Saddle-point masses in the Yukawa + LSD approach

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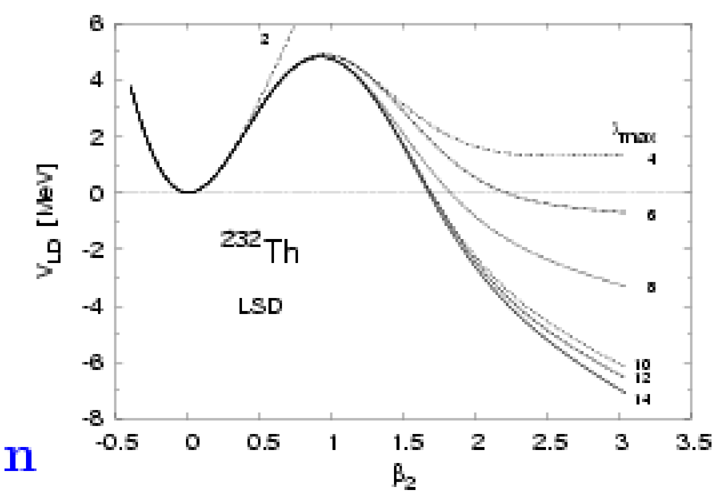
The ingredients

- Shape parametrisations for fissioning nuclei
- Macroscopic-Microscopic Model
- Fission barriers with different proton-neutron deformations
  - ▷ Stiffness of $E_{mac} \Leftrightarrow$ shell + pairing effects
- Fission barriers with left-right asymmetry and non-axiality
- Conclusions

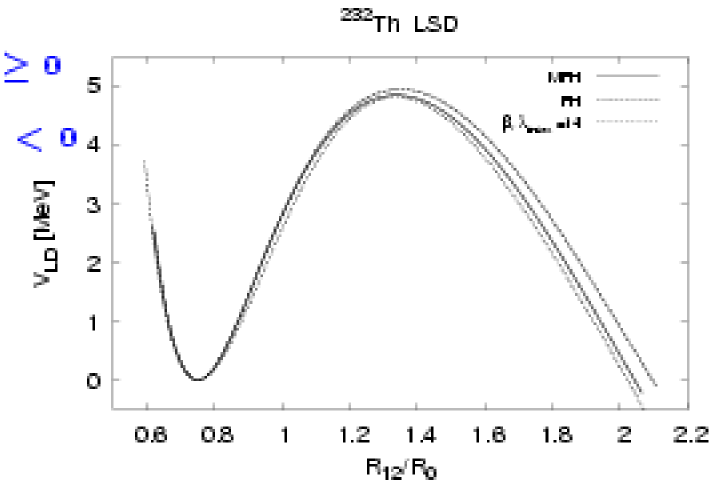
Shape parametrisations for fissioning nuclei

- Huge variety of nuclear shapes (g.s. $\Longrightarrow$ scission point)
- Only a very few relevant deformation parameters
  - Expansion in spherical harmonics



  - Funny-Hills (FH) parametrisation

$$\varrho_s^2(u) = \begin{cases} R_0^2 c^2 \left(1-u^2\right)\left(A+\alpha u+Bu^2\right) & ,\ B \geq 0 \\ R_0^2 c^2 \left(1-u^2\right)(A+\alpha u)\exp\left(Bc^3u^2\right) & ,\ B < 0 \end{cases}$$

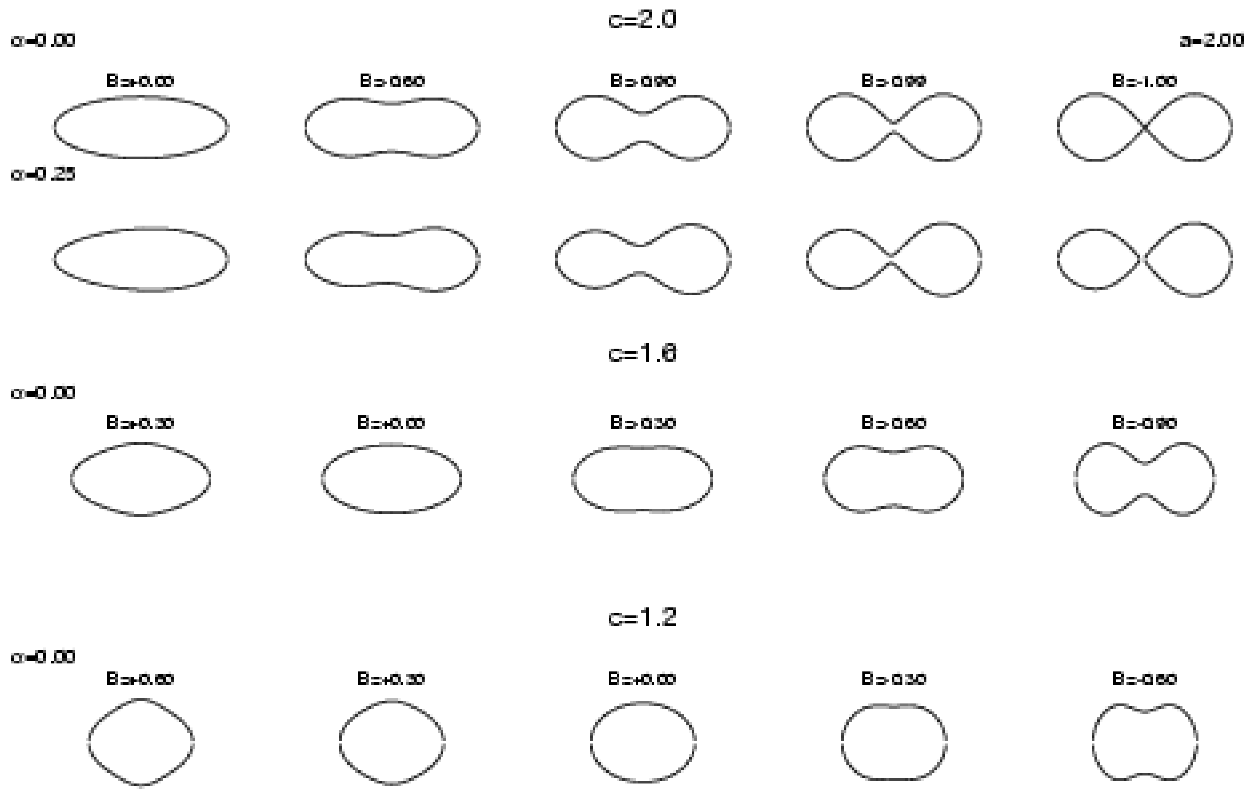


- Modified Funny-Hills shape parametrisation

$$\varrho_s^2(z) = \frac{R_o^2}{c\, f(a,B)} (1-u^2)\,(1+\alpha u - B\, e^{-a^2 u^2}) \ ,$$

where

$$f(a,B) = 1 - \frac{3\,B}{4\,a^2}\left[e^{-a^2} + \sqrt{\pi}(a - \frac{1}{2a})\,\mathrm{Erf}(a)\right]$$



breaking axial symmetry

supose ellipsoidal shape $\perp$ to z axis

and introduce the non-axiality parameter

$$\eta = \frac{a_y^2 - a_x^2}{a_y^2 + a_x^2}$$

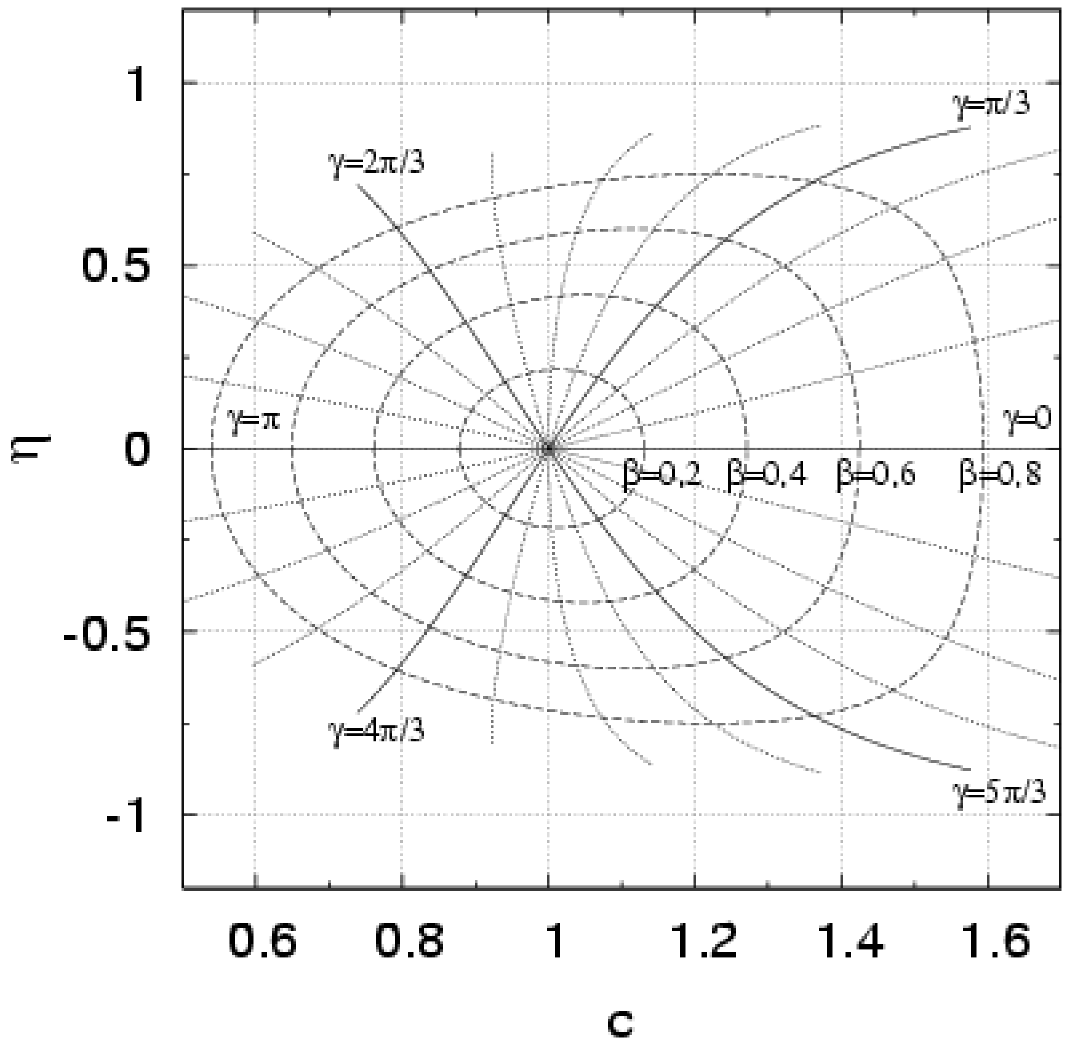
assume that η is independent of z

$$a_x(z) = \varrho_s(z) \left(\frac{1-\eta}{1+\eta} \right)^{1/4}$$

$$a_y(z) = \varrho_s(z) \left(\frac{1+\eta}{1-\eta} \right)^{1/4}$$

volume conservation then leads to

$$\tilde{\varrho}_s^2(z,\varphi) = \varrho_s^2(z) \, \frac{\sqrt{1-\eta^2}}{1+\eta\cos(2\varphi)}$$



Transformation from (c, η) to (β, γ) in the pure ellipsoidal case

Macroscopic-Microscopic Model

According to the Strutinski theorem

$$E_{\rm tot} = \int \mathcal{H}(\rho)\, d^3r = E_{\rm mac} + \delta E_{\rm mic}$$

with Lublin–Strasbourg–Drop (LSD)

$$E_{\rm mac}(Z,N,def) = a_{\rm vol}\,(1-\kappa_{\rm vol}I^2)\,A + a_{\rm surf}\,(1-\kappa_{\rm surf}I^2)\,A^{2/3}\,B_{\rm surf}(def)$$
$$+\,a_{\rm cur}\,(1-\kappa_{\rm cur}I^2)\,A^{1/3}\,B_{\rm cur}(def) + \frac{3\,e^2}{5\,r_o}\,\frac{Z^2}{A^{1/3}}\,B_{\rm Coul}(def)$$
$$-\,C_4\,\frac{Z^2}{A} - E_{\rm cong}$$

with shell and pairing corrections

$$\delta E_{\rm mic} = \delta E_{\rm shell} + \delta E_{\rm pair}$$

$$\delta E_{\rm shell} = \sum_{\rm occ} \varepsilon_\nu - \tilde{E}$$

$$\delta E_{\rm pair} = E_{\rm BCS} - \sum_{\rm occ} \varepsilon_\nu - \langle E_{\rm pair} \rangle$$

Yukawa folded mean-field potentials

$$V_{cen}(\vec{r}) = \frac{V_o}{\rho_o} \int \rho(\vec{r}\,') \, g_\lambda(\vec{r}, \vec{r}\,') \, d^3 r\,' \quad \text{with} \quad \rho(\vec{r}) = \int \rho_{sh}(\vec{r}\,') \, g_a(\vec{r}, \vec{r}\,') \, d^3 r\,'$$

where

$$g_\lambda(\vec{r}, \vec{r}\,') = \frac{1}{4\pi\lambda^2} \frac{e^{-|\vec{r}-\vec{r}\,'|/\lambda}}{|\vec{r} - \vec{r}\,'|}$$

spin–orbit potential

$$V_{s.o.} = i \, \Lambda \, \vec{\nabla} V_{cen} \cdot \left[\vec{\sigma} \times \vec{\nabla} \right]$$

Parameters:

$$V_o^{(p)} = V_s + V_a \, \bar{\delta} \qquad \text{and} \qquad V_o^{(n)} = V_s - V_a \, \bar{\delta}$$

$$\bar{\delta} = \frac{I + D_1 Z^2/A^{5/3}}{1 + D_2/A^{1/3}} \quad , \qquad I = \frac{N - Z}{A}$$

$$\Lambda^{(p)} = C_{1p} \, A + C_{2p} \qquad \text{and} \qquad \Lambda^{(n)} = C_{1n} \, A + C_{2n}$$

Constants used in the Yukawa–folding procedure

constant	value	unit	constant	value	unit
λ	0.8	$[fm]$	a	0.7	$[fm]$
V_s	52.5	$[MeV]$	V_a	48.7	$[MeV]$
C_{1p}	$2.76 \cdot 10^{-4}$	$[MeV]$	C_{2p}	0.3092	$[MeV]$
C_{1n}	$2.07 \cdot 10^{-4}$	$[MeV]$	C_{2n}	0.3479	$[MeV]$
D_1	$1.117 \cdot 10^{-2}$		D_2	3.15	

Fission barriers with different proton-neutron deformations

Potential energy through Yukawa folding

$$E_{\rm pot} = \frac{V_\circ}{2a^3\rho_\circ^2} \int\!\!\int \rho(\vec{r}\,)\, g_\lambda(\vec{r},\vec{r}\,')\, \rho(\vec{r}\,')\, d^3r\, d^3r\,'$$

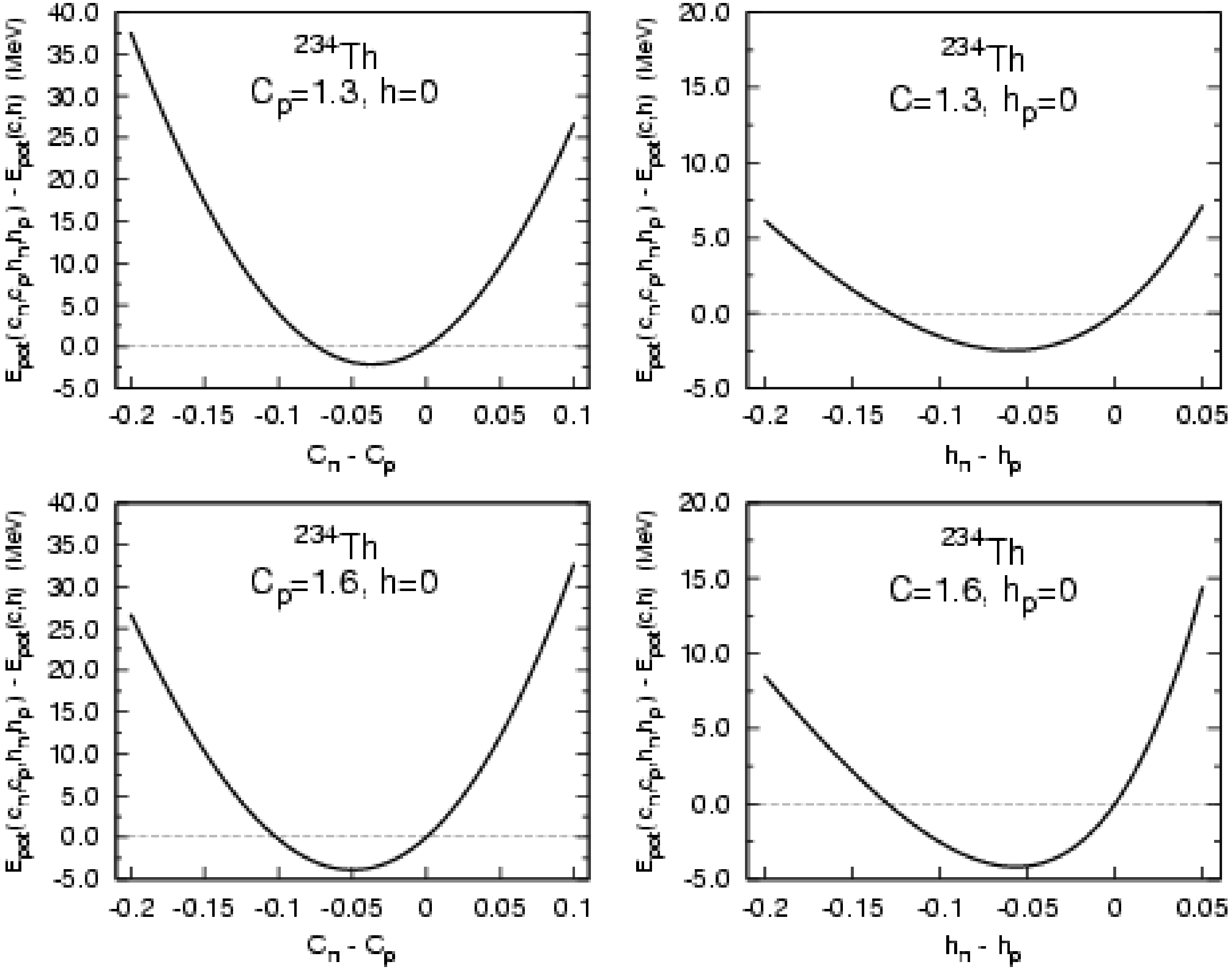
$$\rho(\vec{r}\,) = \rho_n(\vec{r}\,) + \rho_p(\vec{r}\,)$$

$$E_{\rm pot}(\mathrm{def}_p, \mathrm{def}_n) = E_{pp} + E_{nn} + 2\,E_{pn}$$

where

$$E_{qq'} = \frac{V_\circ}{2a^3\rho_\circ^2} \int_{V_q}\!\int_{V_{q'}} g_\lambda(\vec{r},\vec{r}\,')\, \rho_q(\vec{r}\,)\, \rho_{q'}(\vec{r}\,')\, d^3r\, d^3r\,'$$

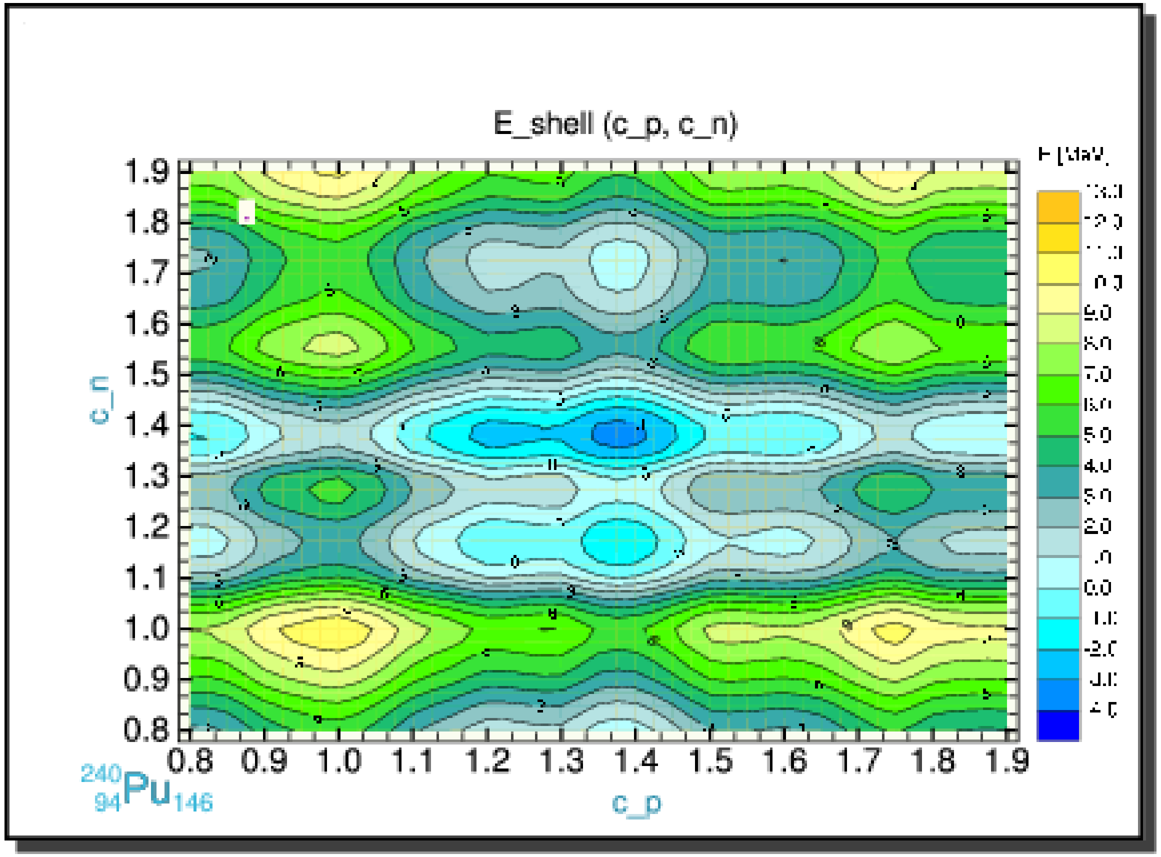
Stiffness of $\mathbf{E_{mac}}$ against different p-n deformations



Variation of macroscopic Yukawa–folded energy for ^{234}Th as function of the proton ⇔ neutron deformation difference

Shell + pairing effects

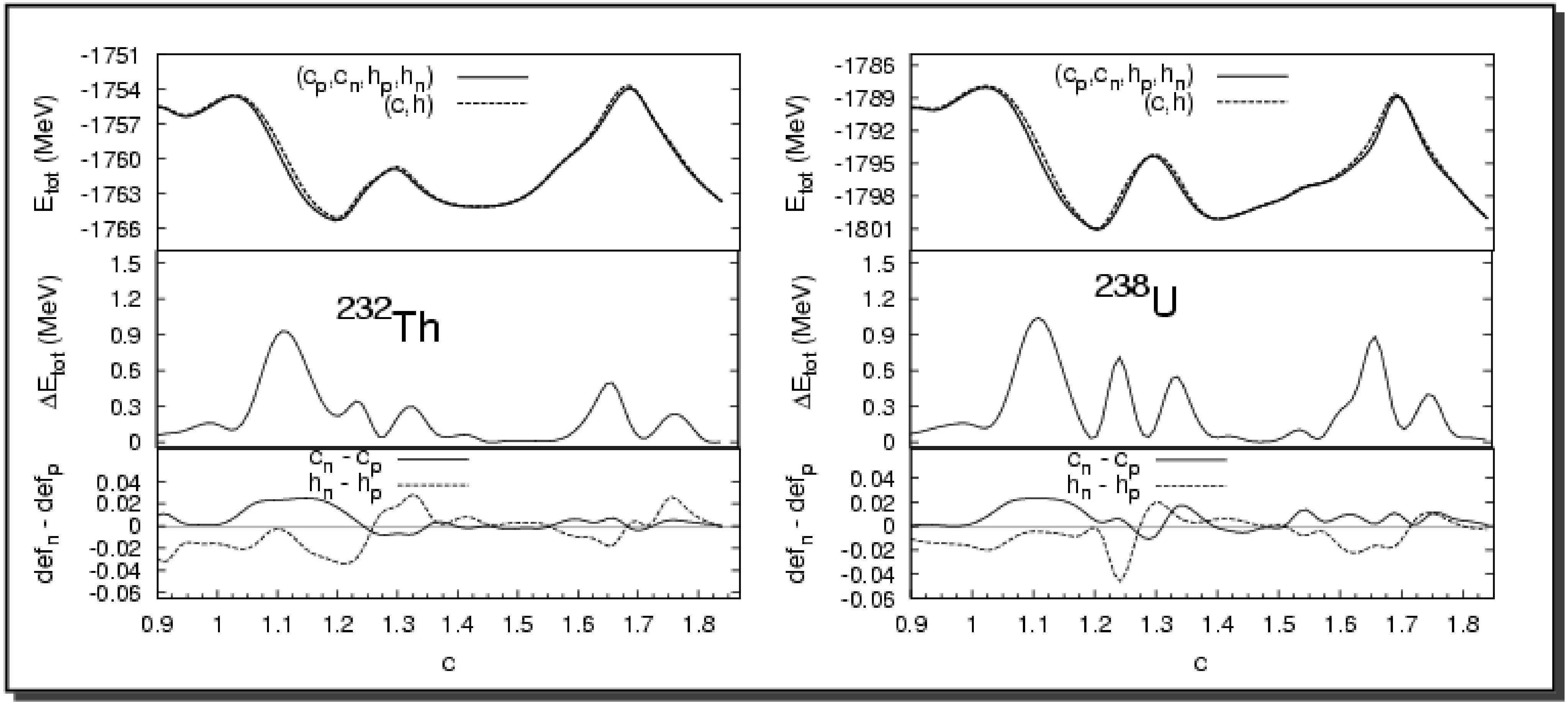
can favour such deformation difference

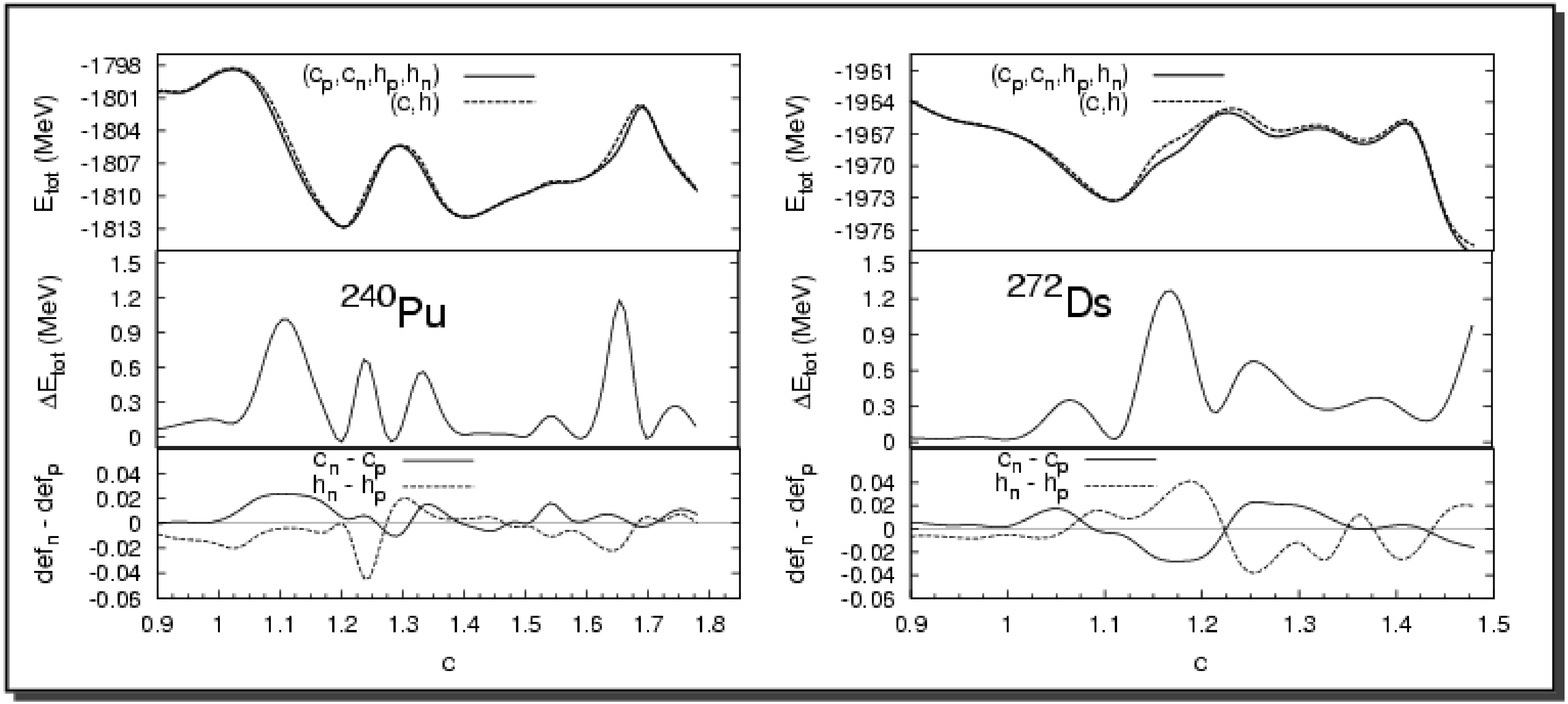


$$E_{tot} = E_{\mathbf{mac}}(\mathrm{def}_p, \mathrm{def}_n) \; + \; \delta E_{\mathbf{mic}}(\mathrm{def}_p, \mathrm{def}_n)$$

$$E_{\mathbf{mac}}(\mathrm{def}_p, \mathrm{def}_n) = E_{\mathbf{LSD}}(\mathrm{def}) + E_{\mathbf{pot}}(\mathrm{def}_p, \mathrm{def}_n) - E_{\mathbf{pot}}(\mathrm{def}, \mathrm{def})$$

$$\delta E_{\mathbf{mic}} = \delta E_{\mathbf{shell}} + \delta E_{\mathbf{pair}}$$


232Th
238U
E_tot (MeV)
ΔE_tot (MeV)
def_n - def_p
(c_p,c_n,h_p,h_n)
(c,h)
c_n - c_p
h_n - h_p
c



(c_p, c_n, h_p, h_n)
(c, h)
^{240}Pu
^{272}Ds
$c_n - c_p$
$h_n - h_p$
E_{tot} (MeV)
ΔE_{tot} (MeV)
$def_n - def_p$
c

Barriers with left-right asymmetric and non-axial shapes

Use now full 4-D $\{c, h, \alpha, \eta\}$ deformation space

generally admitted:

- non axial 1^{st} barrier
- left-right asymmetric 2^{nd} barrier

BUT

- strong variation of shell effects from one nucleus to the next
- strong variation of energy landscape on the way to scission

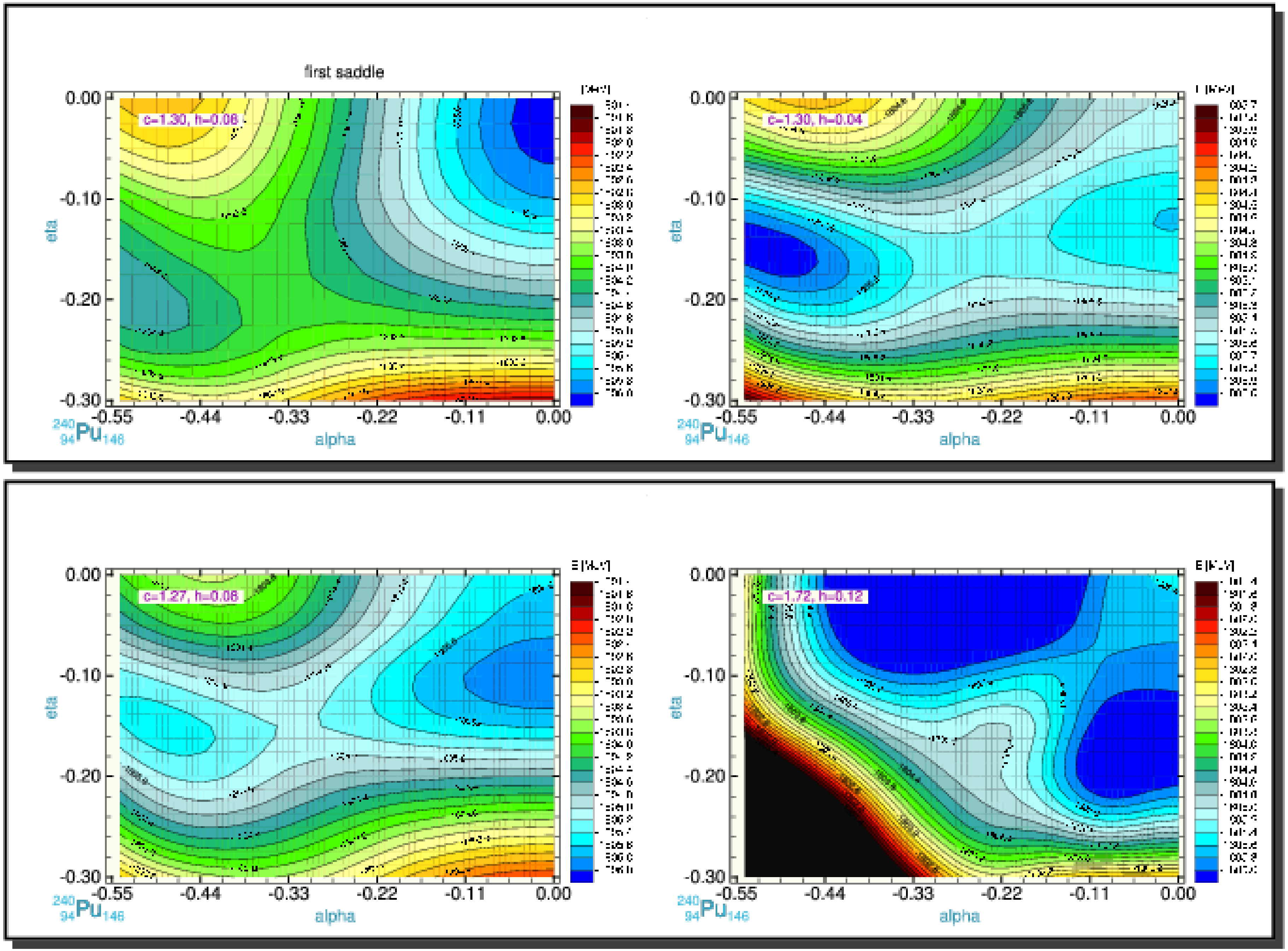
$\Longrightarrow$ location of saddle points is difficult

use gradient method

$$|\vec{\nabla} V_{pot}| = \sqrt{\left(\frac{\partial V_{pot}}{\partial c}\right)^2 + \left(\frac{\partial V_{pot}}{\partial h}\right)^2 + \left(\frac{\partial V_{pot}}{\partial \alpha}\right)^2 + \left(\frac{\partial V_{pot}}{\partial \eta}\right)^2} = 0$$

diagonalize the matrix $\dfrac{\partial^2 V_{pot}}{\partial \alpha_i \, \partial \alpha_j}$

decide whether maximum, minimum or saddle point


first saddle
c=1.30, h=0.08
c=1.30, h=0.04
c=1.27, h=0.08
c=1.72, h=0.12
eta
alpha
$^{240}_{94}Pu_{146}$
E [MeV]
0.00
-0.10
-0.20
-0.30
-0.55
-0.44
-0.33
-0.22
-0.11
0.00

	Ground state	Inner saddle point				Outer saddle point			
Nucleus	Mass (MeV)	α	η	ΔE	B_f^{th}	α	η	ΔE	B_f^{th}
^{232}Th	-1765.3 0.8	0.06	0.10	0.4	5.0 0.0	0.42	0.05	5.5	4.5 -0.9
^{234}Th	-1776.5 0.5	0.03	0.10	0.3	5.2 -0.4	0.39	0.05	6.6	4.4 -1.4
^{234}U	-1777.1 0.8	0.12	0.0	0.4	4.4 -0.7	0.30	0.0	4.9	3.8 -1.1
^{236}U	-1789.3 0.4	0.06	0.0	0.2	5.5 0.3	0.33	0.0	6.3	3.5 -1.7
^{238}U	-1800.8 0.2	0.0	0.05	0.1	6.7 1.2	0.33	0.05	6.9	4.2 -1.4
^{240}U	-1811.8 -0.1	0.06	0.10	0.3	6.5 0.3	0.33	0.0	7.2	3.8 -2.1
^{236}Pu	-1787.2 0.5	0.15	0.05	0.2	5.9 0.7	0.33	0.0	4.3	3.6 -0.4
^{238}Pu	-1800.3 0.2	0.09	0.0	0.1	6.5 0.8	0.36	0.0	4.2	4.5 -0.4
^{240}Pu	-1812.7 0.0	0.06	0.10	0.4	7.0 1.2	0.21	0.0	6.1	3.7 -1.6
^{242}Pu	-1824.5 -0.2	0.09	0.10	0.5	7.1 1.2	0.30	0.0	6.3	4.2 -1.3
^{244}Pu	-1835.6 -0.3	0.09	0.10	0.8	6.9 1.1	0.33	0.05	4.9	5.2 -0.3
^{246}Pu	-1846.8 -0.9	0.03	0.15	1.1	7.2 0.9	0.30	0.05	5.0	4.5 -1.7
^{242}Cm	-1822.7 -0.1	0.09	0.20	0.7	7.1 1.0	0.24	0.0	5.2	3.4 -0.7
^{244}Cm	-1835.3 -0.2	0.06	0.10	0.9	7.2 0.9	0.27	0.05	5.1	4.2 -0.3
^{246}Cm	-1847.1 0.0	0.06	0.15	1.4	6.8 0.8	0.21	0.05	4.7	4.5 -0.2
^{248}Cm	-1858.4 0.0	0.06	0.15	1.8	6.6 0.7	0.21	0.10	3.2	5.2 0.2
^{250}Cm	-1868.8 0.2	0.12	0.10	1.1	5.9 0.7	0.27	0.05	3.5	4.3 0.1
^{250}Cf	-1869.0 0.2	0.09	0.15	2.2	6.5 1.1	0.06	0.05	3.6	3.8 0.2

What can we conclude?

- ground-state masses very well reproduced ($\sim$ 0.5 MeV)
- saddle-point masses $\sim$ **OK** (slightly too high $\sim$ 0.8 MeV)

  But that is good news

  - ▷ Deformation dependence of *Congruence* energy $\sim$ 0.1 MeV
  - ▷ Additional degrees of freedom like proton-neutron deformation difference
  - ▷ Shape dependence of average pairing energy
- masses of 2^{nd} saddle seem to high

  But: exp. masses of 2^{nd} saddle *very* model dependent

Conclusions

- Fission barriers very well described by the macroscopic-microscopic **YF** + **LSD** approach
- different proton-neutron deformations can change fission barriers *locally* by ~1 MeV
- left-right asymmetric shapes also present at the 1st barrier
- non axial shapes also present at the **2**$^{\mathbf{nd}}$ barrier
- same kind of description for super-heavy nuclei (under way)
- include **4-D** shape description in **L**angevin approach