Oak Ridge, March 30-31, 2005

Microscopic calculations of PES : fission barriers, fission paths and fusion barriers

L. Bonneau

Los Alamos National Laboratory

in collaboration with P. Quentin and D. Samsœn,

Centre d'Etudes Nucléaires de Bordeaux-Gradignan (France)

Contents

Introduction

Motivation : fission and fusion static properties from the PES in the Hartree–Fock–BCS approach

Tests of reliability :

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☞ most probable fragmentations : comparison of calculated fusion valleys with experimental mass distributions

Application to super-heavy elements :

☞ stability against fission : comparison with other theoretical works and some experimental data

☞ most favorable reaction channels : fusion barriers and minimal excitation energy of the compound nucleus

Application to the $A = 70$ mass region :

☞ conditional fission barriers below the Businaro–Gallone point

1^{st} part : Formalism and numerical aspects

Approximate resolution of the nuclear many-body problem at low energy

* Basic assumptions : non relativistic nucleons, without internal structure and interacting through an effective 2-body force
* Mean field in the Hartree-Fock approximation with the Skyrme interaction (SkM* parametrization : good surface properties and reasonable spectroscopic properties)
* Pairing correlations : ($T = 1$, $S = 0$) channel and even-even nuclei :
  - ☞ BCS approximation (seniority force G)

Energy corrective terms

Approximate treatment of the symmetries broken by the mean field

☞ Approximate restoration of translation symmetry : removal of the 1-body contribution to the center of mass kinetic energy

$$E_{kin}^{(corr)} \approx \left(1 - \frac{1}{A}\right) E_{kin} \quad \text{assuming } m_n \approx m_p$$

☞ Approximate restoration of rotation symmetry : approximate projection of $|\Psi_{intr}\rangle$ onto 0^+
⇝ rotational zero-point motion correction

$$E_{0^+} \approx E_{intr} - \frac{\langle \hat{\mathbf{J}}^2 \rangle}{2\,\mathcal{I}} \quad \text{where } E_{intr} = \frac{\langle \Psi_{intr}|\hat{H}_{\text{eff}}|\Psi_{intr}\rangle}{\langle \Psi_{intr}|\Psi_{intr}\rangle}$$

$\langle \hat{\mathbf{J}}^2 \rangle$: expectation value of $\hat{\mathbf{J}}^2$ in a BCS state

$\mathcal{I}$: moment of inertia, Belyaev formula

Vibrational zero-point motion : no systematic effect expected as function of deformation

⇒ **not taken into account**

⇝

Constrained calculations

Variational calculations with several constraints :

- ☞ approximate restoration of particle number within HF+BCS (good N and Z on average)
- ☞ position of the center of mass of the fissioning nucleus : reference point for global multipole moments calculations
- ☞ shape of the fissioning nucleus : elongation $\langle \hat{Q}_{20} \rangle$, triaxiality $\langle \hat{Q}_{22} \rangle$, left-right asymmetry $\langle \hat{Q}_{30} \rangle$, neck formation $\langle \hat{Q}_{40} \rangle$ (axial and parity symmetries non simultaneously broken)
- ☞ characteristics of fragments : mass A_H and charge Z_H of the heavy fragment, elongations $\langle \hat{Q}_{20}^{(i)} \rangle$ of both fragments and distance between their centers of mass $D = \left| z_{cm}^{(1)} - z_{cm}^{(2)} \right|$

$$\Longrightarrow \quad \delta\left[\langle \hat{H} \rangle - \sum_q \lambda_q \langle \hat{N}_q \rangle - C_{20} \Big(\langle \hat{Q}_{20} \rangle - \underbrace{\mu_{20}}_{\text{targeted } \langle \hat{Q}_{20} \rangle} \Big)^2 - \cdots \right] = 0$$

⇝

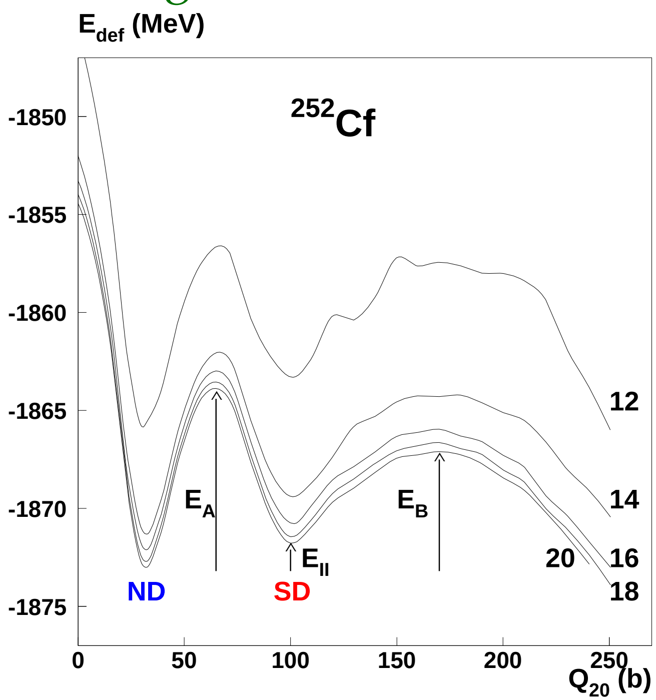
Truncated expansion basis for single-particle wave-functions

Decomposition of sp wave-functions onto the axial harmonic oscillator (HO) truncated basis :

$$\hbar\omega_\perp(n_\perp + 1) + \hbar\omega_z\left(n_z + \frac{1}{2}\right) \leqslant \hbar\omega_0(N_0 + 2) \qquad N_0 \rightsquigarrow \text{basis size}$$

☞ optimization of the basis parameters : $b = \sqrt{m\omega_0/\hbar}$ and $q = \omega_\perp/\omega_z$

☞ convergence with N_0 :

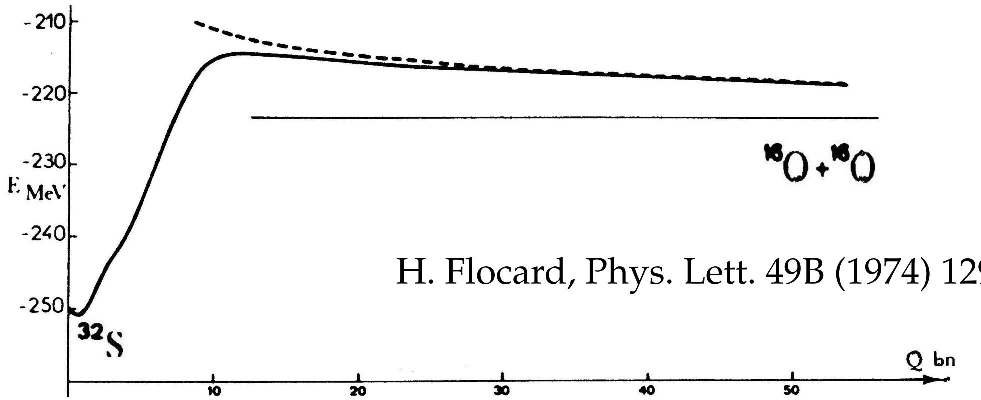


N_0	E_A (MeV)	E_{II} (MeV)	E_B (MeV)
12	10.8	2.5	8.6
14	10.9	1.9	7.1
16	10.1	1.3	6.0
18	10.2	1.3	6.1
20	10.2	1.2	5.9

$\rightsquigarrow$

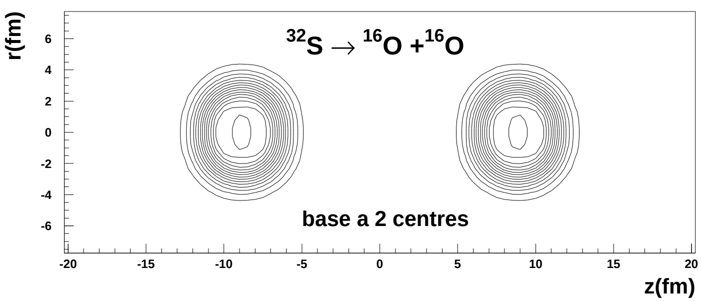
Relevance of the HO basis at scission and beyond

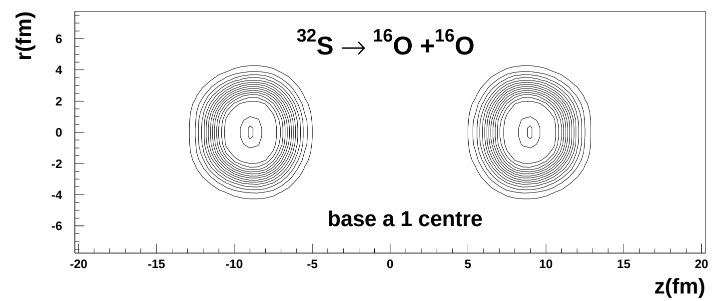
Comparison with a "2-center basis" : orthogonal polynomials associated with a weight function proportional to the sum of two gaussians : $G_{z_0}(z) \propto e^{-\beta_z^2(z-z_0)^2} + e^{-\beta_z^2(z+z_0)^2}$ (along z only)



H. Flocard, Phys. Lett. 49B (1974) 129

$\rightsquigarrow$





$$\left.\begin{array}{l} b = 0.54 \text{ fm}^{-1} \\ q = 1.7 \\ z_0 = 8.84 \text{ fm} \\ Q_{20} = 50.0 \text{ b} \end{array}\right\} \Rightarrow E^*_{\text{def}} = 29.85 \text{ MeV}$$

$$\left.\begin{array}{l} b = 0.54 \text{ fm}^{-1} \\ q = 3.5 \\ Q_{20} = 50.0 \text{ b} \end{array}\right\} \Rightarrow E^*_{\text{def}} = 34.06 \text{ MeV}$$

$\Rightarrow$ HO basis $\rightsquigarrow$ reasonable description of the whole system wave function

2nd part :
Fission barriers of actinides

Method of calculating the fission barrier heights

- ☞ Deformation energy curve : constraint on $\langle\hat{Q}_{20}\rangle$ step by step from the spherical point imposing axial and left-right symmetries
- ☞ Determination of extrema : local minima (GS, isomeric states) and maxima (saddle points)
- ☞ Checking the stability of extrema against asymmetric degrees of freedom :
  - ✻ inner barrier : triaxial shapes
  - ✻ outer barrier : left-right asymmetric shapes
- ☞ Relative energies of maxima with respect to GS : upper limits of barrier heights (partial exploration of a limited deformation space)

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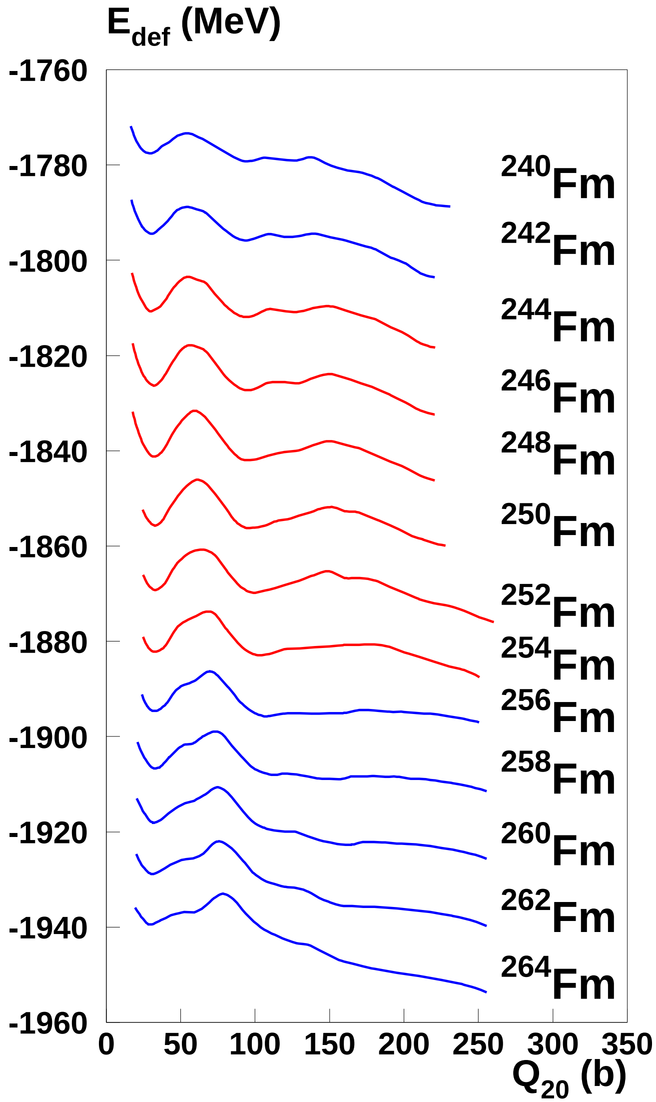
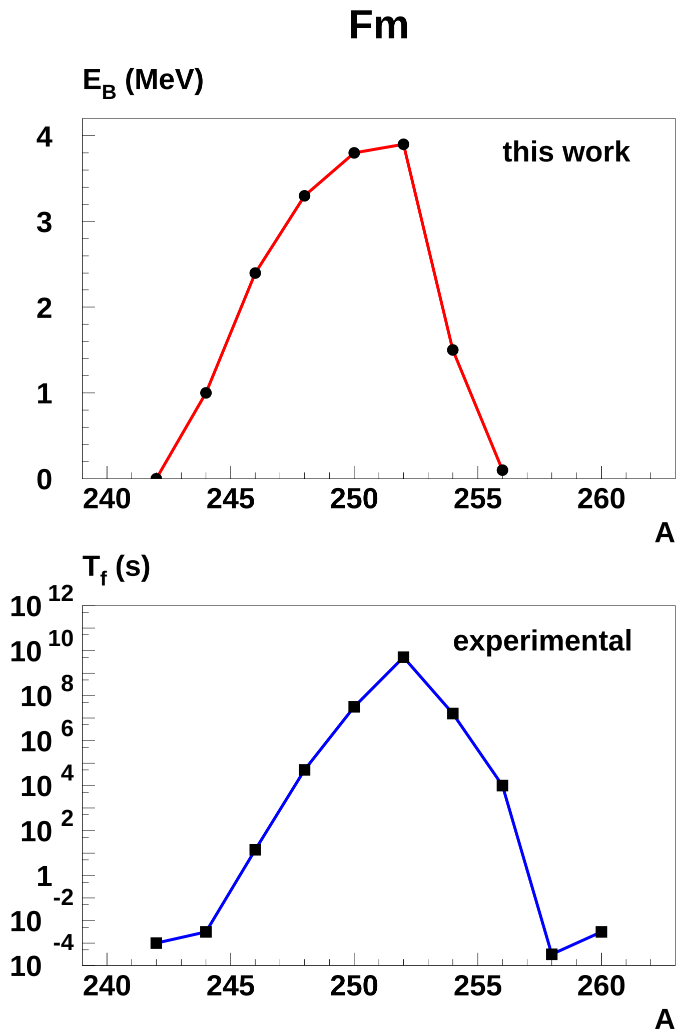
The outer barrier of even Fm isotopes

☞ Existence of the outer barrier only for $242 < A < 258$



Isotope	E_A (MeV)	E_{II} (MeV)	E_B (MeV)
^{240}Fm	4.2		
^{242}Fm	5.6	-1.4	0.0
^{244}Fm	7.2	-1.2	1.0
^{246}Fm	8.1	-1.0	2.4
^{248}Fm	9.6	-0.7	3.3
^{250}Fm	9.6	-0.1	3.8
^{252}Fm	8.1	-0.6	3.9
^{254}Fm	8.2	-0.7	1.5
^{256}Fm	8.3	-1.1	0.1
^{258}Fm	7.5		
^{260}Fm	7.4		
^{262}Fm	6.7		
^{264}Fm	6.5		

☞ Correlation between the outer barrier height and the experimental fission half-life[a]

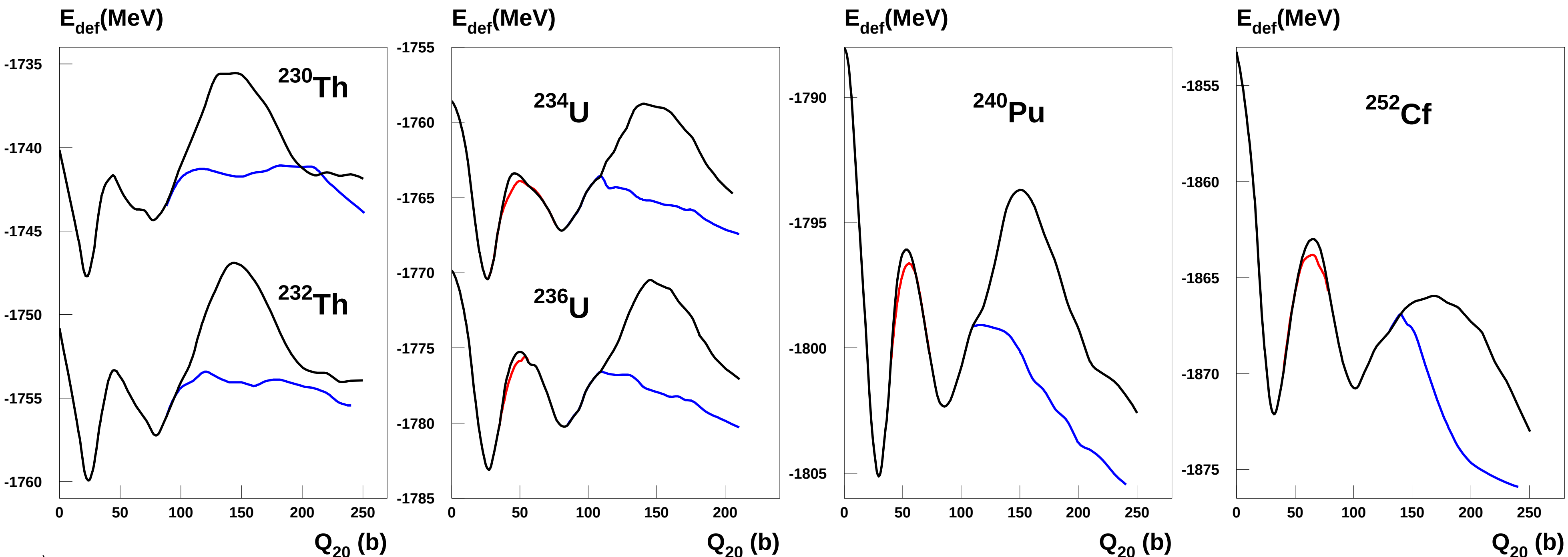


⇝

[a] D. Hoffman *et al.*, Nucl.Phys. A502 (1989) 21c

Axial or reflection symmetry breaking

☞ Deformation energy curves (without rotational correction) :



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☞ Comparison with experimental data :

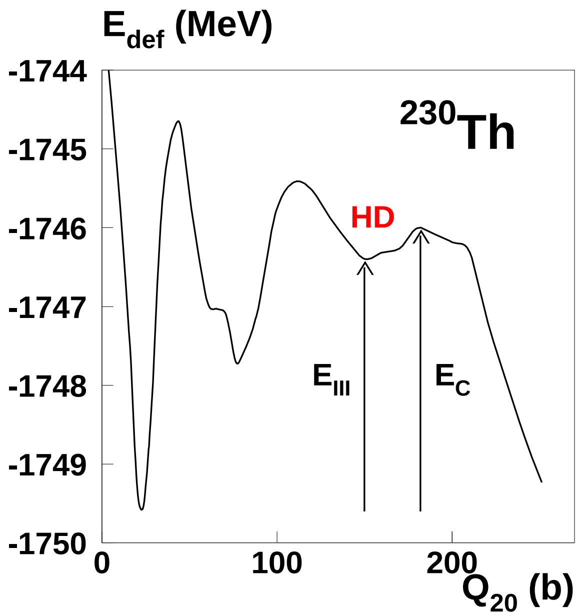
Nucleus	E_A (MeV)		E_{II} (MeV)		E_B (MeV)	
	exp. [a]	th. [b]	exp. [a]	th. [b]	exp. [a]	th. [b]
^{230}Th	6.1	4.9	–	1.8	6.5	4.4
^{232}Th	5.8	5.5	2.8 [d]	1.2	6.2	4.1
^{234}U	5.6	5.3	–	1.8	5.5	5.1
^{236}U	5.6	6.2	2.3	1.5	5.6	4.6
^{240}Pu	5.6	7.1	2.4	1.3	5.1	4.1
^{252}Cf	5.3 [c]	7.1	–	-0.3	3.5 [c]	2.9

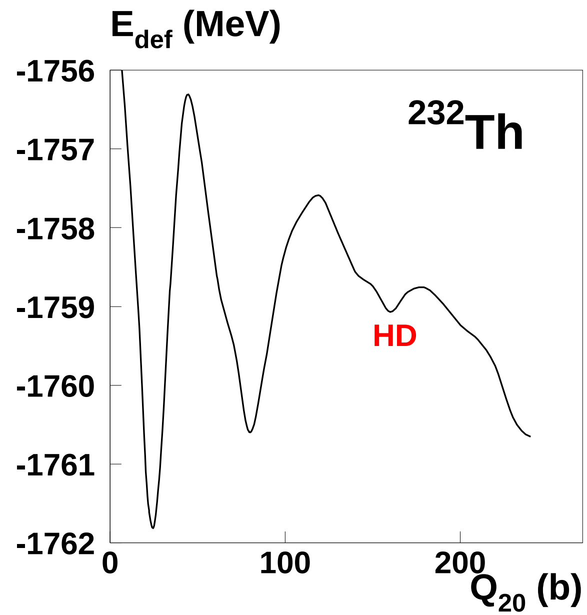
⇝

rms error (E_A)=1.0 MeV, rms error (E_B)=1.8 MeV ⇒ global rms error=1.5 MeV

[a] S. Bjørnholm, J.E. Lynn, Rev. Mod. Phys. 52 (1980) 725
[b] L. Bonneau, P. Quentin and D. Samsœn, Eur. Phys. J. A21 (2004) 391
[c] G. N. Smirenkin, IAEA Report (1993) INDC(CCP)-359
[d] H. X. Zhang *et al.*, Phys. Rev. C34 (1986) 1397

☞ Hyperdeformed left-right asymmetric well in ^{230,232}Th isotopes [a]





Isotope	E_{III} (MeV)		E_C (MeV)		$E_C - E_{III}$ (MeV)		
	Berger [b]	this work [c]	Berger [b]	this work [c]	Berger [b]	this work [c]	exp.[a]
^{230}Th	5.0	3.2	5.7	3.6	0.7	0.4	0.3
^{232}Th	4.2	2.7	4.3	3.0	0.1	0.3	–

[a] J. Blons *et al.*, Nucl. Phys. A477 (1988) 231
[b] J.-F. Berger *et al.*, Nucl. Phys. A502 (1989) 85c
[c] L. Bonneau, P. Quentin and D. Samsœn, Eur. Phys. J. A21 (2004) 391

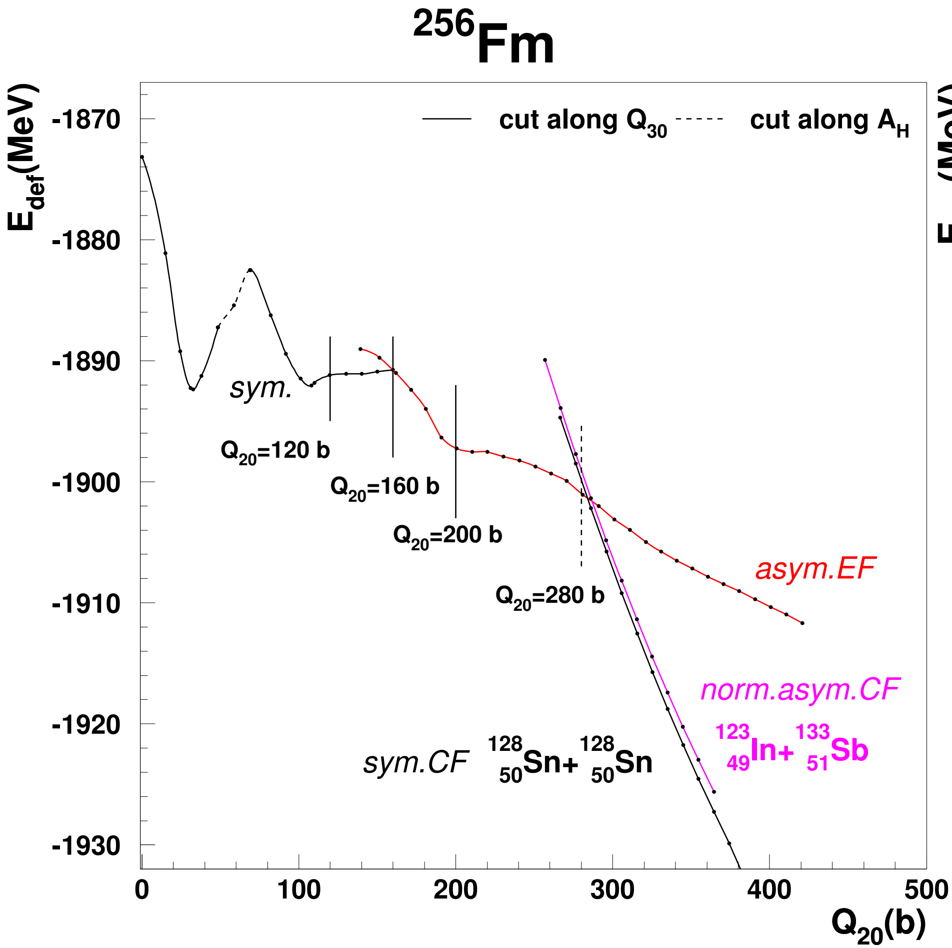
3rd part :

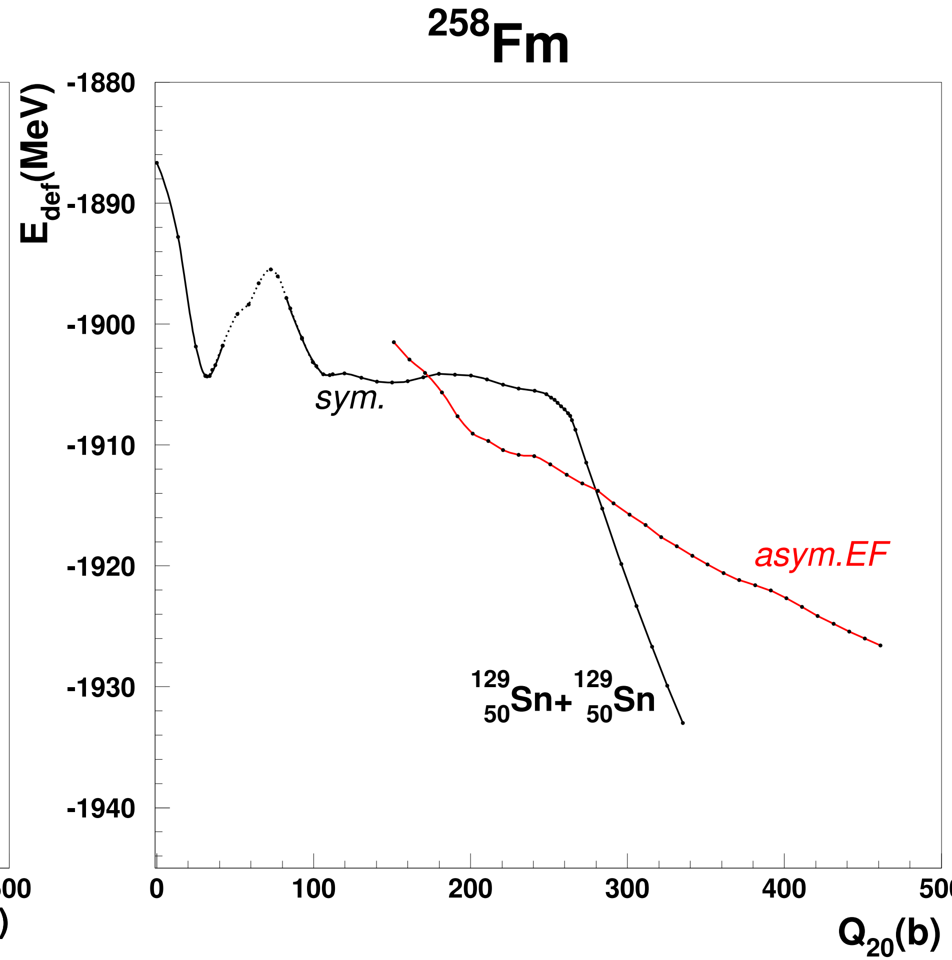
Fission and fusion properties of the PES of heavy nuclei

Method of exploring the PES

* Determination of fission valleys :
  - ☞ searching for local minima in the $\langle \hat{Q}_{30} \rangle$ direction at given $\langle \hat{Q}_{20} \rangle$-values
  - ☞ following the corresponding valleys : deformation energy curves by constraining $\langle \hat{Q}_{20} \rangle$ step by step from each of these minima until they become unstable
* Determination of fusion valleys :
  - ☞ searching for local minima in the $\langle \hat{A}_{heavy} \rangle$ direction at given $\langle \hat{Q}_{20} \rangle$-values
  - ☞ following the corresponding valleys : deformation energy curves by constraining $\langle \hat{Q}_{20} \rangle$ step by step from each of these minima until corresponding two-body shapes become unstable

Shape transition of the fragments mass distribution of the Fm isotopes

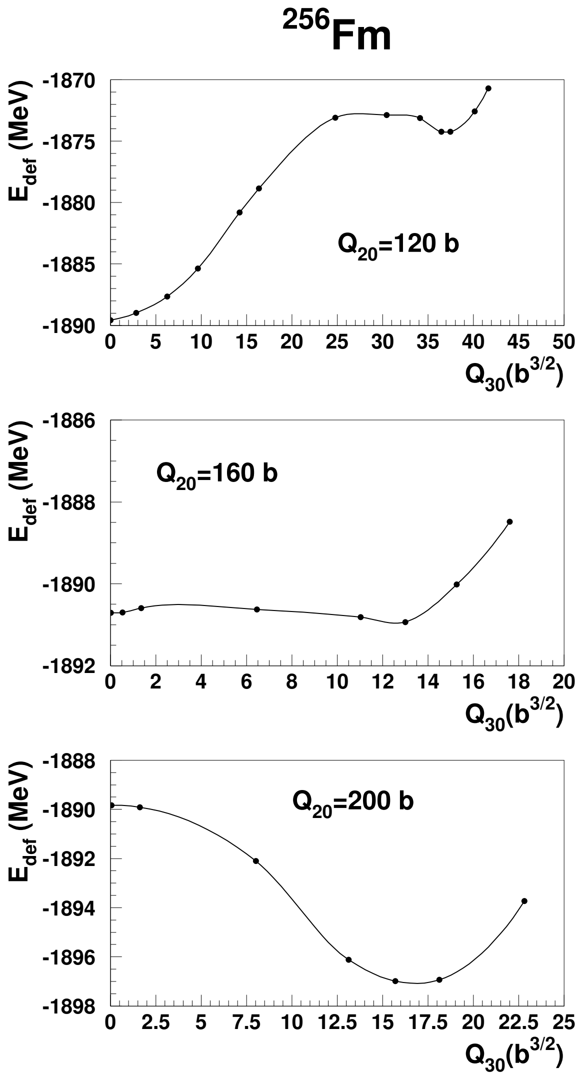


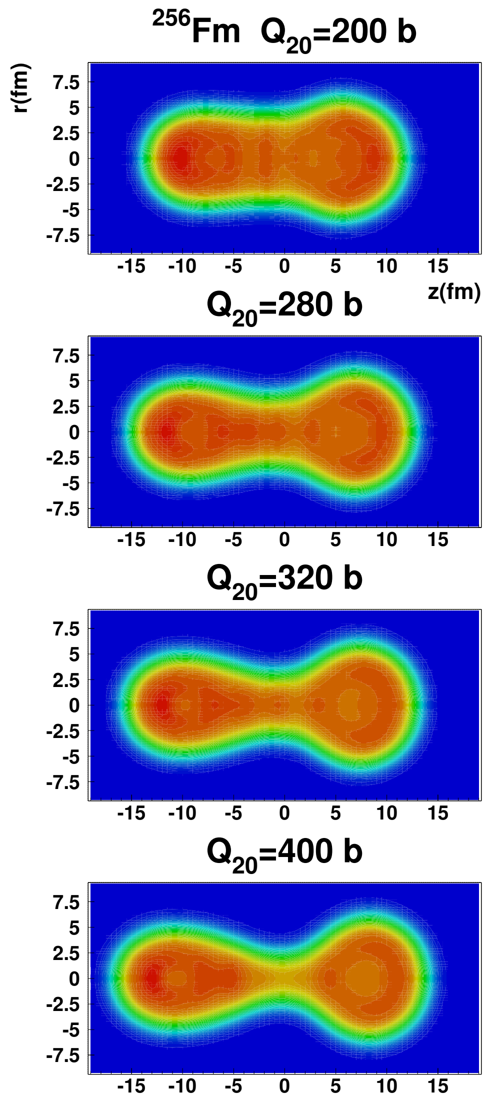


⇒ asymmetric mass distribution

⇒ symmetric mass distribution

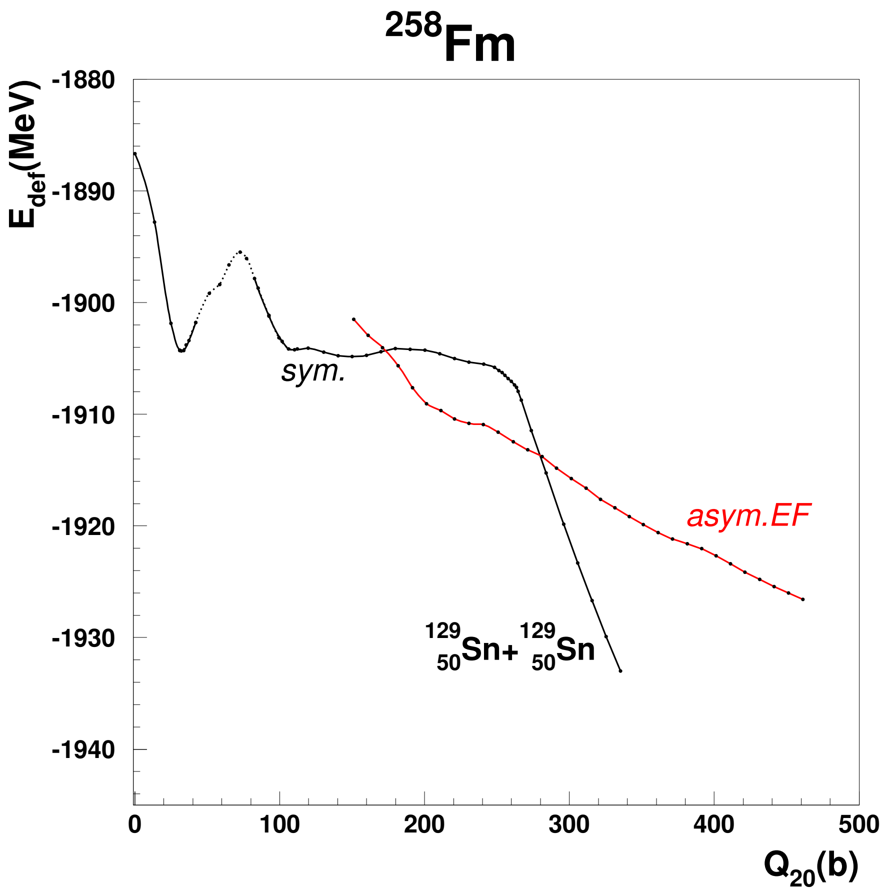
Asymmetric fission path of ^{256}Fm

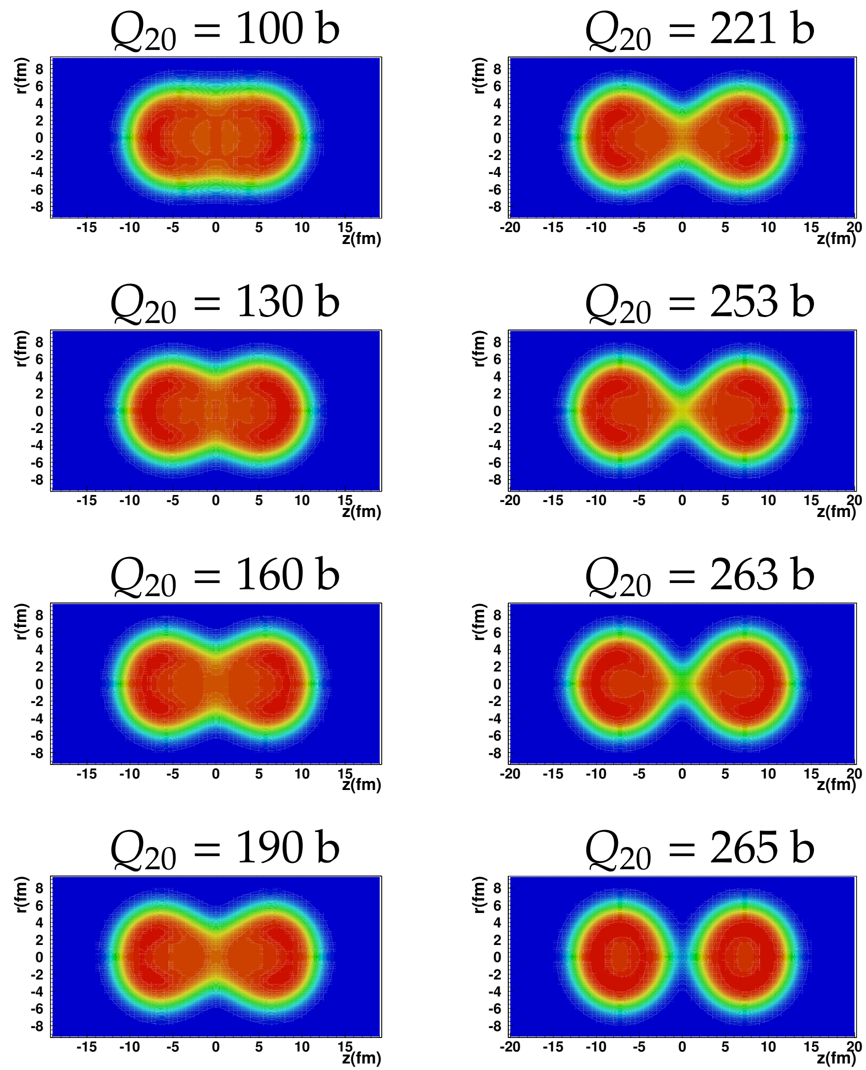




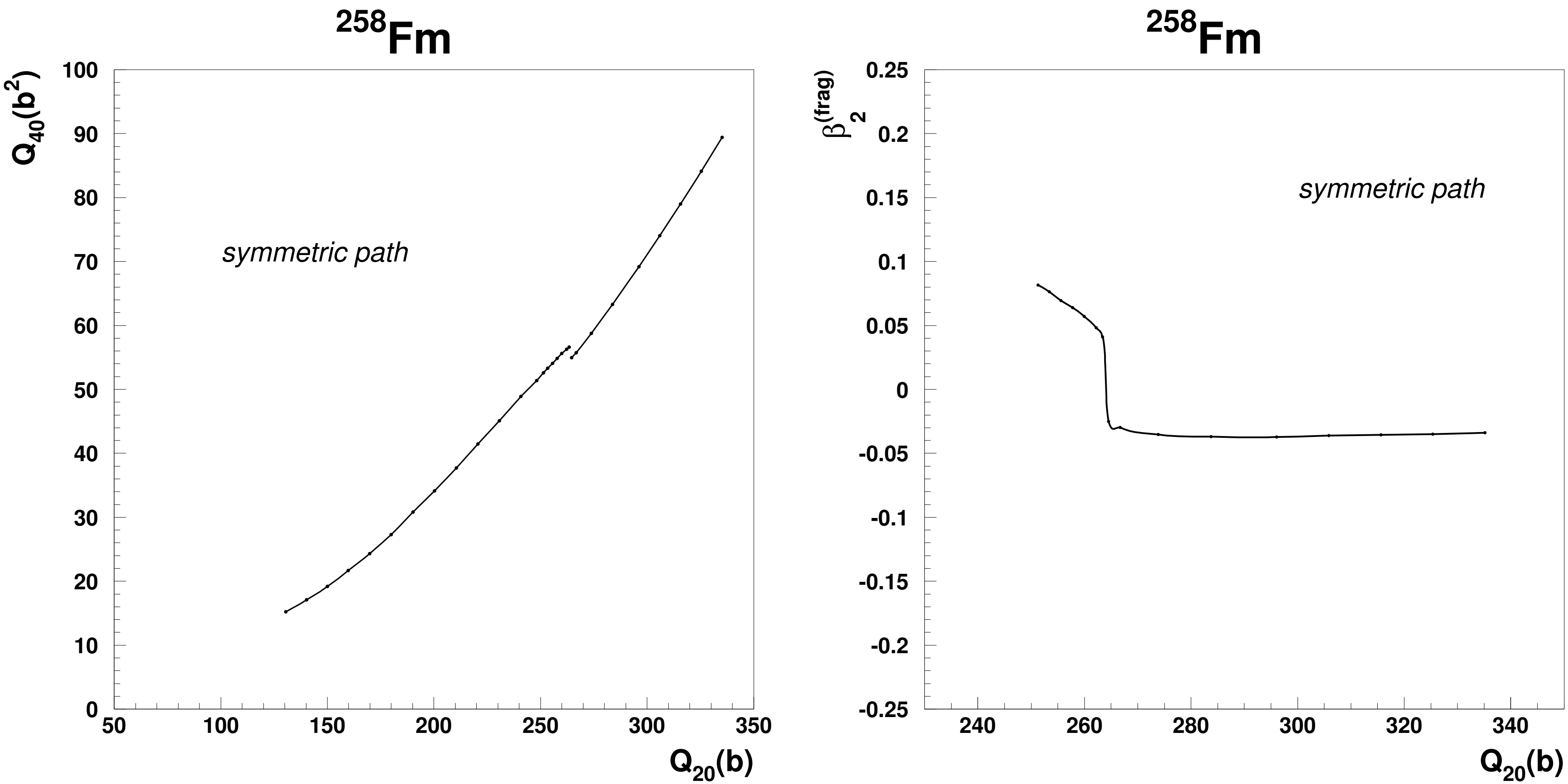
Symmetric fission path of ^{258}Fm

☞ continuity of the energy variation



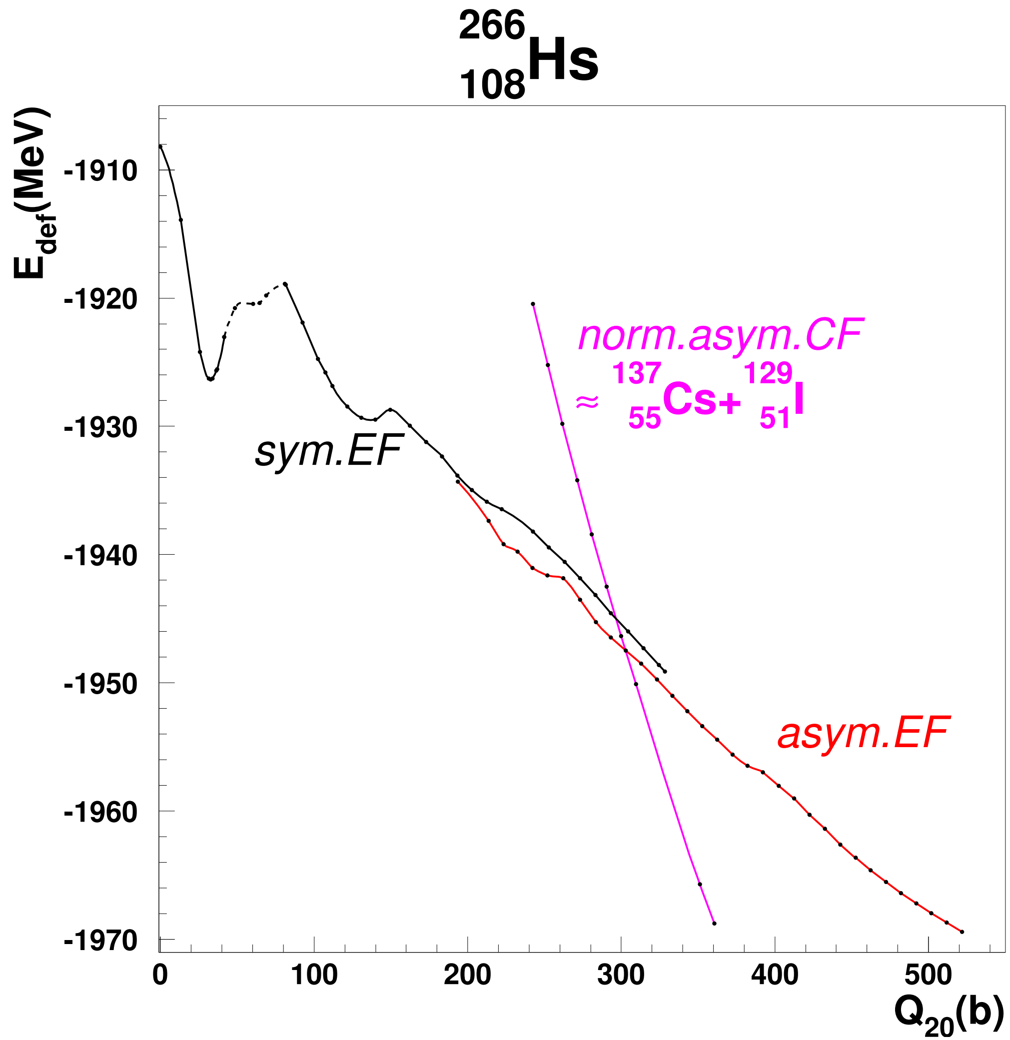


☞ discontinuity of the Q_{40} and $\beta_2^{(frag)}$ variations



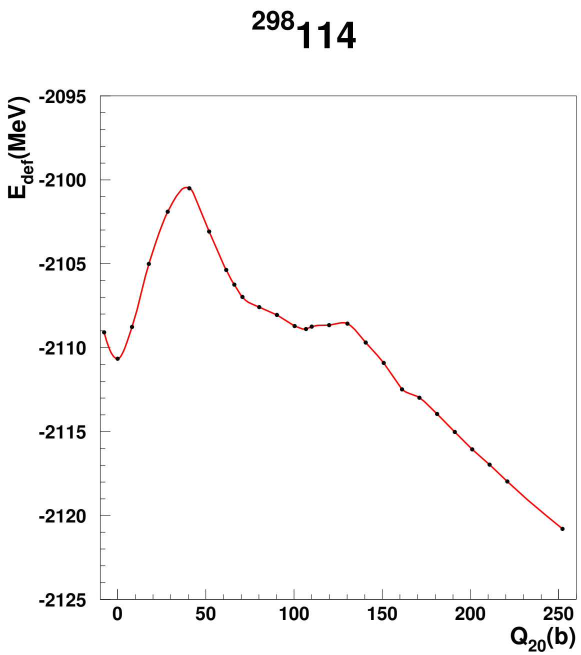
Stability of super-heavy nuclei against fission

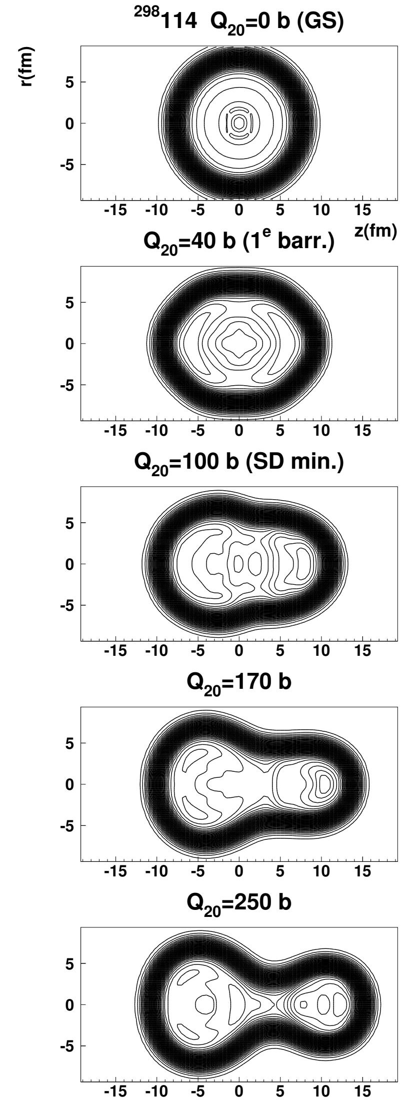
☞ ^{266}Hs (Z = 108) : E_A = 7.4 MeV ; P. Moller *et al.* : 7.5 MeV (priv. comm.)



☞ doubly-magic SH nucleus $Z = 114$, $N = 184$: $E_A = 7.8$ MeV

Exp. $E_A(^{292}114) > 6.8$ MeV [a] ; Smolanczuk[b] : $E_A(^{298}114) = 6.2$ MeV ; Bürvenich[c] : $E_A(^{290}114) =$ 3.56 – 8.57 MeV

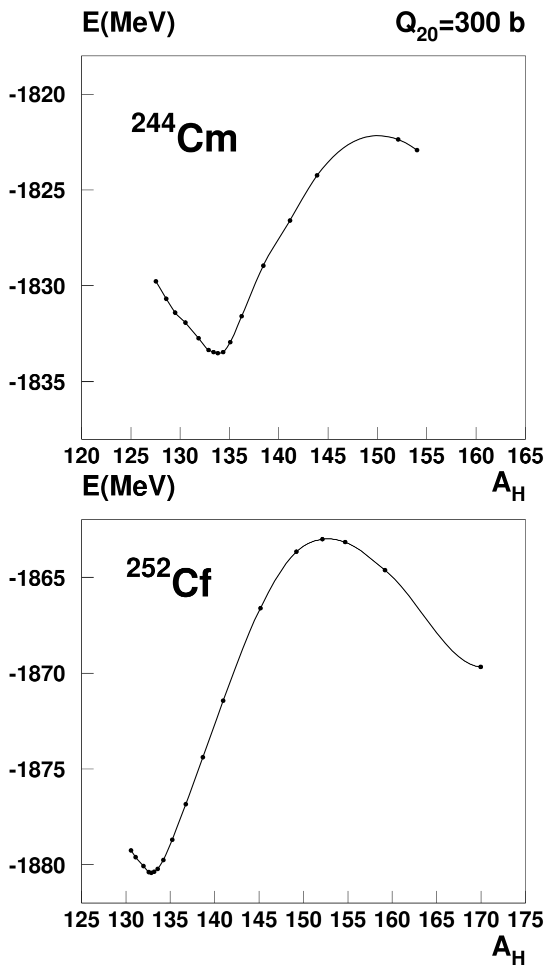


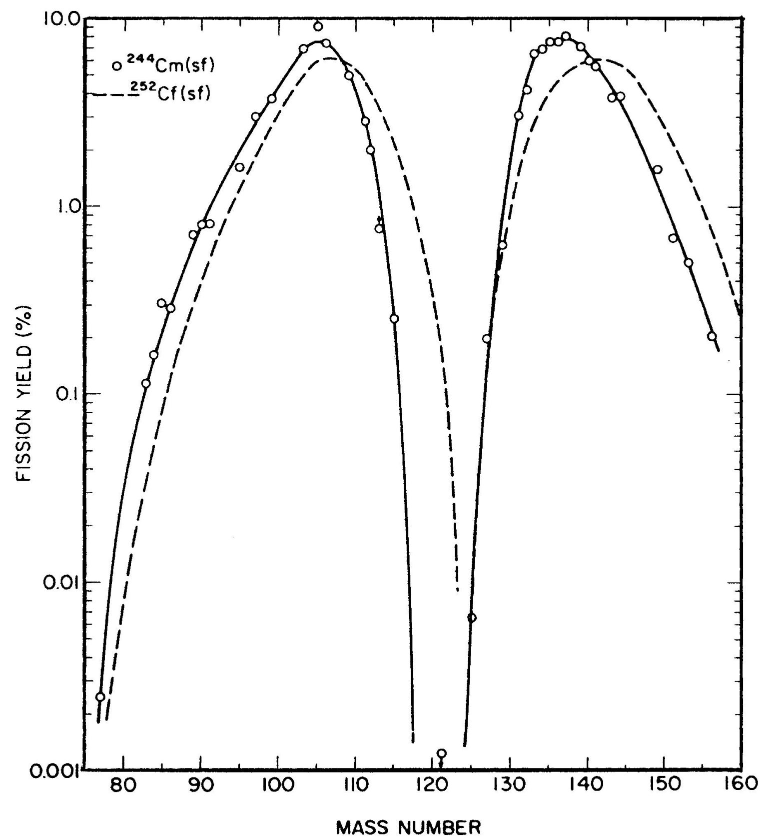


[a] M.G. Itkis, Yu.Ts. Oganessian and V.I. Zagrebaev, PRC65, 044602 (2002)
[b] R. Smolanczuk, PRC56, 812 (1997)
[c] T. Bürvenich, M. Bender, J.A. Maruhn and P.-G. Reinhard, PRC69, 014307 (2004)

Most probable fragmentation

☞ Configuration energy curves (at a fixed Q_{20}-value) compared with experimental mass distributions : minimal energy ⇒ ≈ maximal yield





K.F. Flynn *et al.*, Phys. Rev. C6 (1972) 2211

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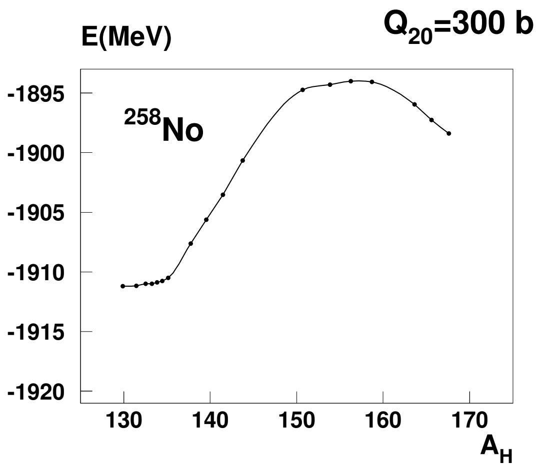
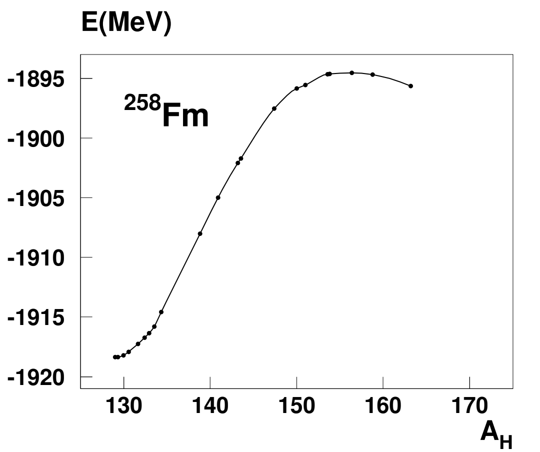




rather shallow minimum at $A/2$

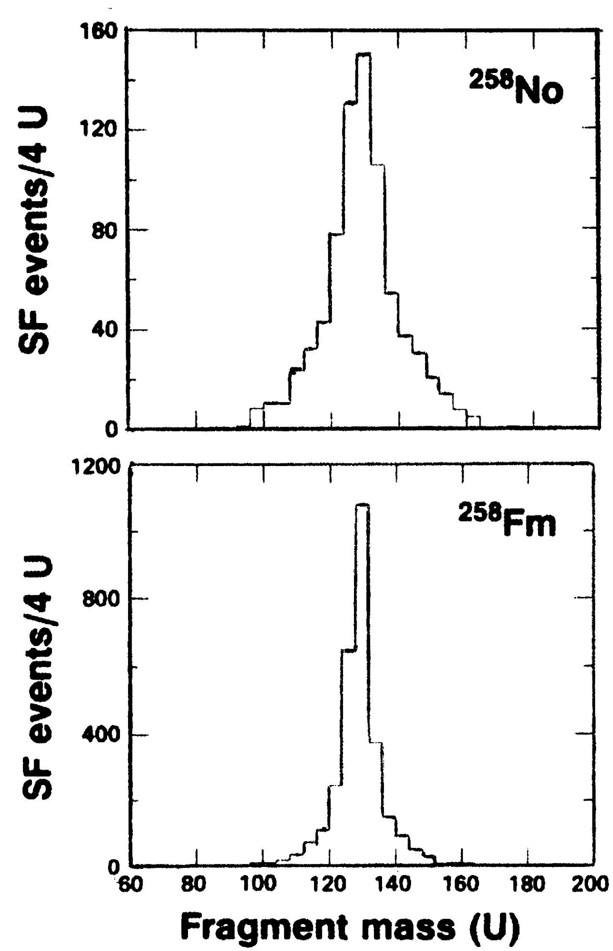
⇓

symmetric mass distribution with a rather large base

more pronounced minimum at $A/2$

⇓

symmetric mass distribution more peaked at $A/2$



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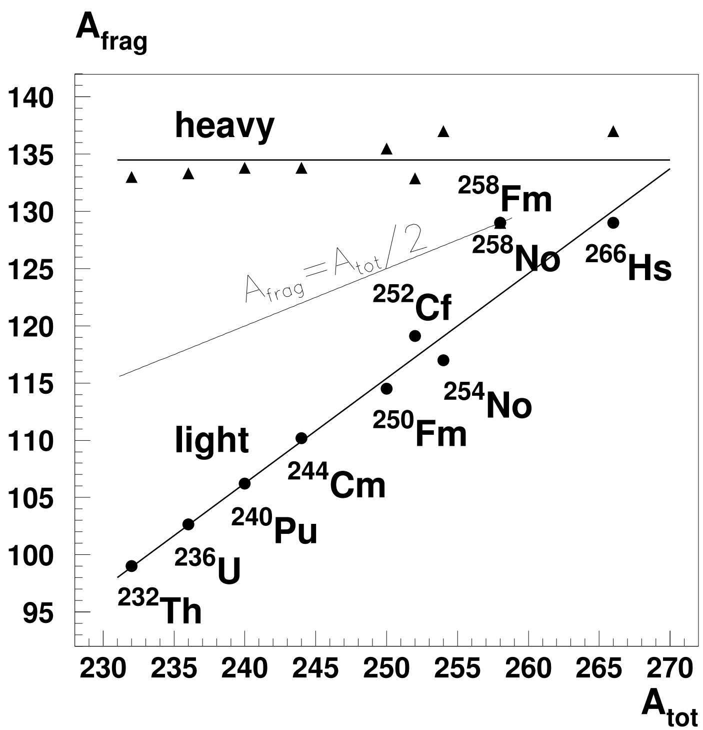
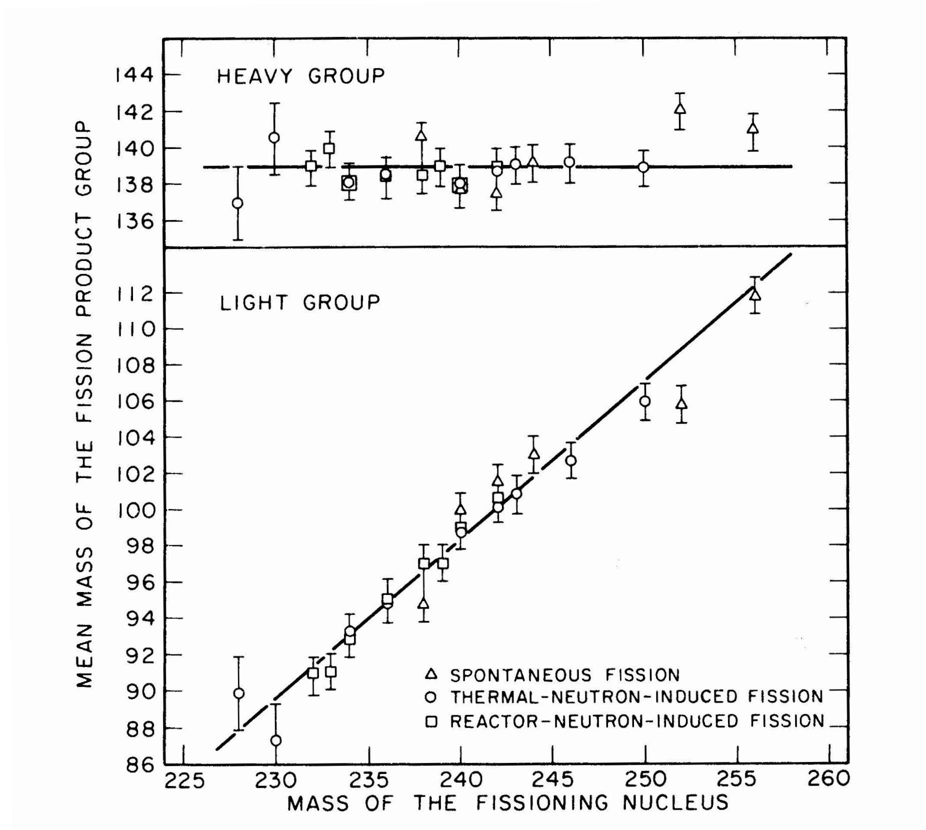
E.K. Hulet *et al.*, Phys. Rev. Lett. 56 (1986) 313

☞ Most probable masses of fragments as a function of the mass of the compound nucleus





K.F. Flynn *et al.*, Phys. Rev. C5 (1972) 1725

$\Longrightarrow$ reasonably close to the experimental mean fragment masses

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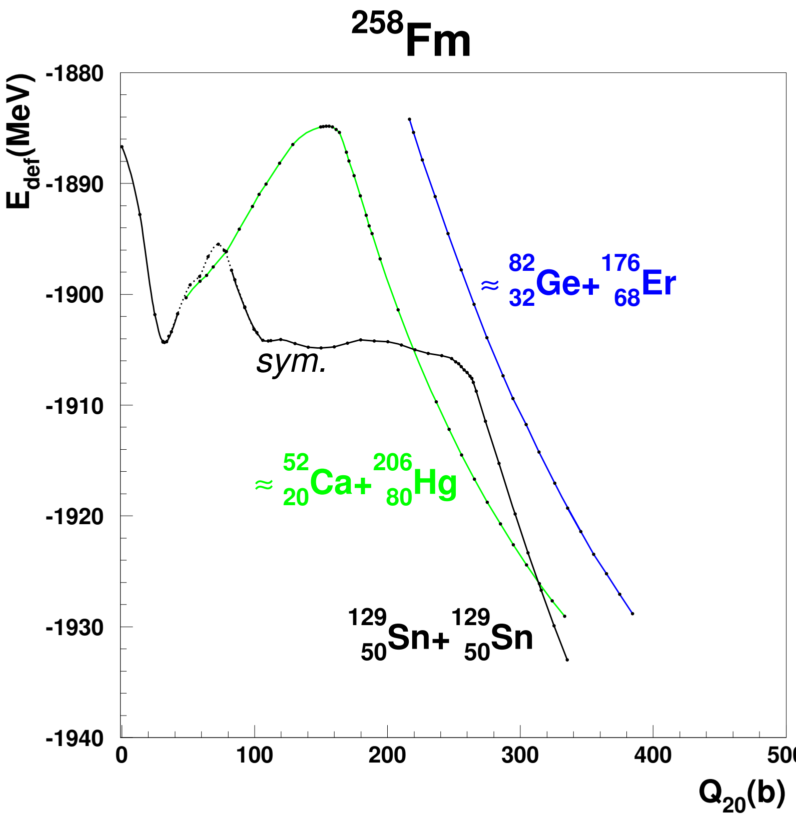
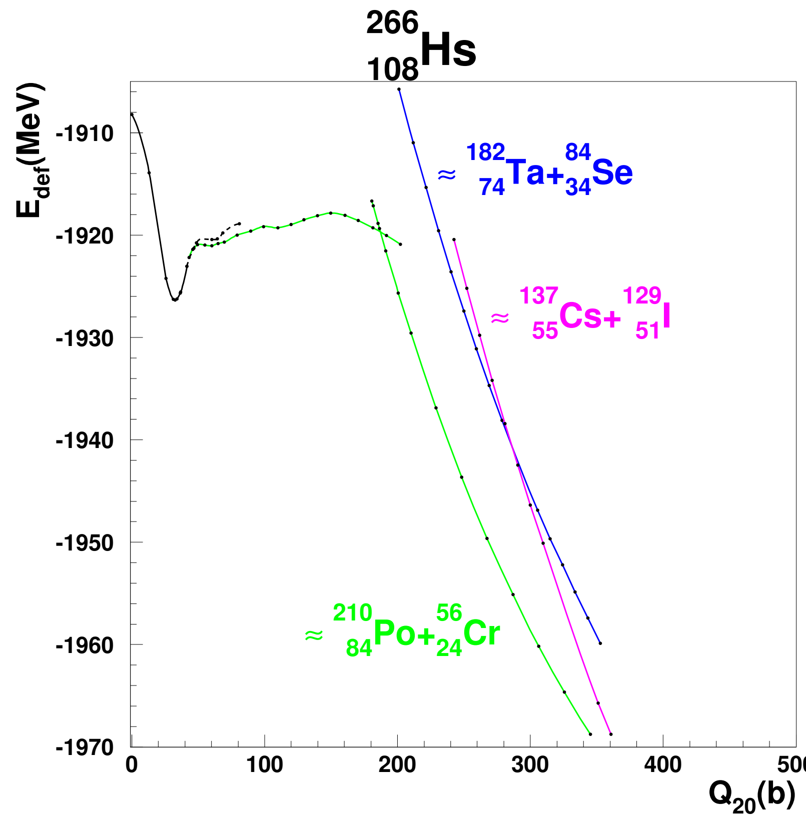
Fusion properties of the PES of heavy nuclei

☞ Fusion valleys of ^{258}Fm and ^{266}Hs





most favorable fusion reaction channel : ^{56}Cr(^{210}Po,1n)^{265}Hs (1*n* channel experimentally predominant in the ^{58}Fe(^{208}Pb,1n) ^{265}Hs[a])

[a] S.Hoffman *et al.*, Z.Phys. A358,377 (1997)

☞ Fusion barrier heights

$$B_{fus} = Q_{fus} + E_{CN}^{(min)}$$

Q_{fus} : Q-value of the reaction (involving the CN, not the evaporation residue)
$E_{CN}^{(min)}$: energy at the top of the fusion barrier with respect to the GS of the CN

CN	reaction	$E_{CN}^{(min)(exp)}$	$E_{CN}^{(min)(HF)}$	$B_{fus}^{(HF)}$	$B_{fus}^{(mic-mac)}$	$B_{fus}^{(ETF)}$ [b]	$B_{fus}^{(Bass)}$
^{256}Fm	^{206}Hg+^{50}Ca		20.0	166.3		175.5	
^{258}Fm	^{206}Hg+^{52}Ca		19.5	163.3		174.7	
^{266}Hs	^{210}Po+^{56}Cr		9.7	202.1		219.8	
^{266}Hs	^{208}Pb+^{58}Fe	~10 [a]			223.89 [c]	232.5	226.8

[a] S.Hoffman *et al.*, Z.Phys. A358,377 (1997)

[b] A. Dobrowolski, K. Pomorski and J. Bartel, Nucl. Phys. A729 (2003) 713

[c] P. Moller, priv. comm.

4th part :

Conditional fission barriers of the light nucleus ^{70}Se

Strategy

Fissility parameter $x < 0.35$

$\Downarrow$

below the Businaro–Gallone point

$\Downarrow$

conditional barriers

☞ deformation energy curve from the GS

☞ determination of the energetically favored exit channels

☞ determination of a continuous to each exit channel

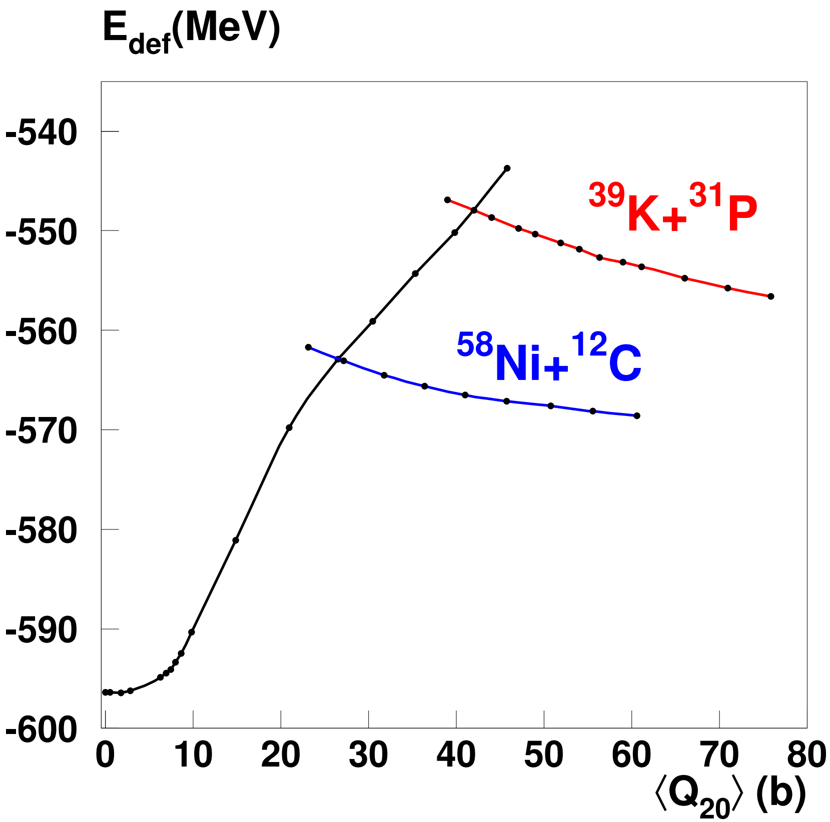
$\Downarrow$

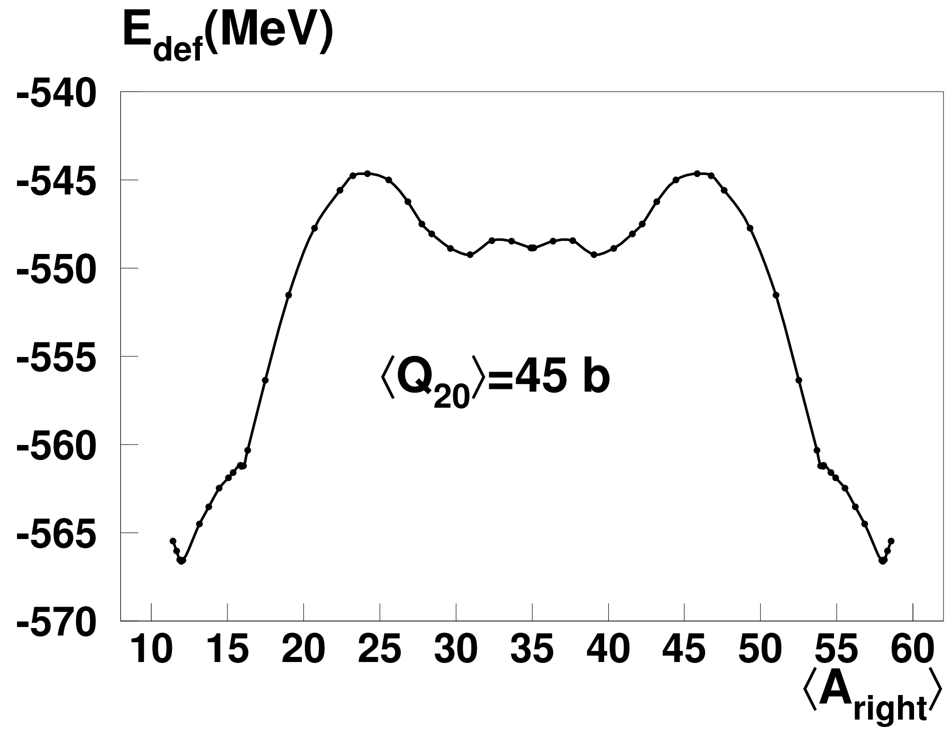
upper limit of barrier height B_Z

=

relative energy of the highest point along the path (saddle point)

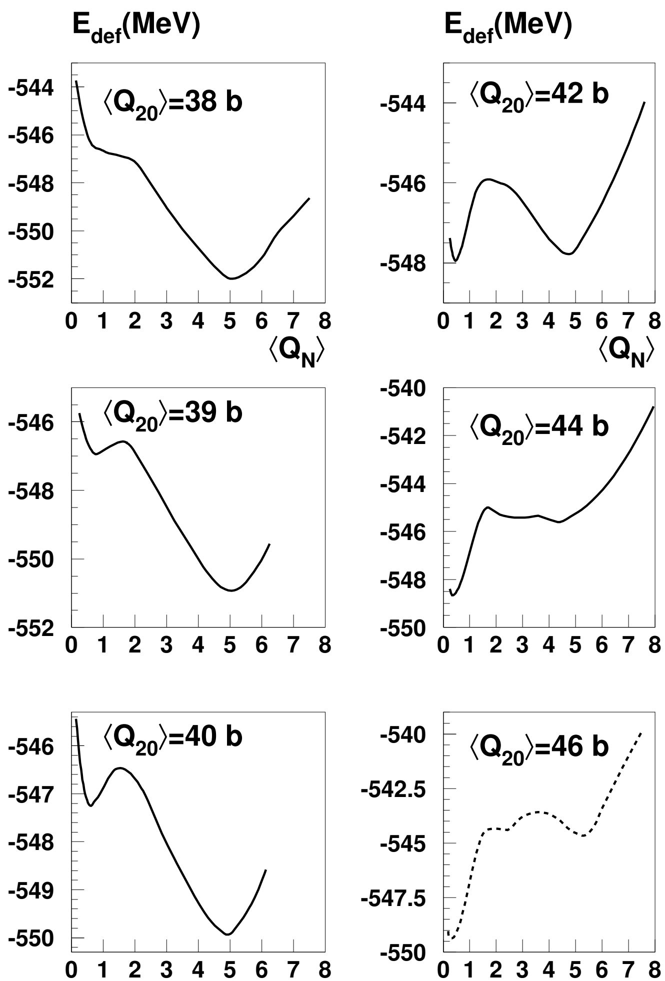
Energetically favored exit channels

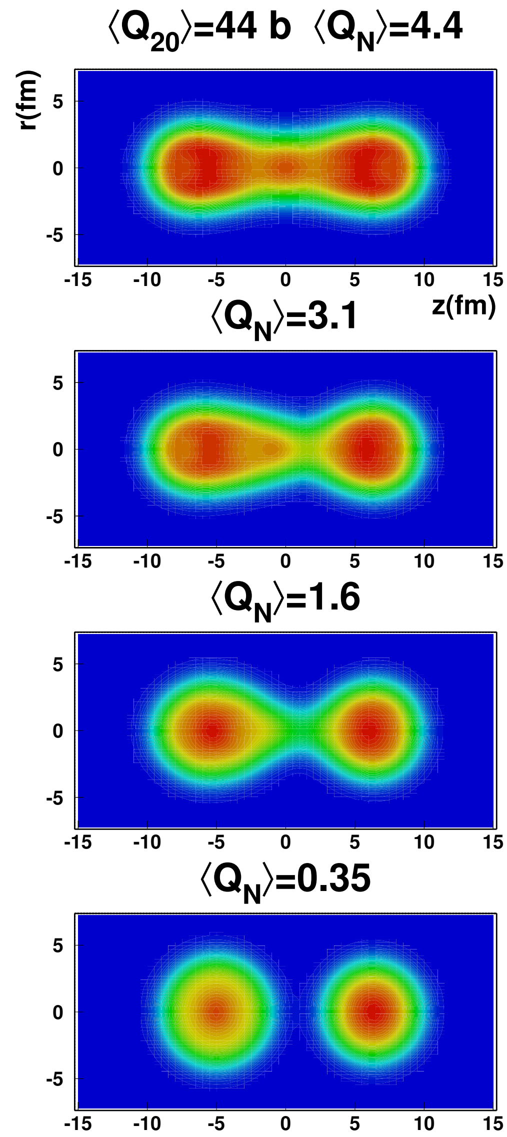




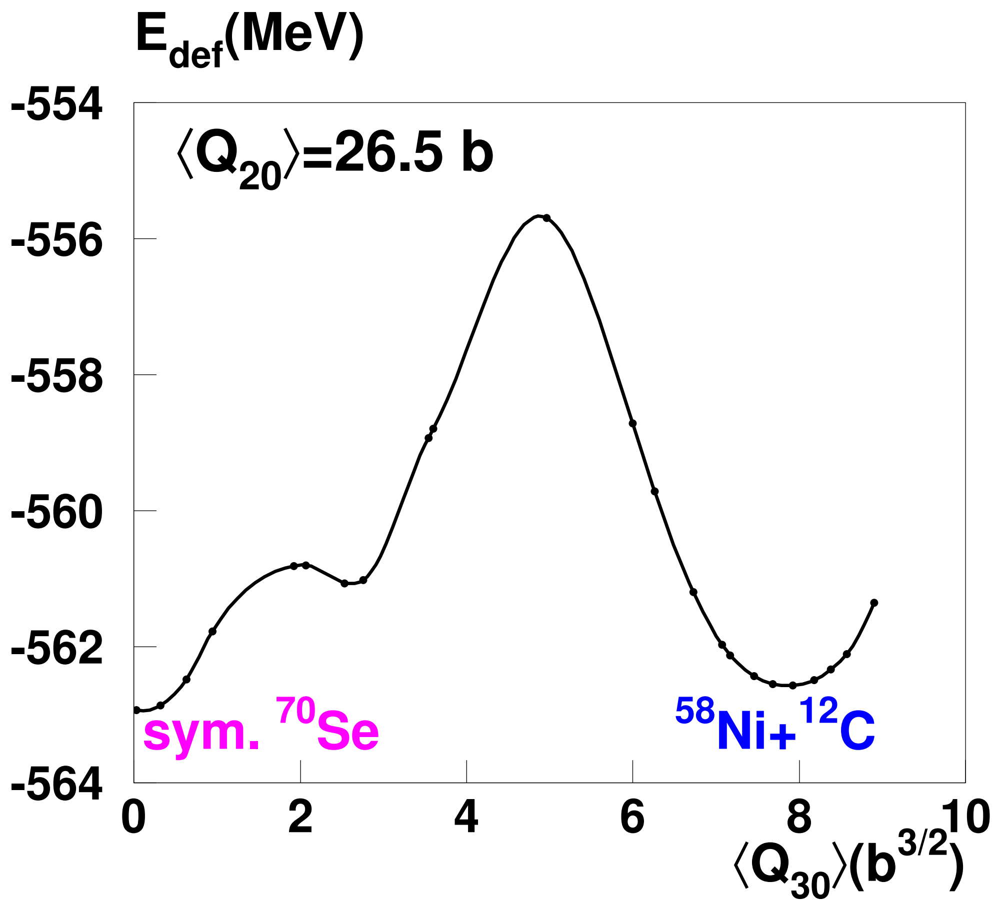
Searching for saddle points

☞ From the GS to the ^{39}K+^{31}P valley





☞ From the GS to the ^{58}Ni+^{12}C valley



Heights of the conditional fission barriers B_Z

Z_{light}	exp.[a]	this work [b]	exp.macro.[a]	Royer *et al.* [c]	Möller *et al.* [d]
6	25.3±0.8	34.7	29.5±0.8	34.5	–
15	35.1±0.8	44.9	39.3±0.8	40.5	–
17	35.2±0.8	–	39.4±0.8	40.6	37.6

☞ upper limits of our B_Z-values : 30 to 35 % (~10 MeV) above the experimental values

[a] T.S. Fan *et al.*, Nucl. Phys. A679, 121 (2000)
[b] L. Bonneau and P. Quentin, submitted to PRC
[c] G. Royer and K. Zbiri, Nucl. Phys. A697, 630 (2002)
[d] P. Möller, A. J. Sierk and A. Iwamoto, Phys. Rev. Lett. 92, 072501 (2004)

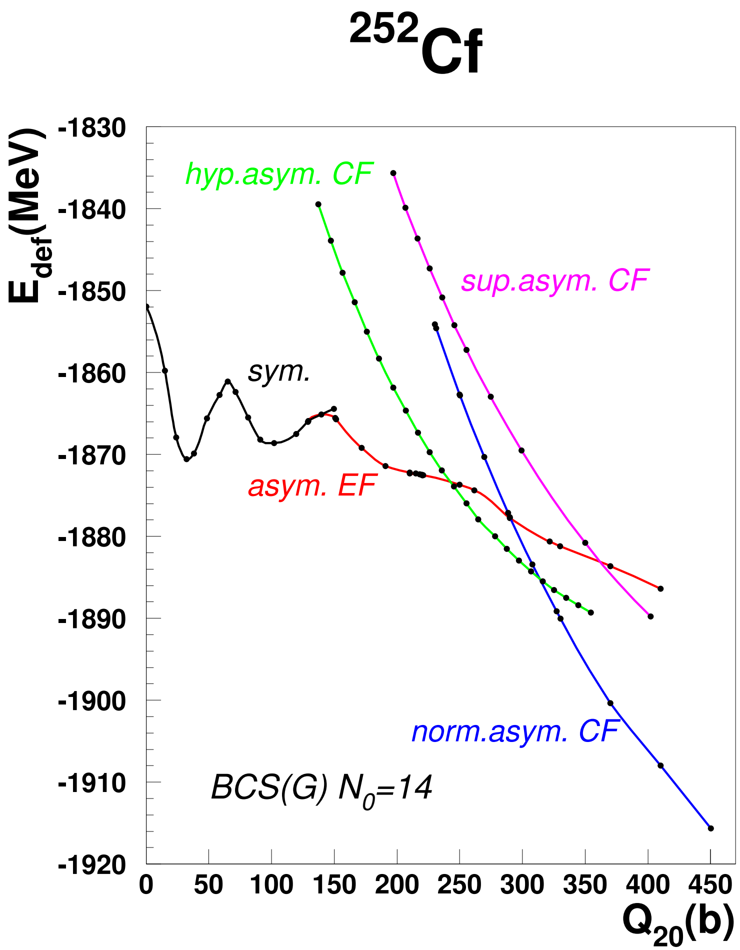
Conclusions

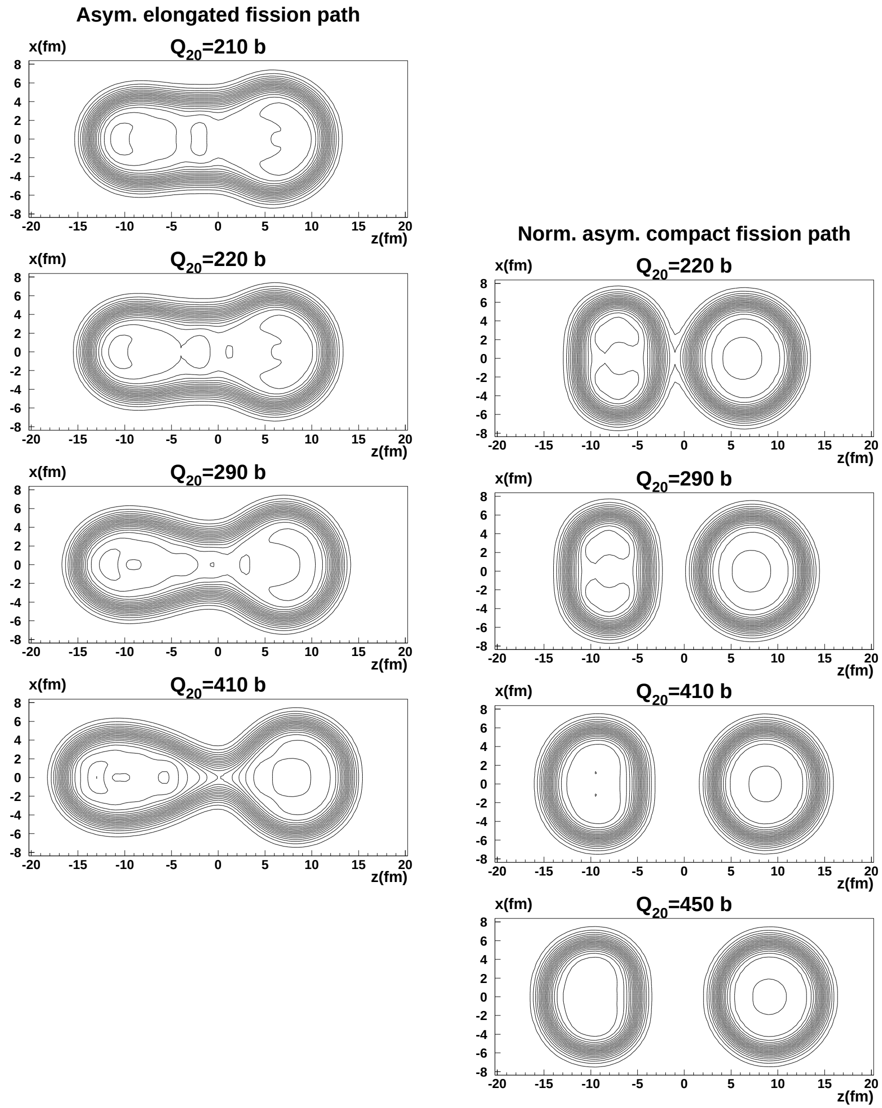
- ∗ Satisfactory description of fission barriers of actinides
- ∗ Reasonable reproduction of most probable fragmentations (fragments shell effects)
- ∗ Overestimation of the ^{70}Se conditional barriers but lower than expected (despite overestimation of the curvature energy by $\sim$ 10 MeV)
- ∗ Reasonable static fusion properties (min. excitation energy of CN)

Perspectives

- ∗ Formalism : better treatment of pairing correlations in separated fragments shapes (exact particle number approach+δ pairing force
- ∗ Fully microscopic study of fragments properties : excitation energy, spin
- ∗ Dynamical aspects : pre-scission kinetic energy, distributions (of scission configurations, fragments mass, TKE)

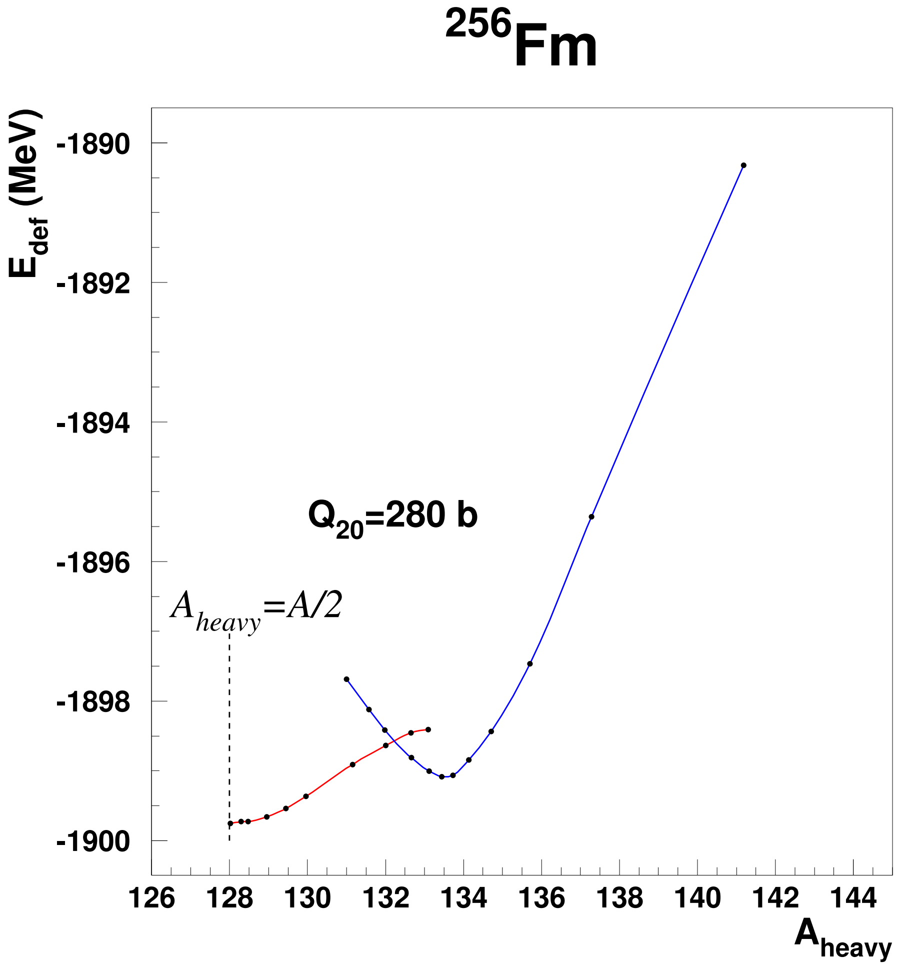
PES of ^{252}Cf

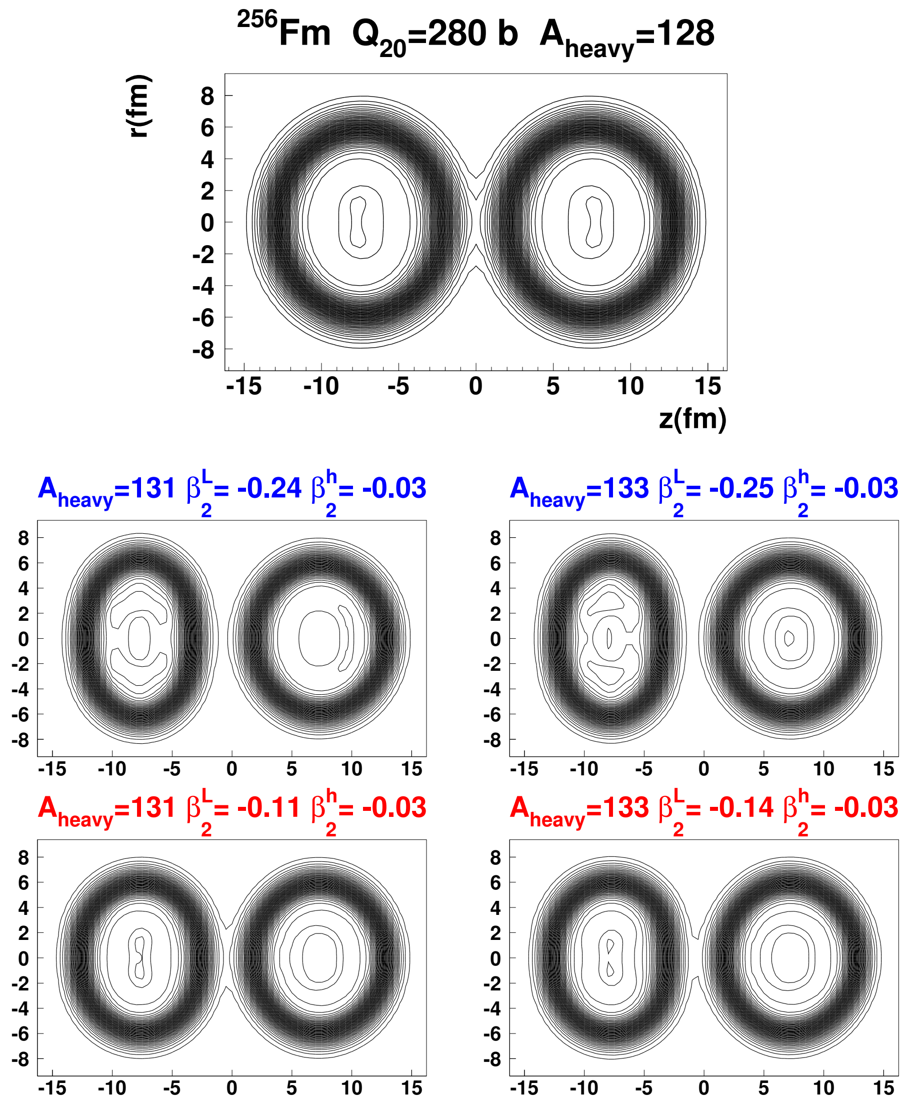


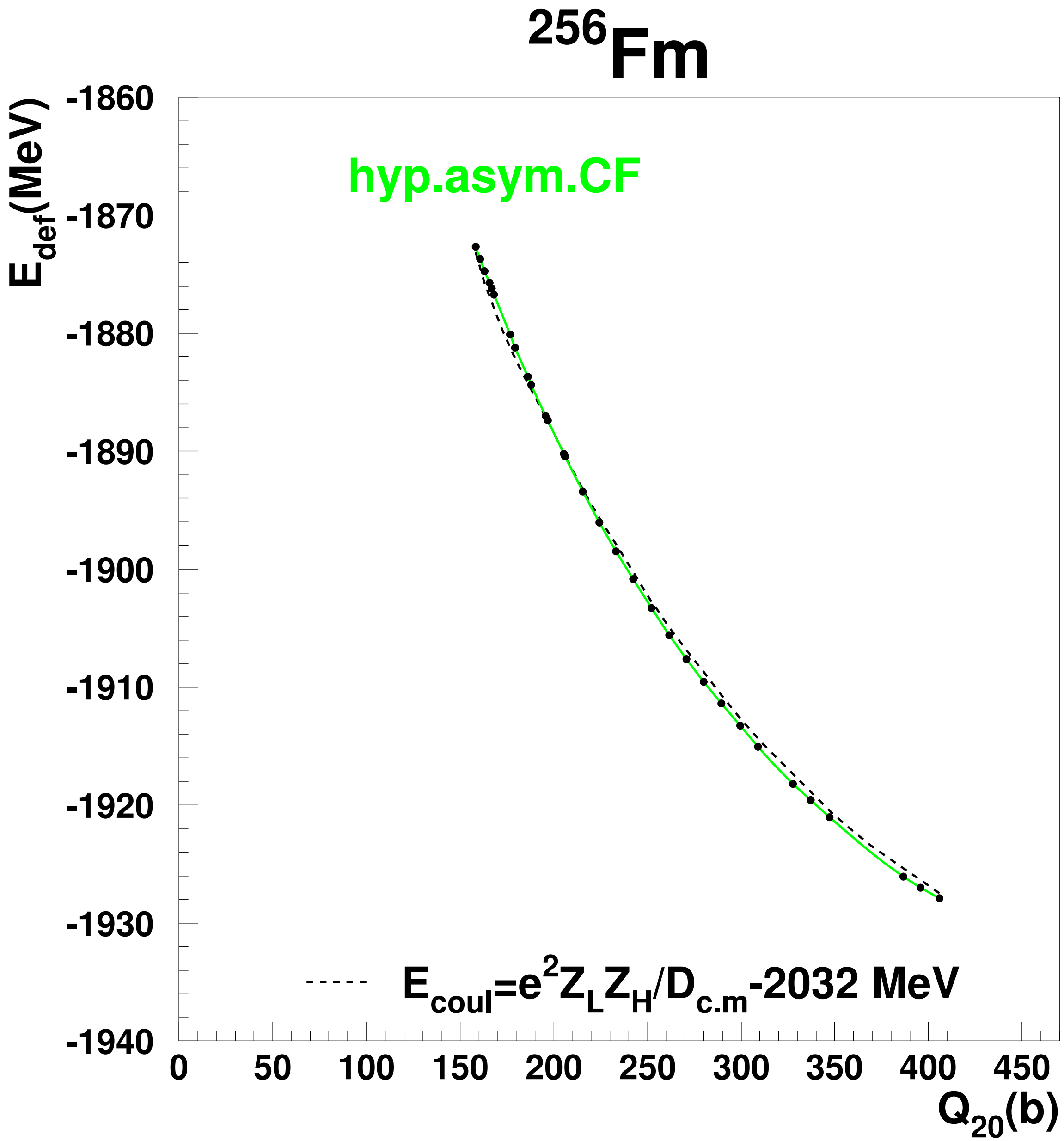


similar to results of M. Warda with HFB(Gogny D1S) (priv. comm.) and P. Möller with micro-macro model (priv. comm.)

Symmetric and asymmetric fusion valleys of ^{256}Fm

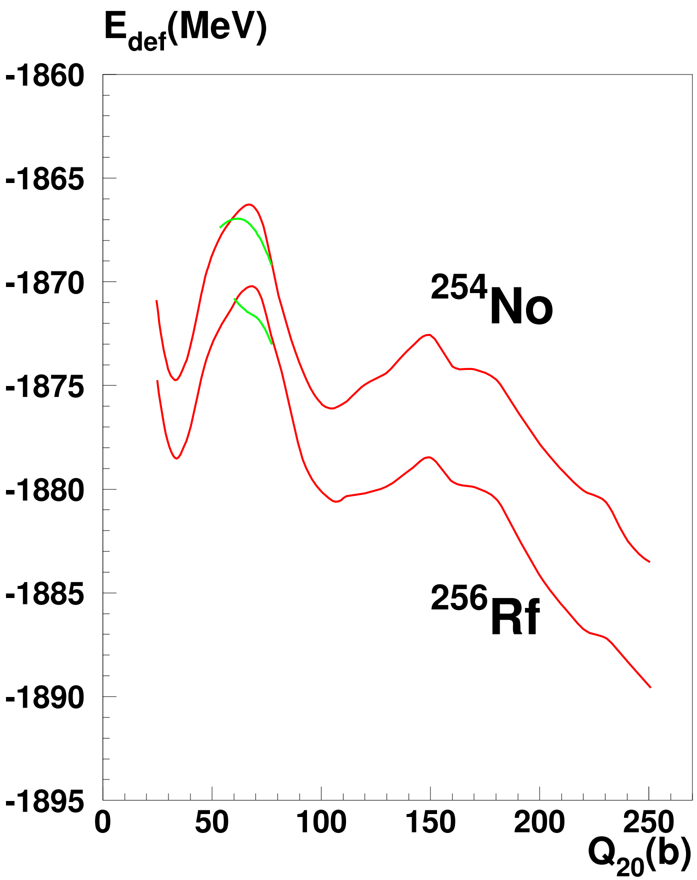





^{256}Fm
hyp.asym.CF
E_{def}(MeV)
-1860
-1870
-1880
-1890
-1900
-1910
-1920
-1930
-1940
0
50
100
150
200
250
300
350
400
450
Q_{20}(b)
$E_{coul}=e^2Z_LZ_H/D_{c.m}$-2032 MeV

Stability of super-heavy nuclei against fission

☞ Even isotopes of No ($Z = 102$) and Rf ($Z = 104$) :



Isotope	E_A (MeV)	E_{II} (MeV)	E_B (MeV)
^{252}No	8.6	-1.5	2.2
^{254}No	8.0 (7.8)	-1.4	2.2
^{256}No	8.7	-1.5	0.1
^{256}Rf	8.1 (7.6)	-2.0	0.0
^{258}Rf	7.9		
^{260}Rf	7.5		
^{262}Rf	7.8		