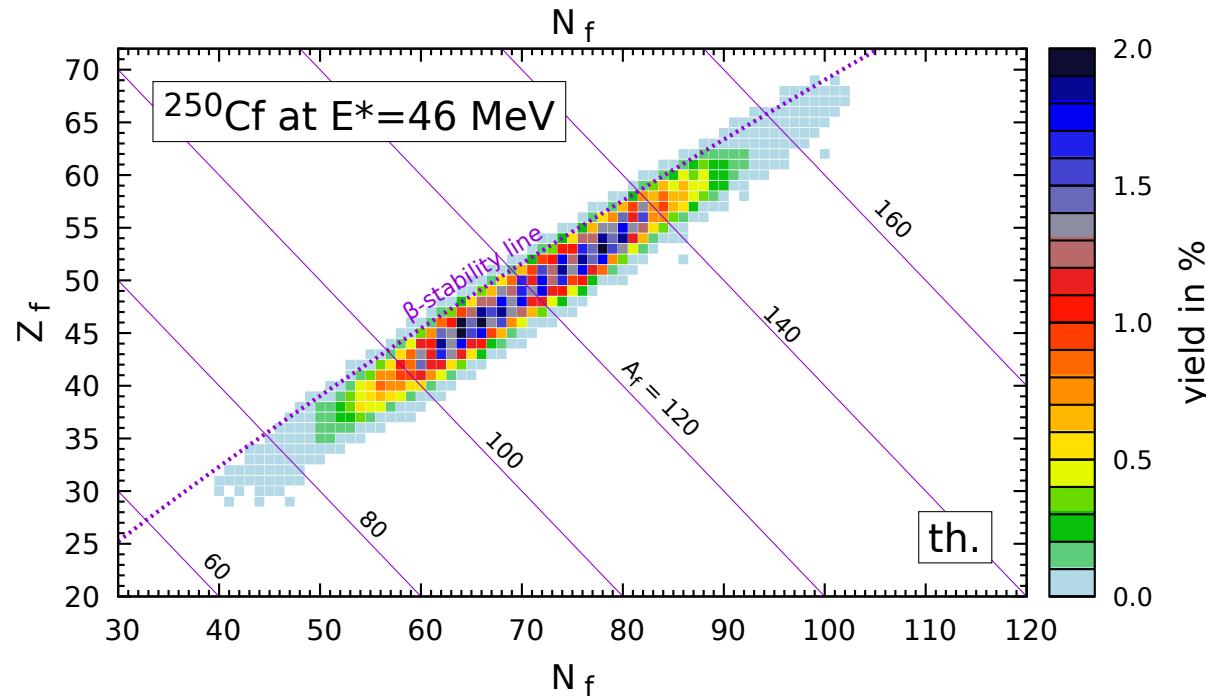
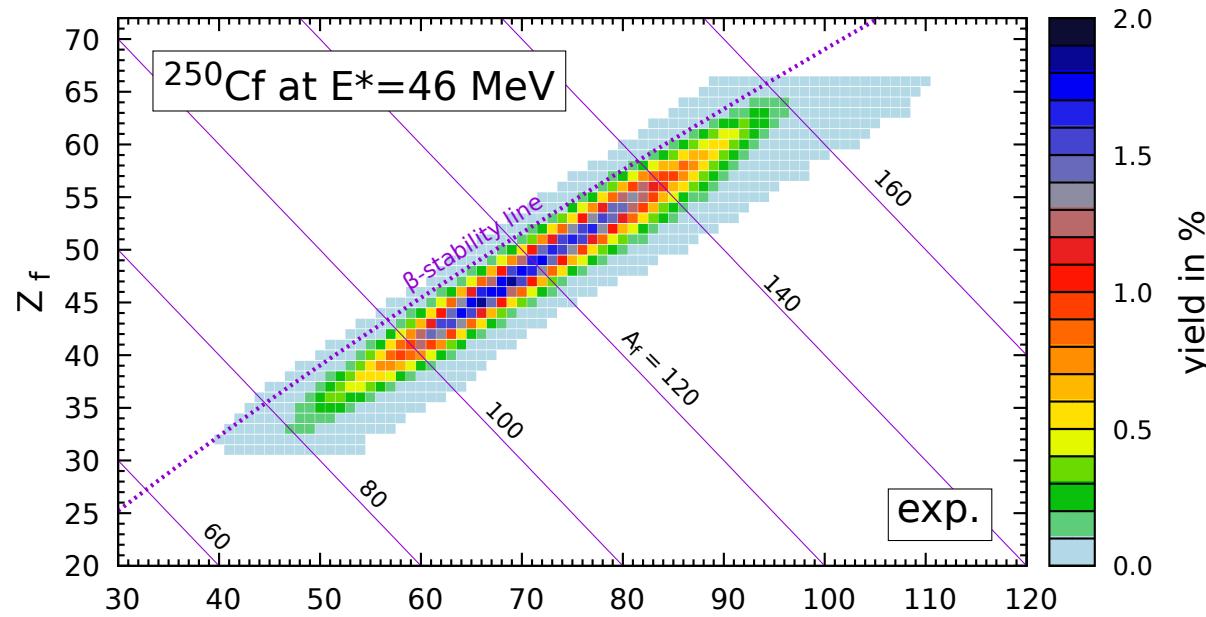
Fission fragment mass yield of ^{250}Cf at $E^*=46$ MeV



All parameters of the calculation are the same as those used to describe fission of $^{236}\text{U}_{\text{th}}$ and $^{246-262}\text{Fm}_{\text{sf}}$ isotopes. Nothing is adjusted.

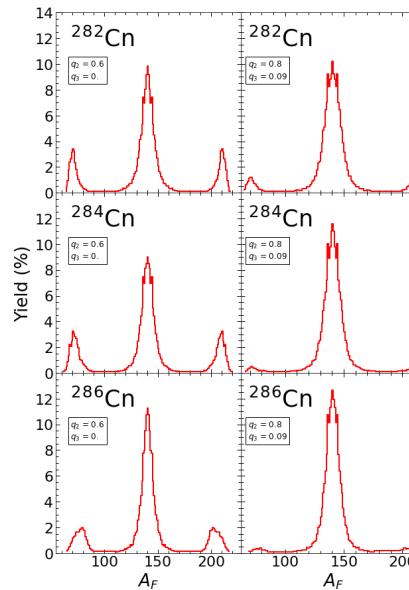
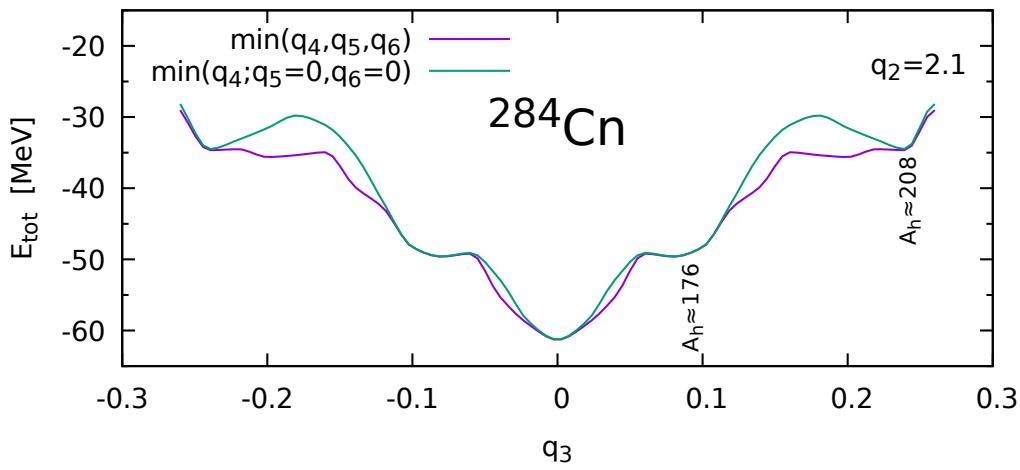
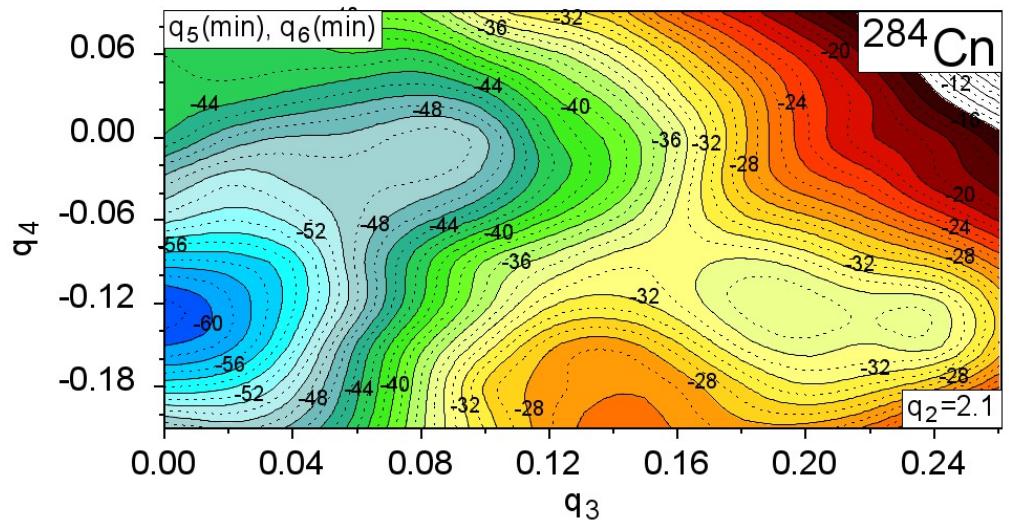
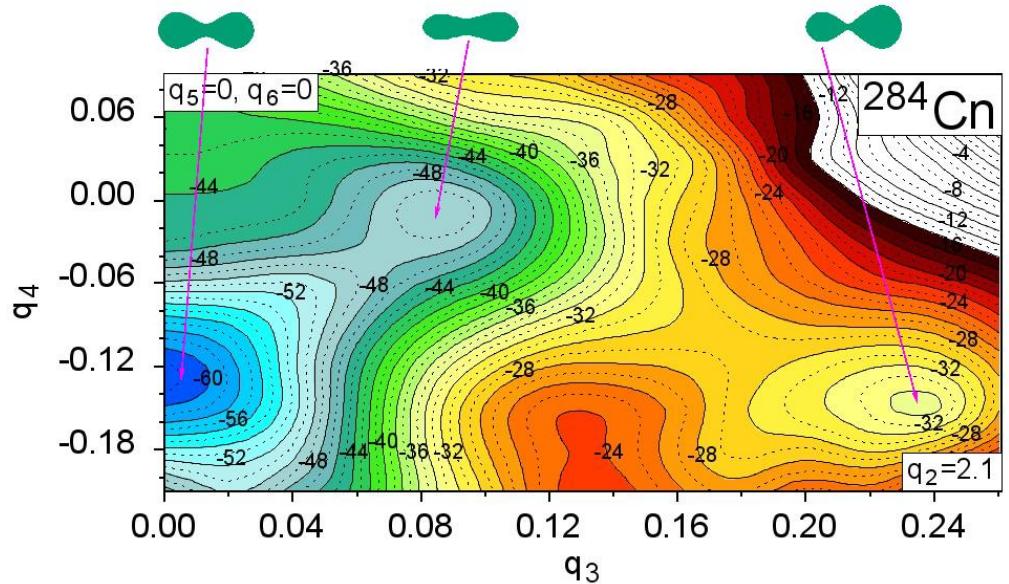
Exp. data: D. Ramos et al. Phys. Rev. c **99**, 024615 (2019).

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



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

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. Kostryukov, 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).

Summary:

- Rapidly convergent Fourier expansion of nuclear shape offers a very effective way of describing shapes of fissioning nuclei both in the vicinity of the ground-state and the scission point,
- Potential energy surfaces are evaluated in the macro-micro model using the LSD formula for the macroscopic part of energy and the Yukawa-folded single-particle potential to obtain the microscopic energy correction,
- The irrotational flow model and the Świątecki wall-formula are used to evaluate the mass and friction tensors,
- It was shown that a 3D Langevin model which couples the fission, neck and mass asymmetry modes describes well the main features of the fragment mass and kinetic energy yields.
- Multiplicity of neutrons emitted by the fission fragments is well reproduced by our model,
- Inclusion of the charge equilibration mode at scission allows to reproduce the measured isotopic yields,
- A very asymmetric fission mode with $A_h \approx 208$ is predicted in some super-heavy nuclei.

FISSION FRAGMENT MASS AND KINETIC ENERGY YIELDS OF FERMIUM ISOTOPES

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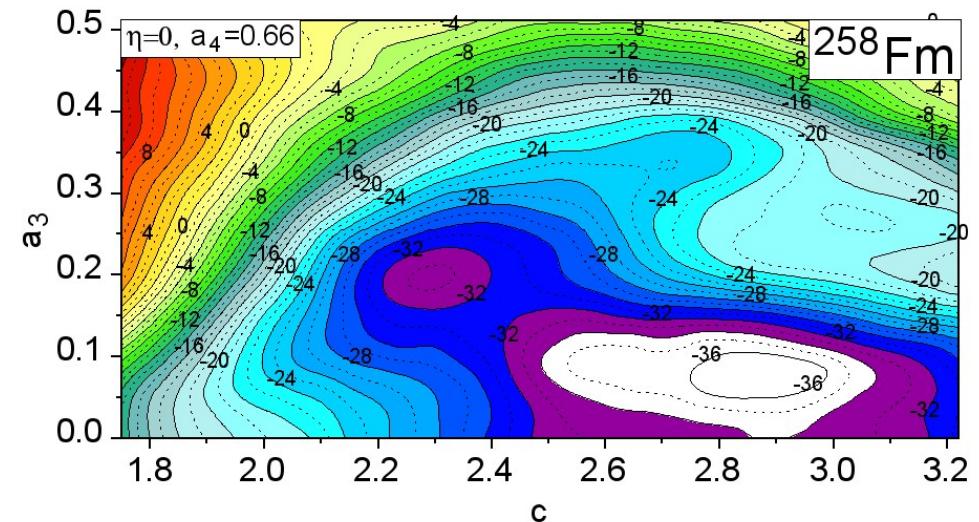
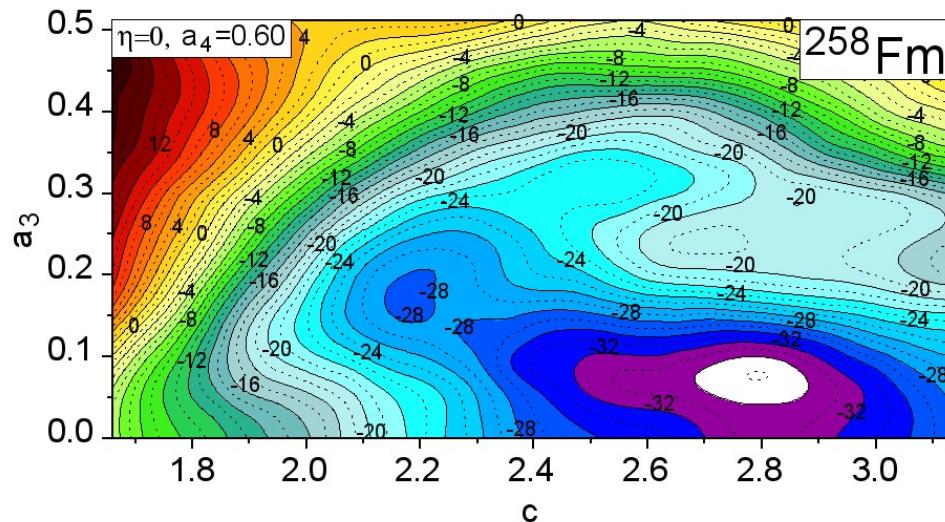
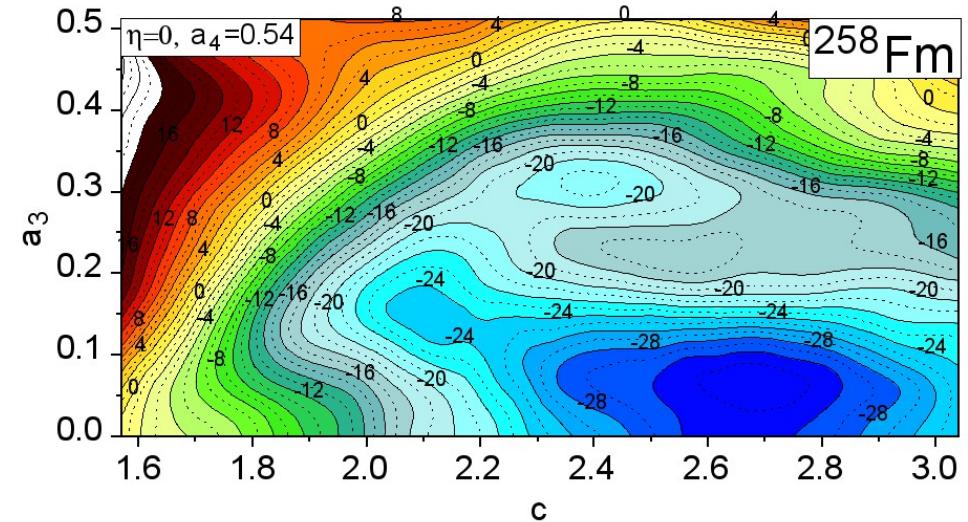
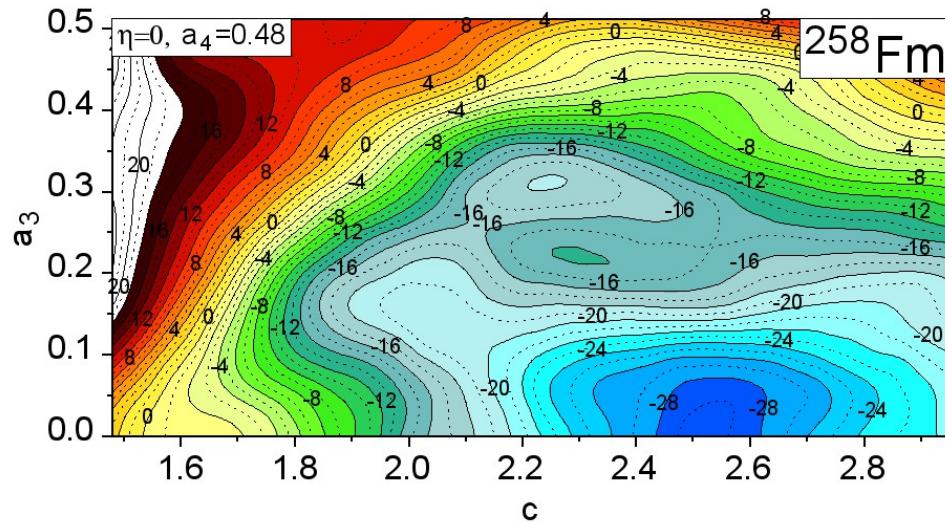
*Received 14 September 2023, accepted 18 September 2023,
published online 21 September 2023*

Thank you for your attention

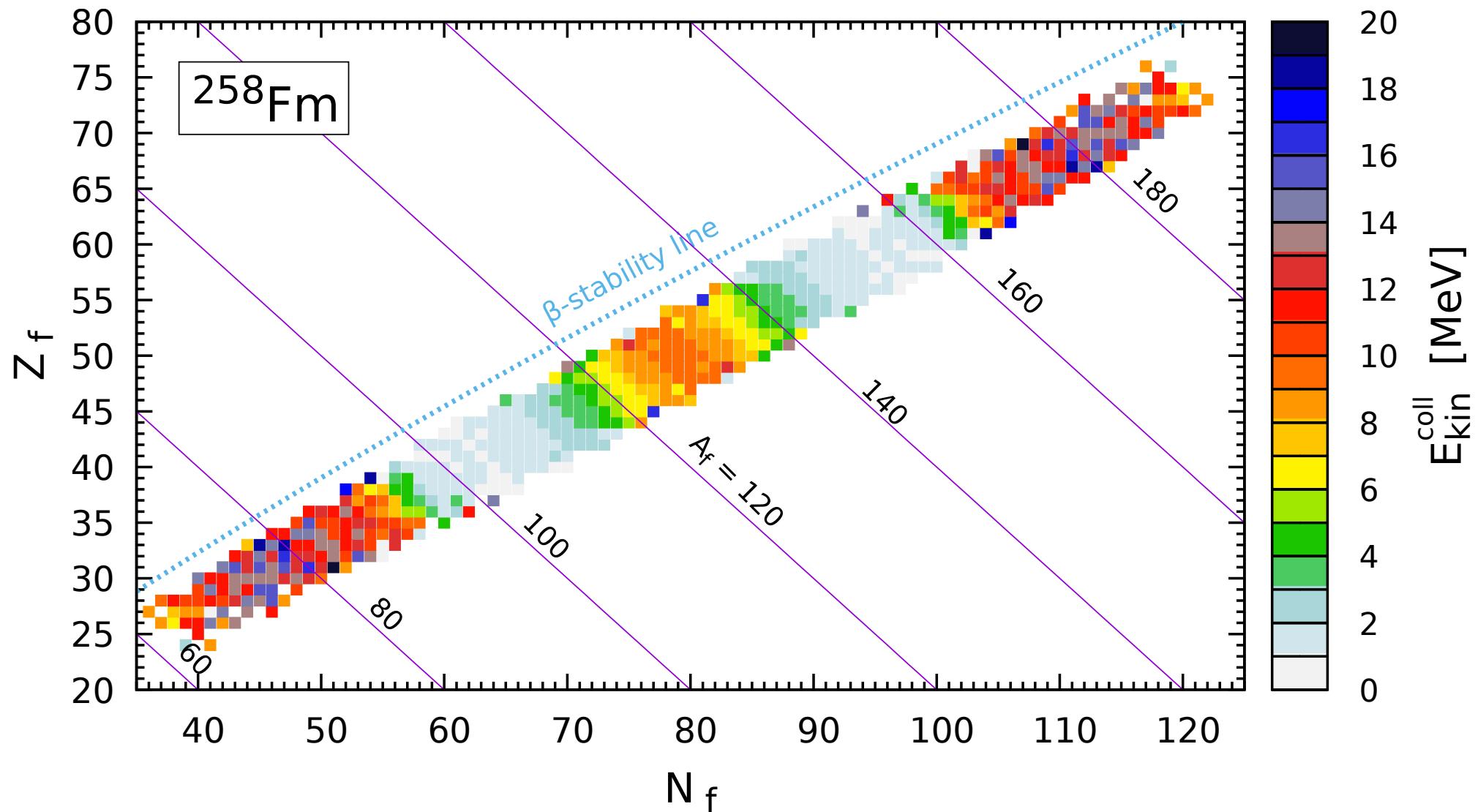
谢谢！

Dziękuję Państwu za uwagę

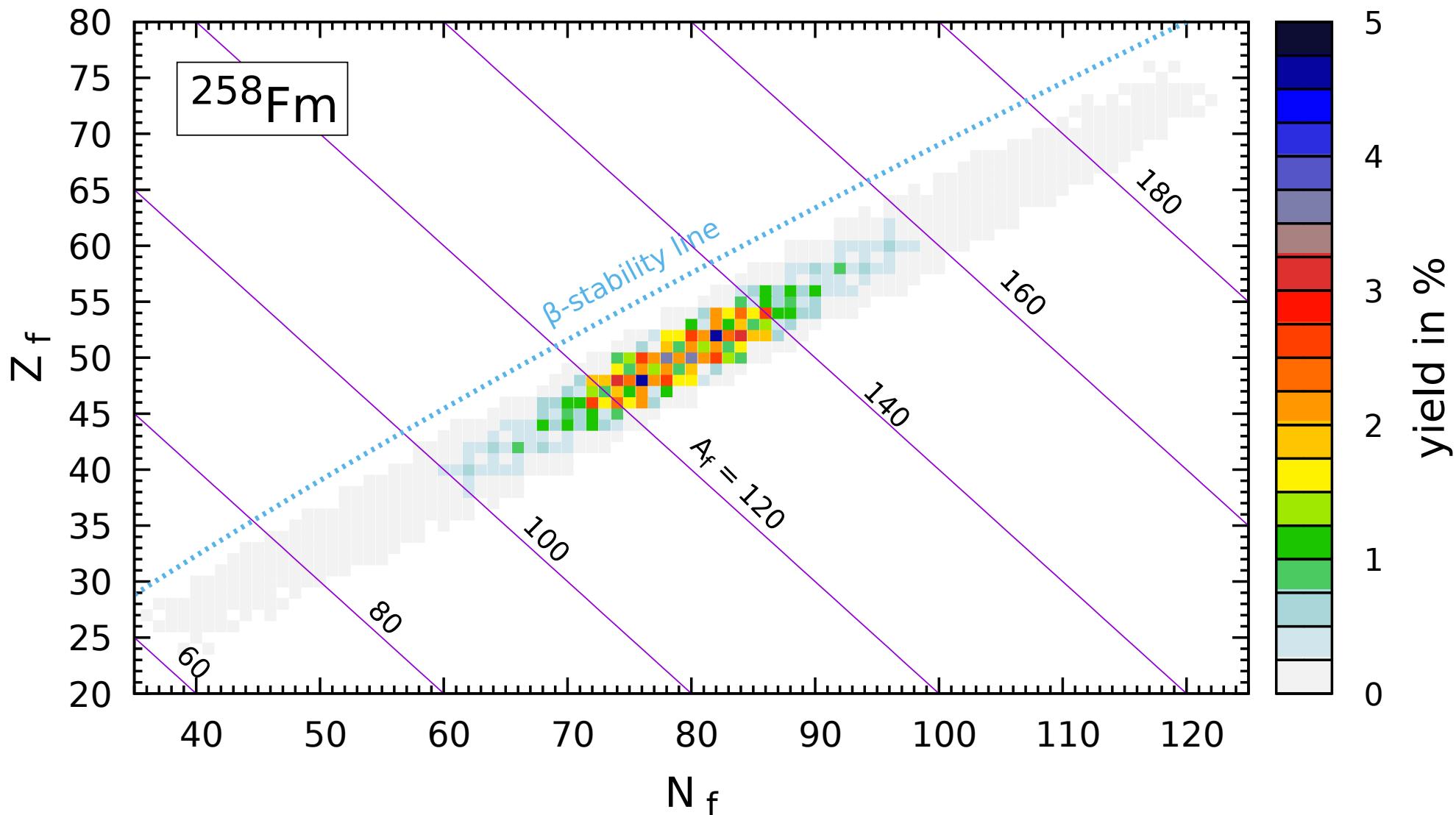
Few (c , a_3) cross-sections of the PES of ^{258}Fm



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



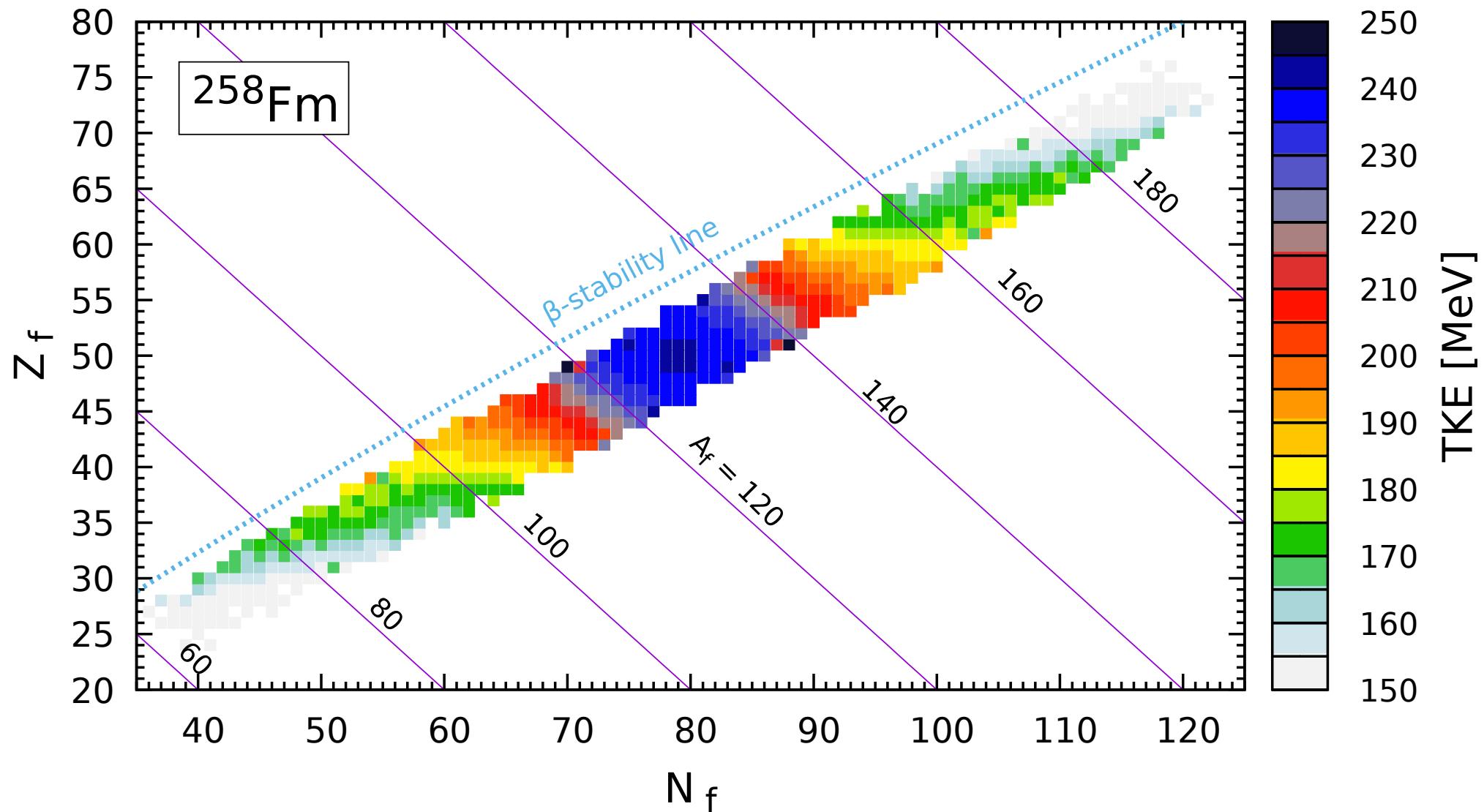
Fission fragment mass-yield of $^{258}\text{Fm}_{\text{sf}}$ *



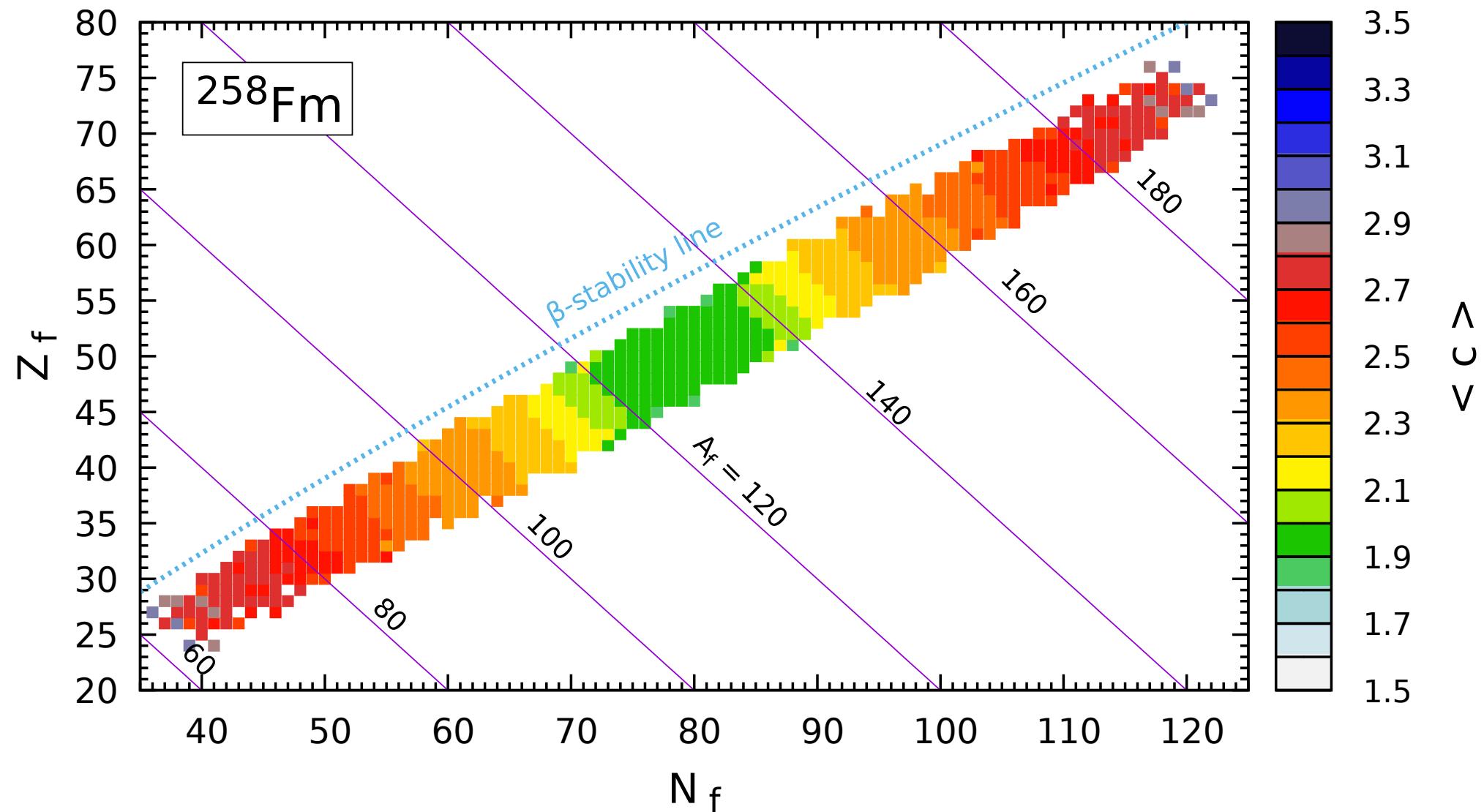
This and the following maps are made on basis of 300k Langevin trajectories.

* 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).

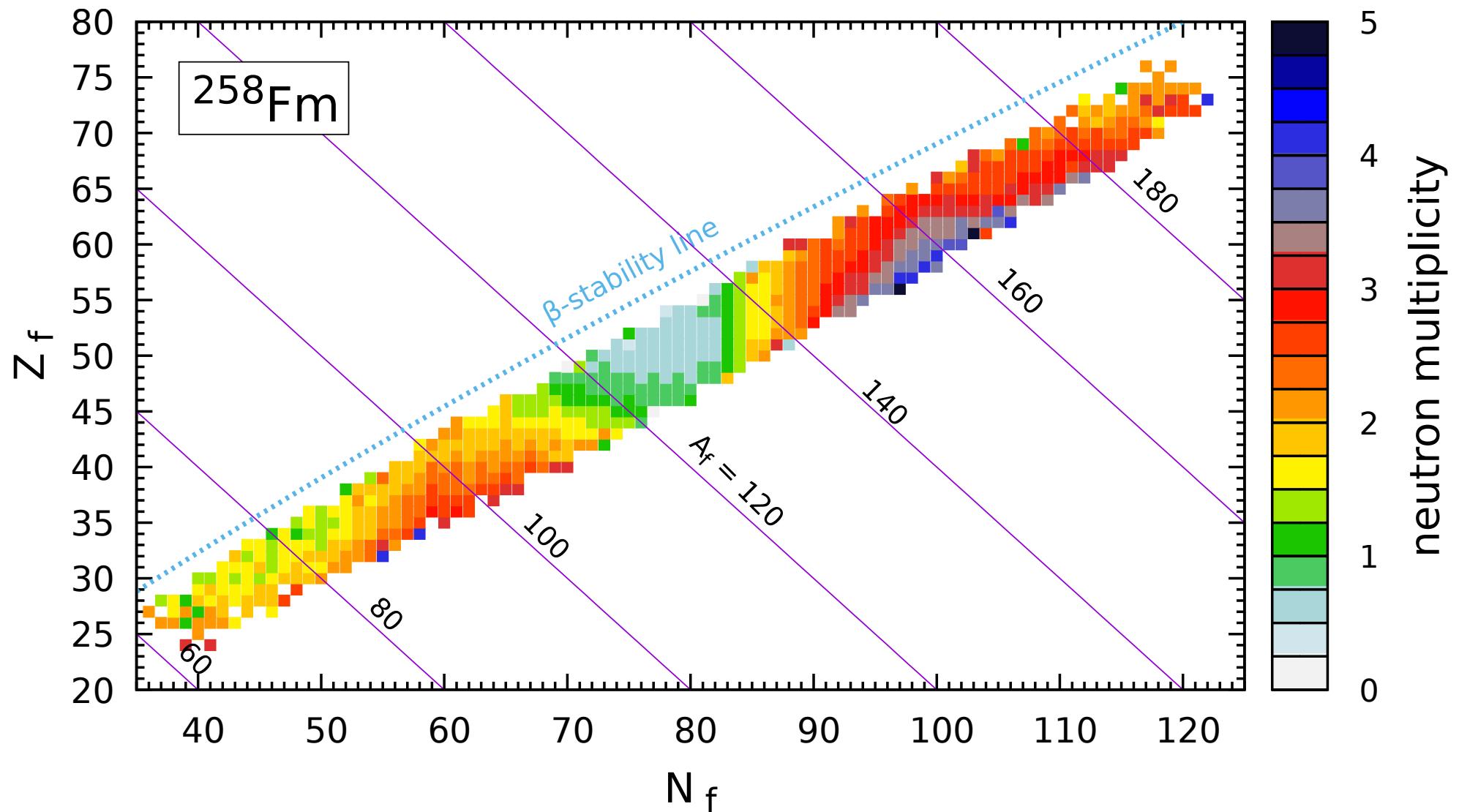
Fragment TKE of $^{258}\text{Fm}_{\text{sf}}$



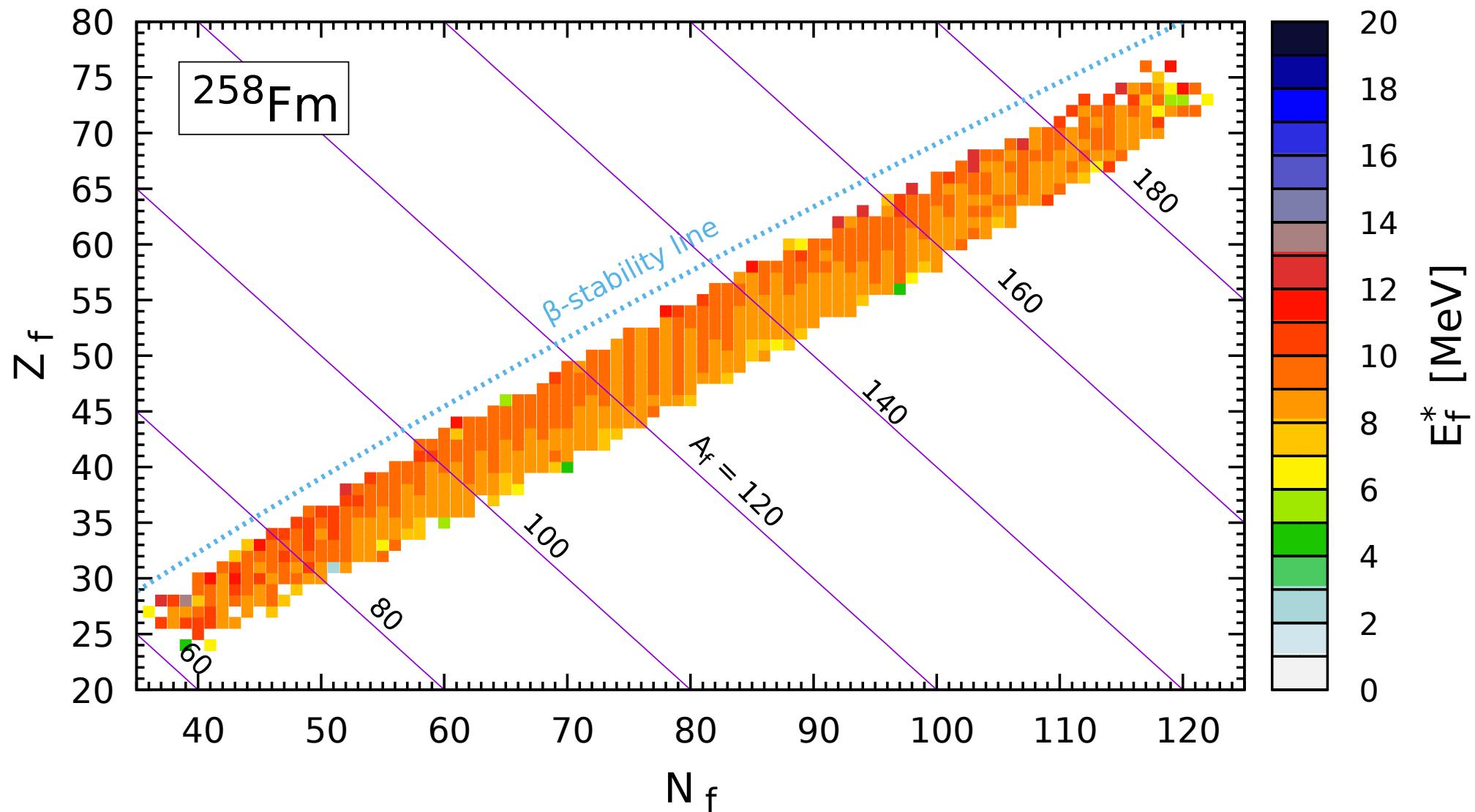
Average elongation of $^{258}\text{Fm}_{\text{sf}}$ at scission



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



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



An example of a grid on the (β, γ) plane and its projection on the (c, η)

