Status of the general description of fission observables by the GEF code

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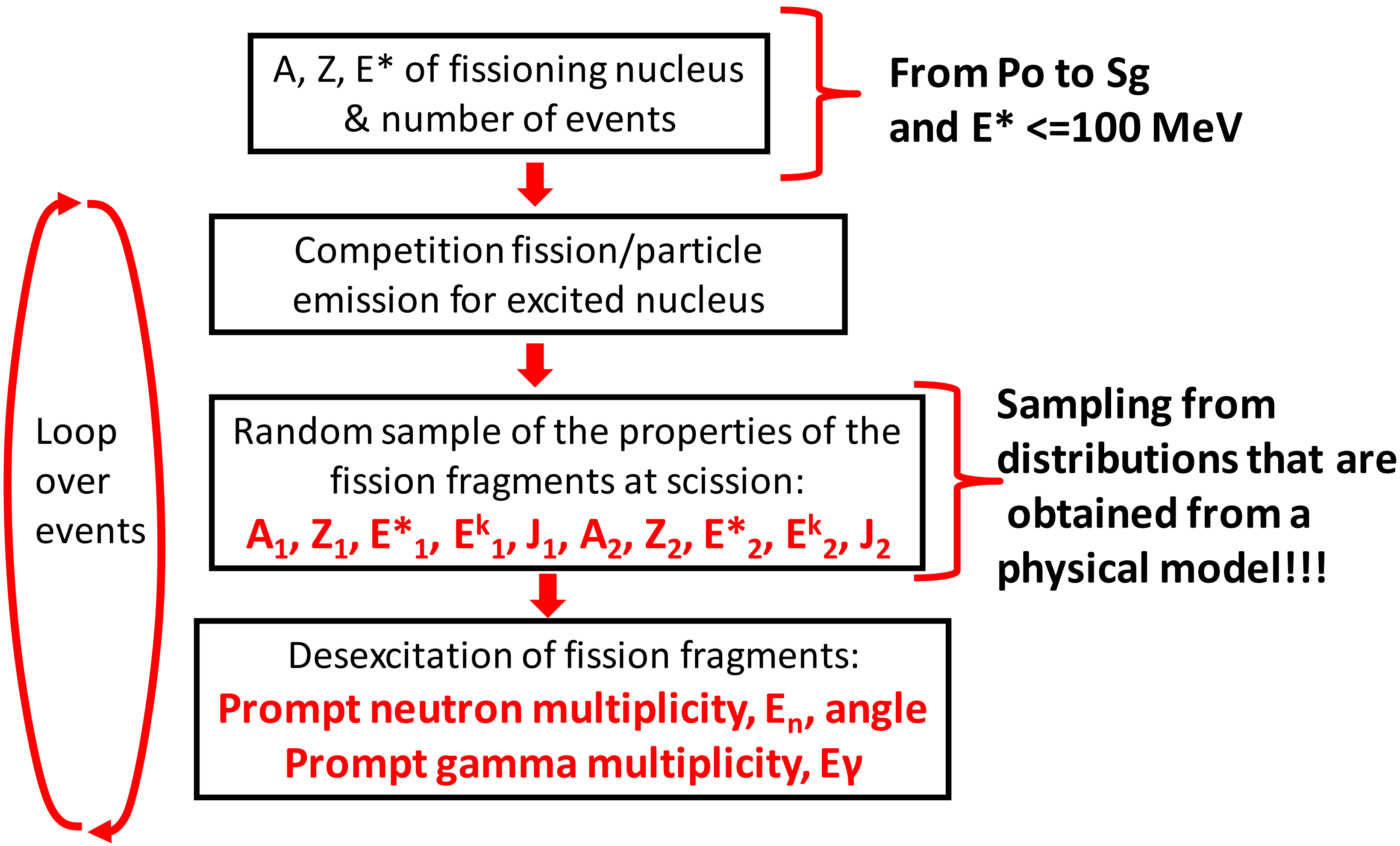
The GEneral Fission (GEF) code

Structure



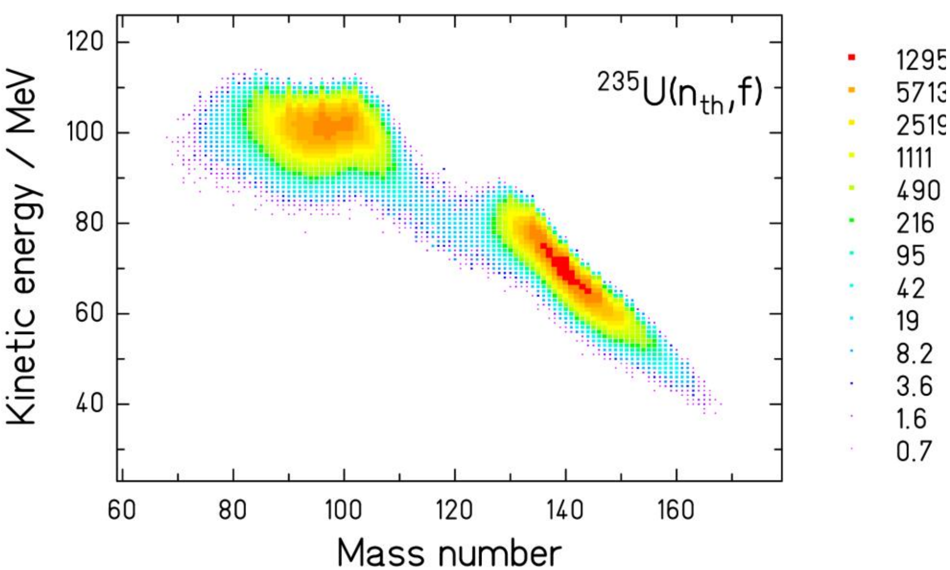
Output of GEF

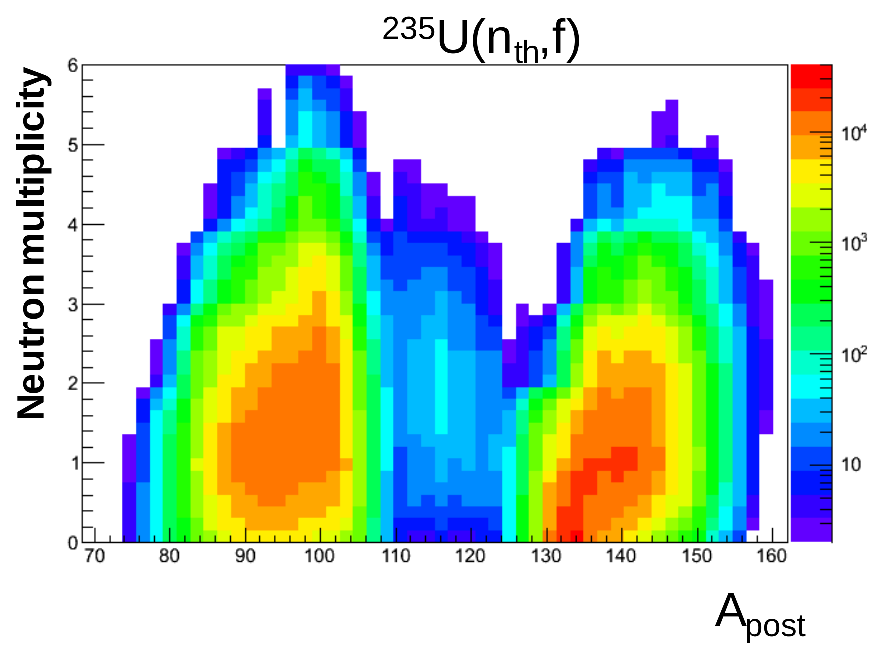
Results for essentially all fission observables

List-mode output can be used as an event generator

```
Fichier  Edition  Format  Affichage  ?
* Z1 Z2 A1post A2post I1pre I2pre n1 n2 TKEpre TKEpost
* Calculation with nominal model parameters
 38  54  94  139  1.5  7.5  1  2  169.3808  167.3484
 37  55  92  140  3  0  2  2  161.8703  158.89
 35  57  88  146  4.5  8.5  1  1  161.9046  160.3561
 35  57  90  143  0.5  14.5  1  2  158.5806  156.6665
 36  56  90  145  3  4  0  1  177.1083  176.6457
 36  56  92  143  4  11  0  1  174.0105  173.5394
 35  57  88  147  2  16  0  1  169.2923  168.8658
 37  55  93  141  5  8  1  1  172.1861  170.601
 40  52  98  135  3.5  3.5  1  2  178.0875  175.9526
 40  52  102  132  7.5  13.5  1  1  171.735  170.2318
 38  54  97  137  5  5  1  1  180.9156  179.2917
```

All possible correlations between quantities





Ideas behind GEF

Combination of physical concepts and experimental information

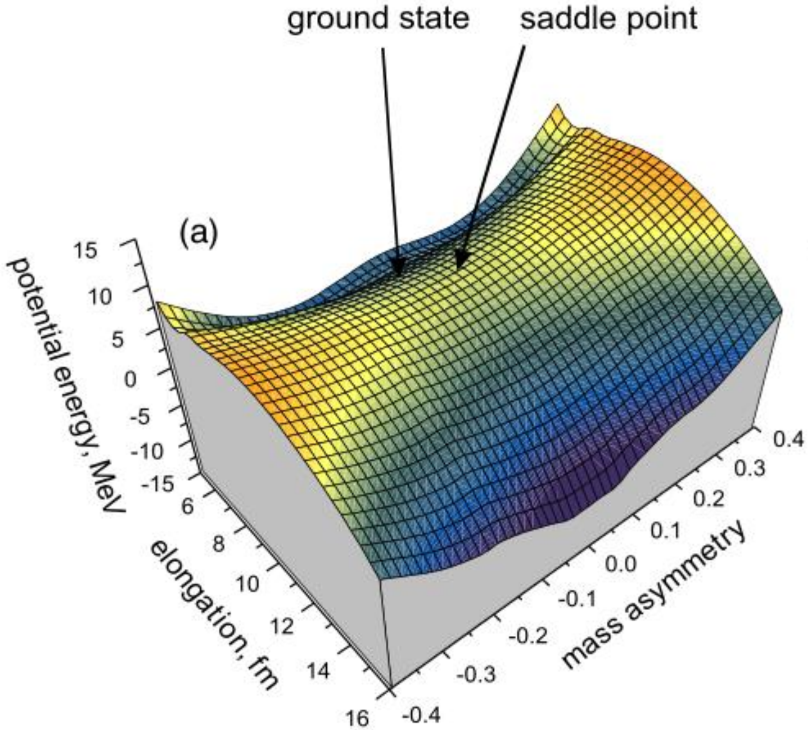
Two examples:

→Fragment yields

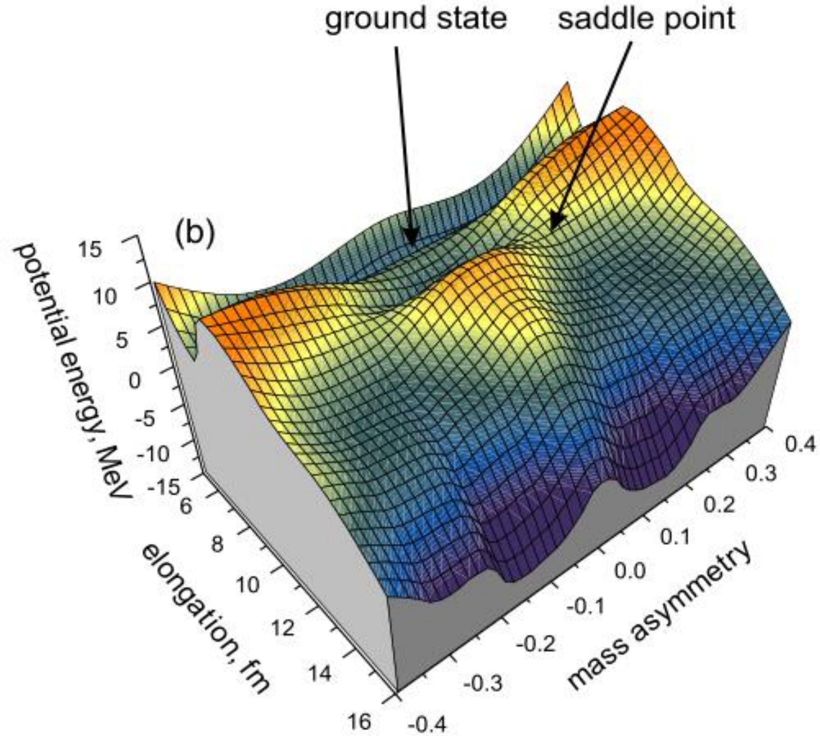
→Partition of excitation energy

Potential energy landscape

2-dim. calculation by A. Karpov, 2008



liquid-drop potential

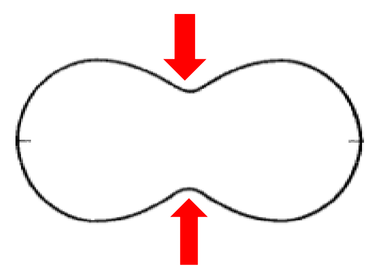


With shell effects

Shells behind outer saddle:

Property of the nascent fragments

Quantum-mechanical effect caused by the neck!



Use of the separability principle in GEF

Separability principle
- Macroscopic potential depends on fissioning nucleus
- Shell effects depend essentially on the fission fragments

Stiffness of macroscopic potential

→ Deduced from experimental yields of symmetric mode for each fissioning nucleus

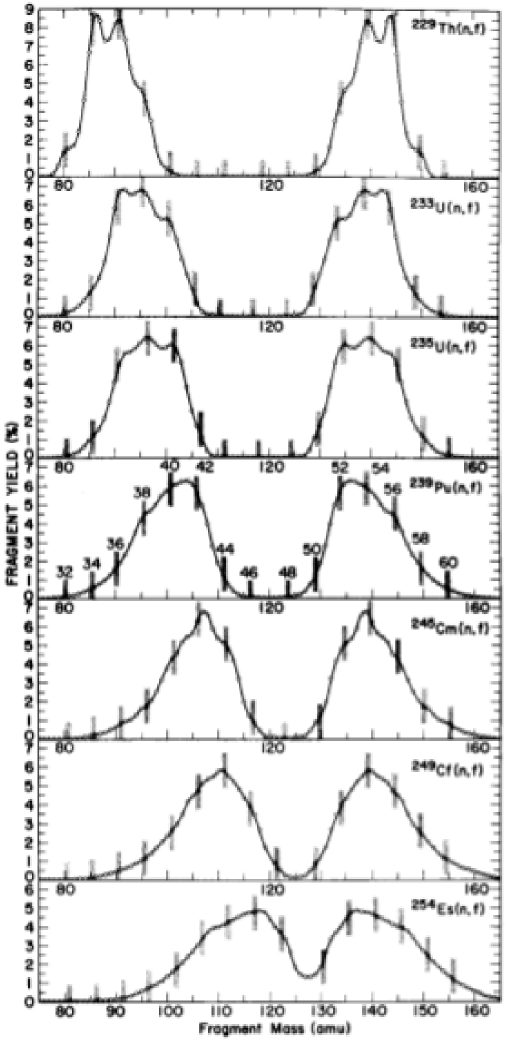
Position, strength and curvature of shells

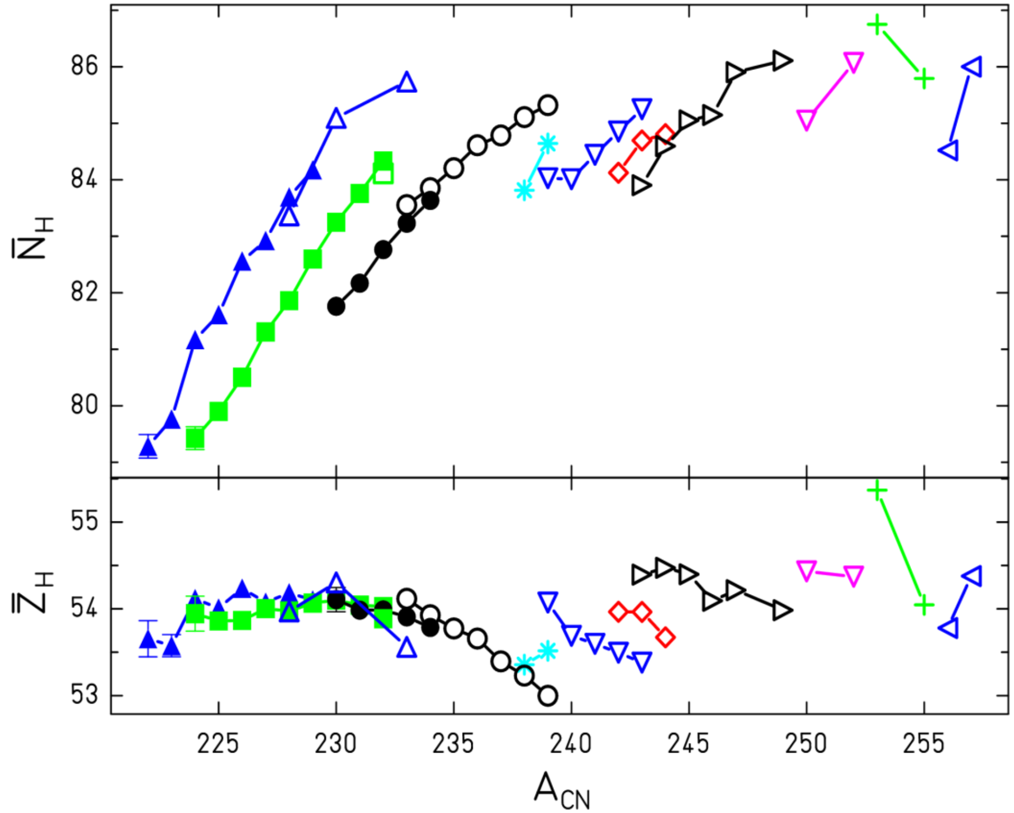
→ Deduced from experimental yields and shapes of asymmetric modes, essentially the same for all fissioning nuclei

↓

Description of a large variety of fissioning systems with the same set of parameters!!

Empirical information on the main shells





Unik et al., 1973

<A> ≈ 140

Shell effects in neutron number

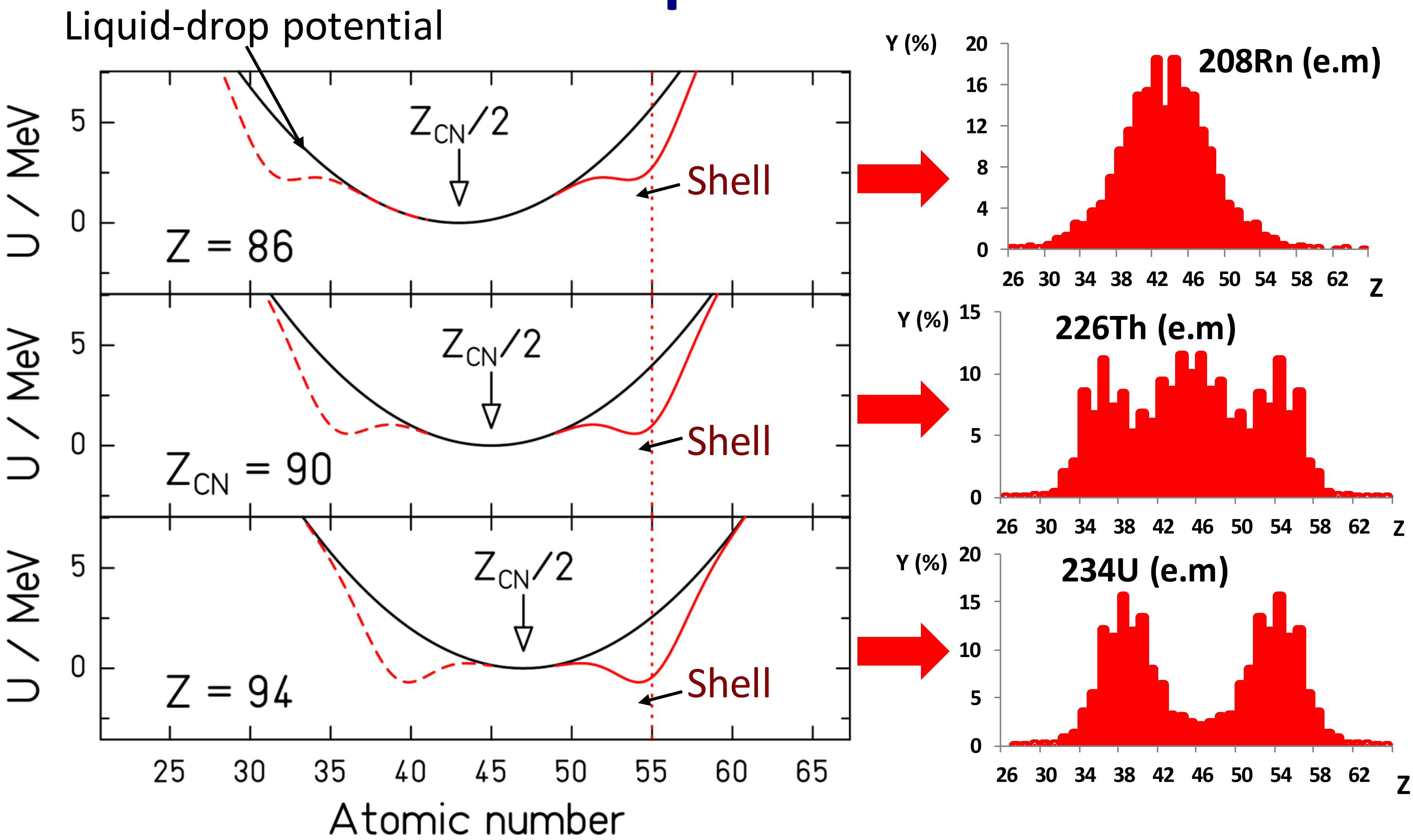
Böckstiegel et al., NPA 802 (2008) 12

GSI data with long isotopic chains:

New empirical result: <Z> ≈ 54

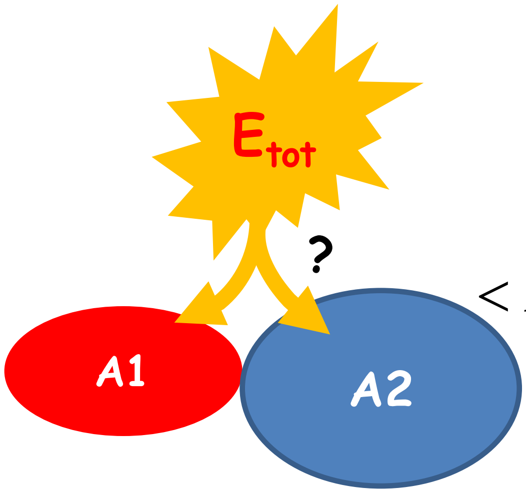
Strong variation of <A> !

Final potential



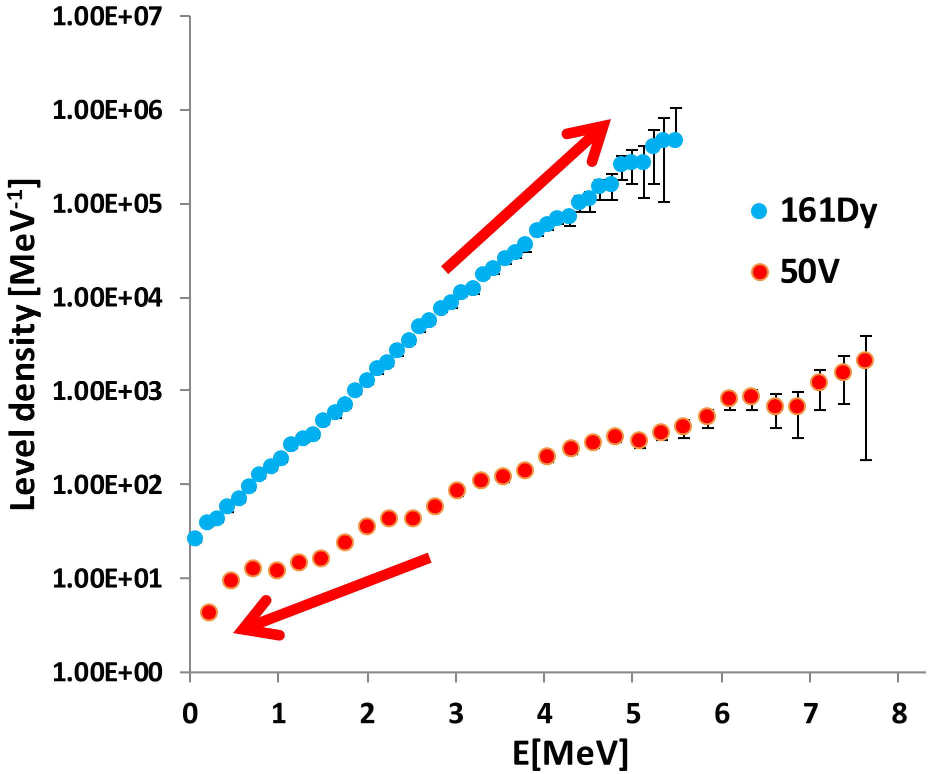
Interplay between liquid-drop potential and shells explains observed transition from symmetric to asymmetric fission

Partition of excitation energy before scission (Statistical mechanics)



$$<E_L>=\frac{\int_0^{E_{tot}} E\rho_L(E)\rho_H(E_{tot}-E)dE}{\int_0^{E_{tot}} \rho_L(E)\rho_H(E_{tot}-E)dE}$$

Only constrain:
$E_L+E_H=E_{tot}$

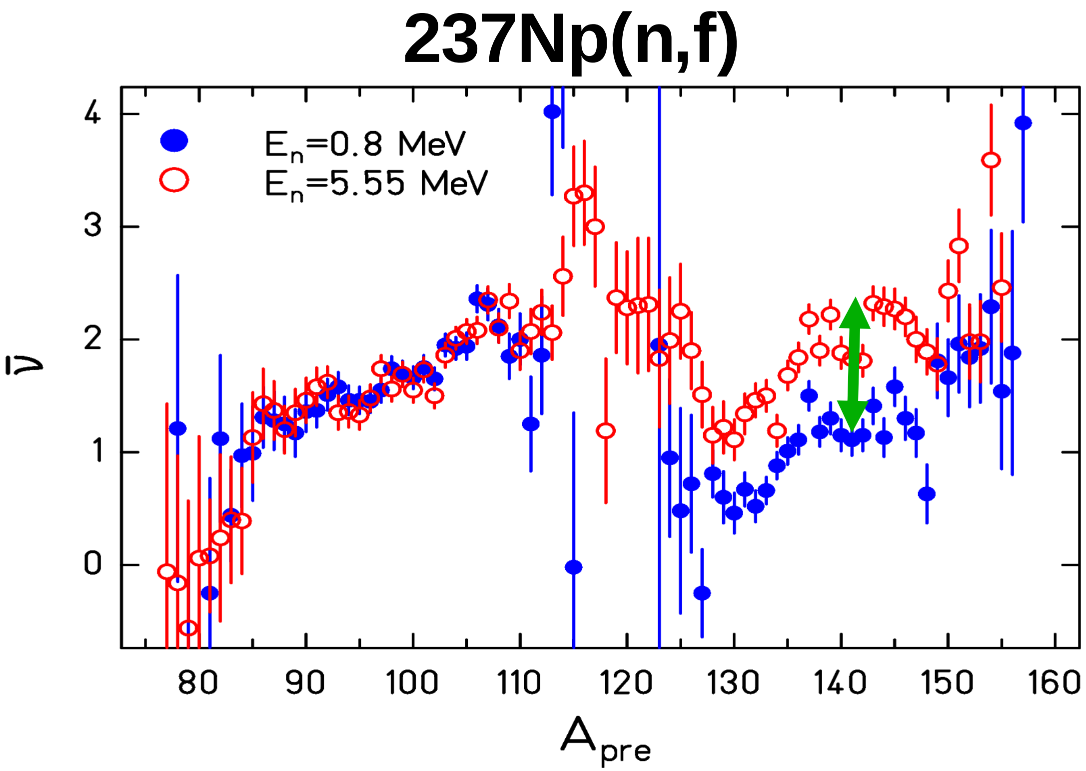


Highest statistical weight for configurations with a cold light fragment!

Due to the constant-temperature behaviour, the excitation energy is transferred to the heavy fragment → Energy Sorting!

Neutron yields at different energies

Signature of energy sorting



The increase in emitted neutrons corresponds to an increase in E^*_{heavy} of 4.8 ± 0.2 MeV.

All the additional E* is found in the heavy fragment!

K.-H. Schmidt, B. Jurado, Phys. Rev. Lett. 104 (2010) 212501

K.-H. Schmidt, B. Jurado, Phys. Rev. C 83 (2011) 014607

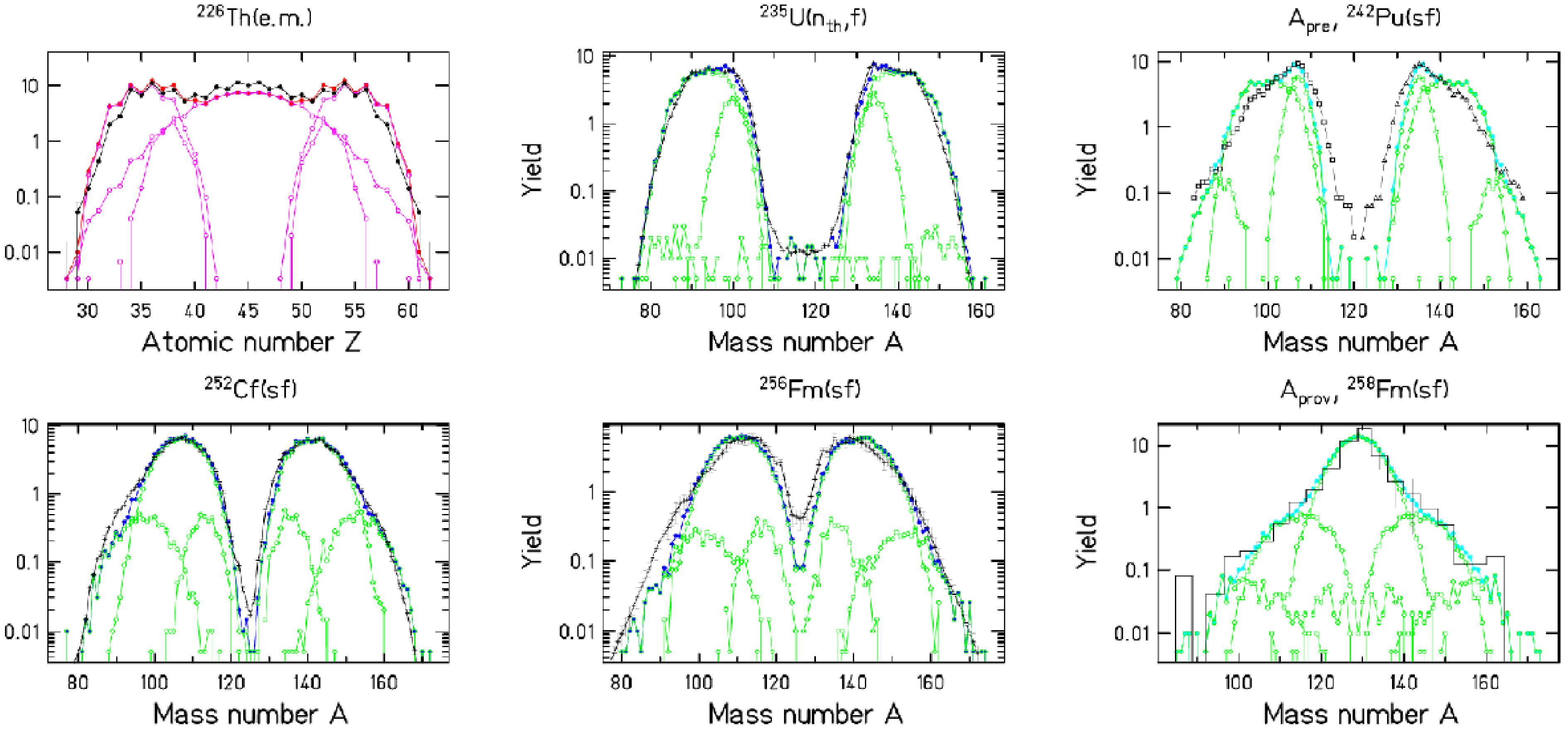
K.-H. Schmidt, B. Jurado, Phys. Rev. C 83 (2011) 061601 (R)

K.-H. Schmidt, B. Jurado, submitted to Phys. Rev. Lett (2013)

Comparison with experimental data and evaluations

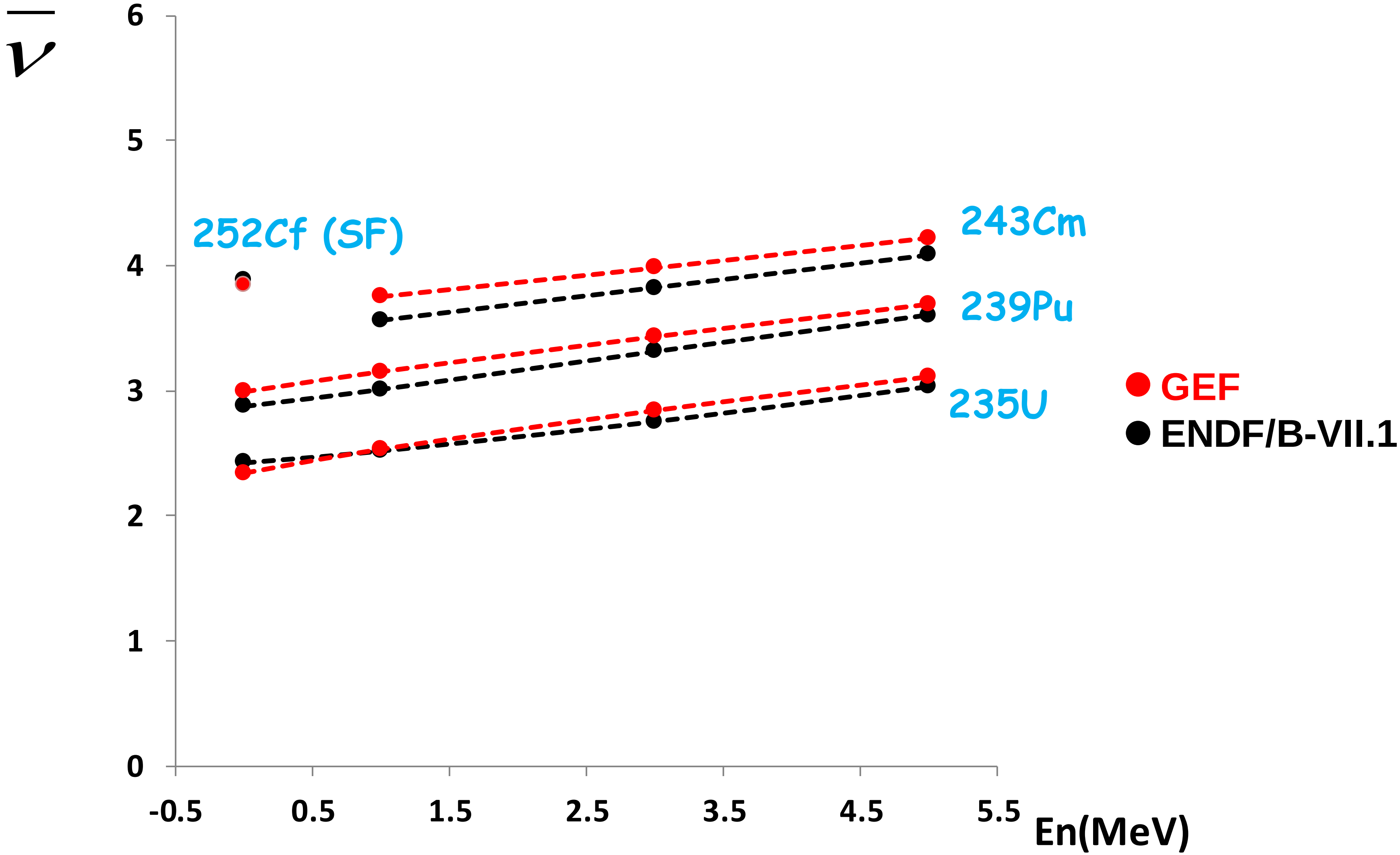
All the results obtained with a single parameter set!

Yields



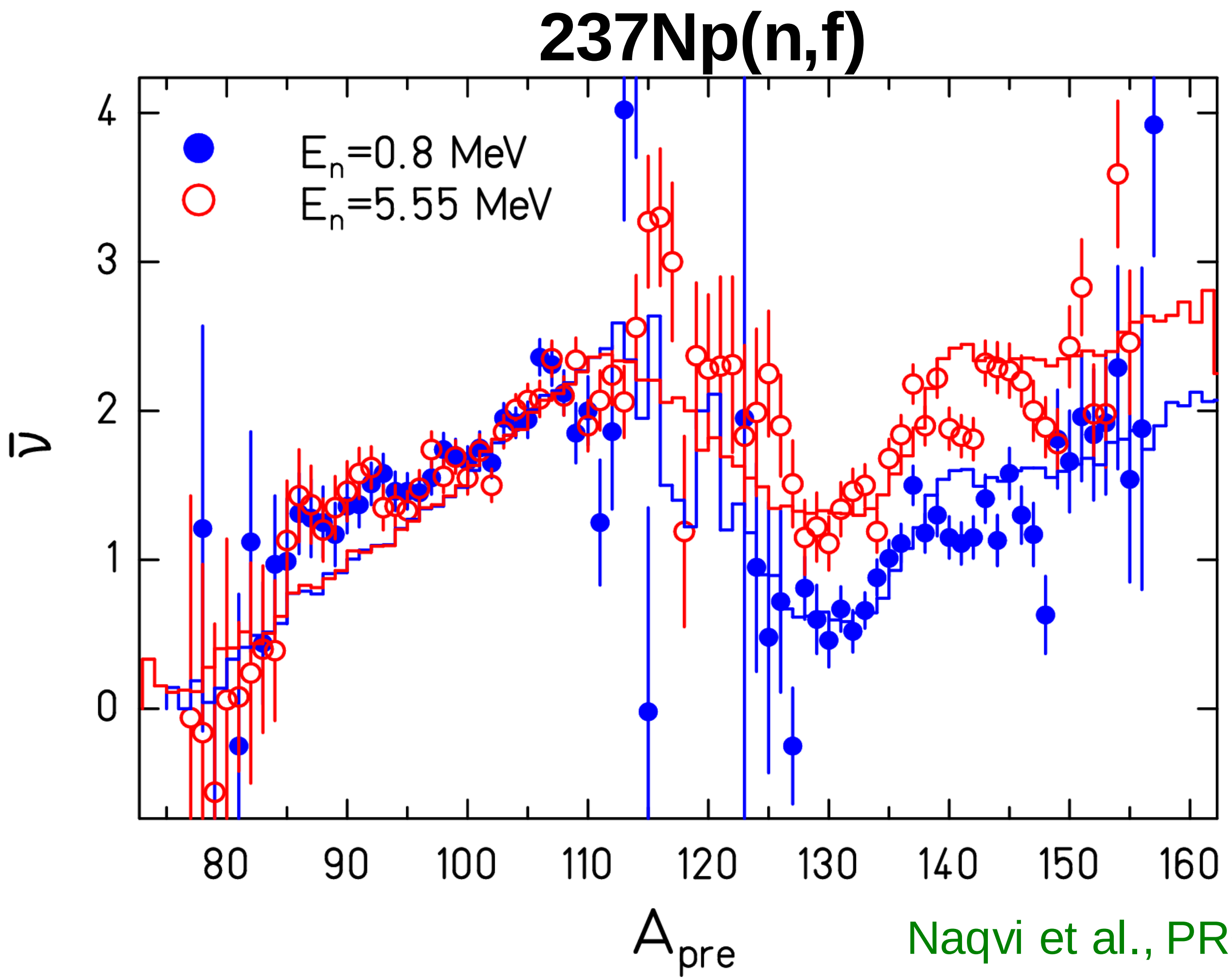
226Th(e.m.)
Atomic number Z
235U(nth,f)
Yield
Mass number A
Apre, 242Pu(sf)
Yield
Mass number A
252Cf(sf)
Mass number A
256Fm(sf)
Yield
Mass number A
Aprov, 258Fm(sf)
Yield
Mass number A

Average number of prompt neutrons



Differences <0.2 neutrons for all systems!

Prompt neutrons as a function of fragment mass

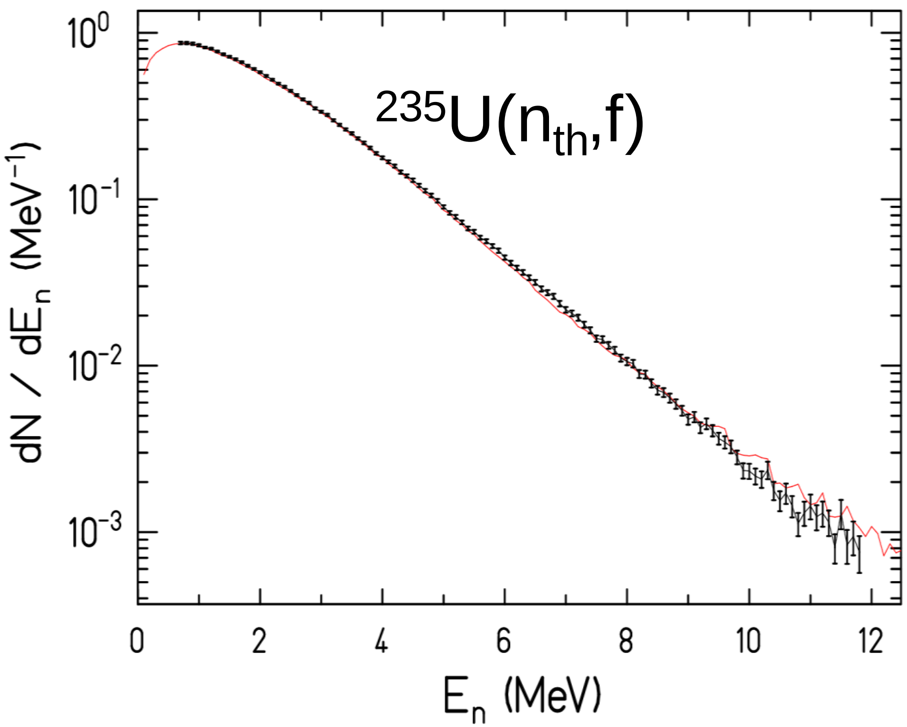


Naqvi et al., PRC 34 (1986) 21

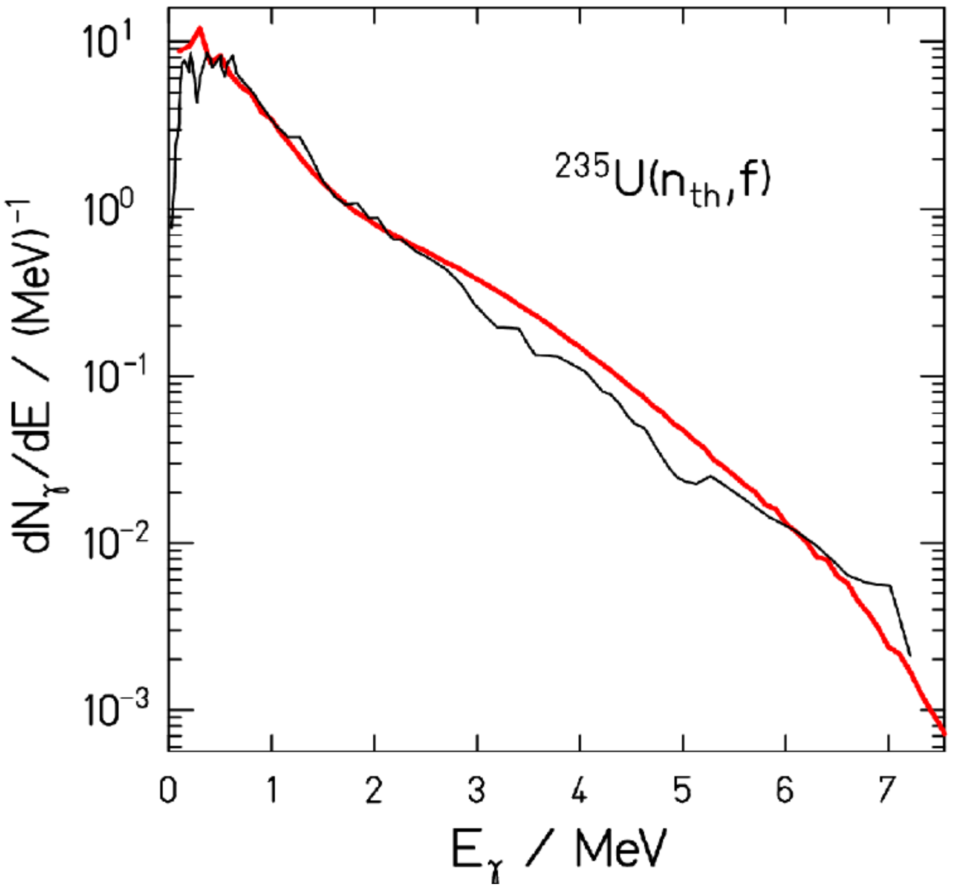
Good description thanks to energy sorting!

Prompt-neutron and gamma spectra

Neutrons



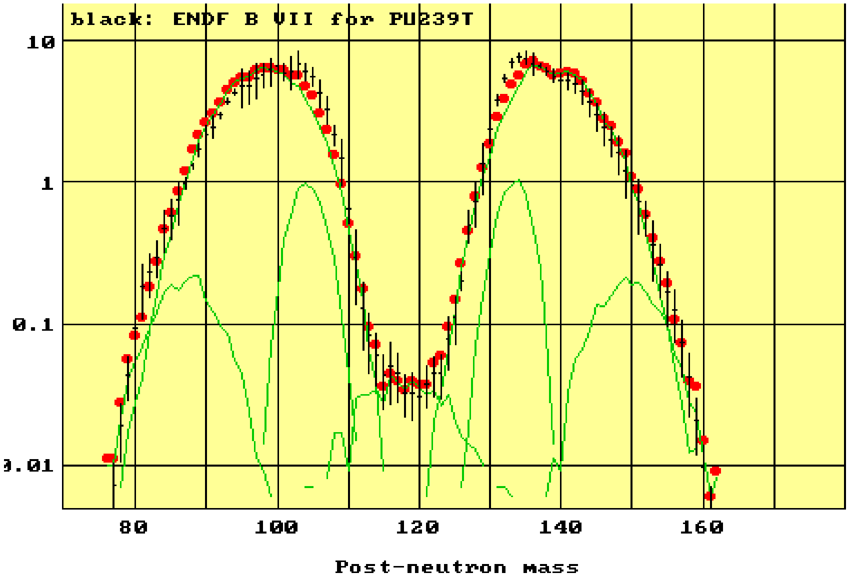
Gammas

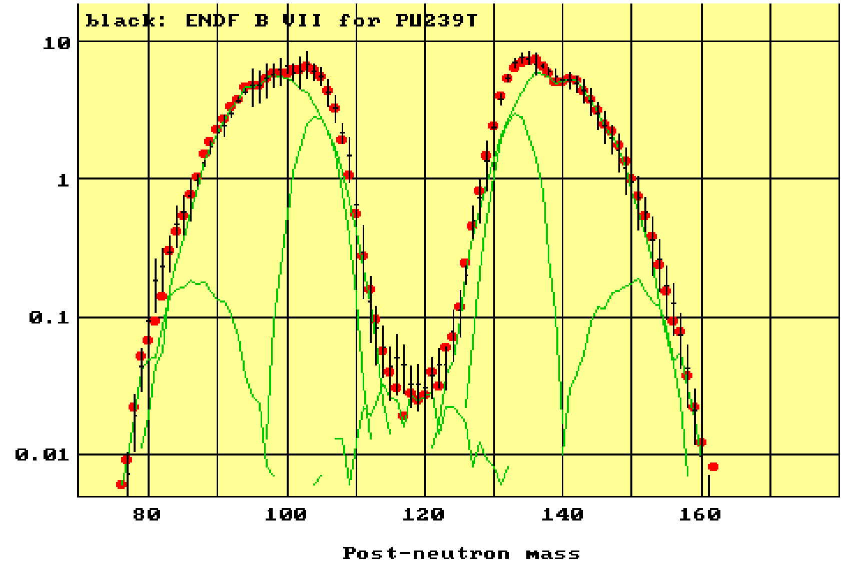


GEF: a useful tool for reactor physics

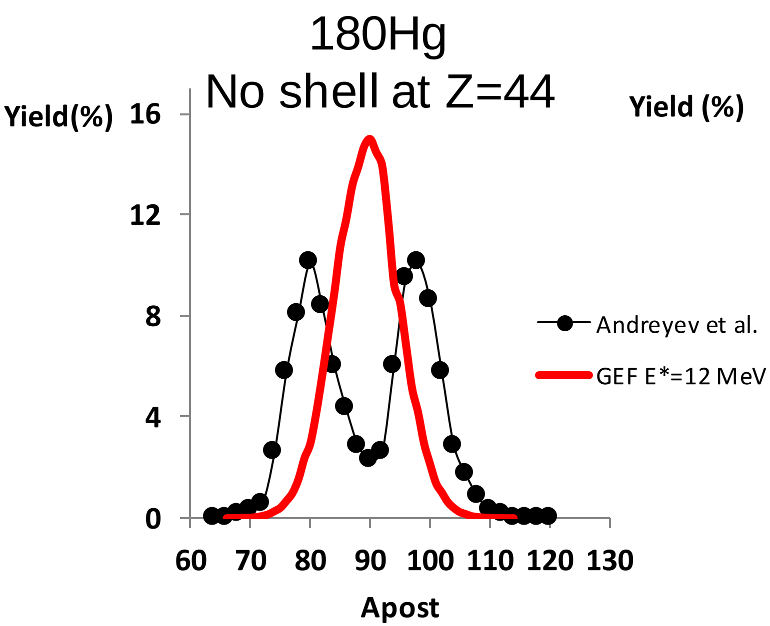
- → Independent and cummulative yields in ENDF format (GEFY)
- → Deterministic version of GEF, subroutine (GEFSUB)
- → Error bars for yields from perturbed model parameters (covariance matrix for yields)
- → Production of isomers

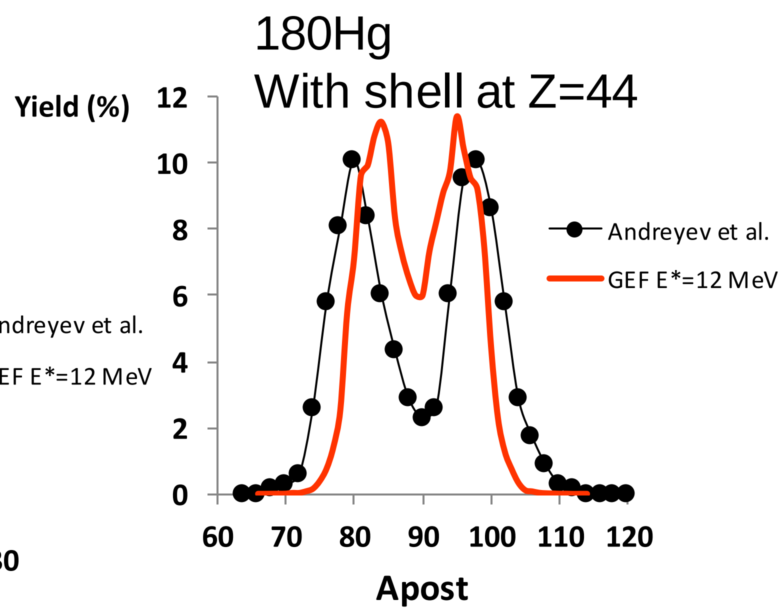
GEF: a useful tool for fundamental physics





Shell effect at Z=44 needed to reproduce all the data in a coherent way!





This shell is responsible for the asymmetric fission observed for light, neutron-deficient fissioning nuclei!!!

Conclusions

- → GEF combination of physical concepts from quantum mechanics and statistical mechanics and specific experimental information within a general approach
- → GEF gives reliable predictions for essentially all fission observables, also for nuclei where no data exist!
- → It is a very useful tool for reactor physics (GEF Yields will be part of next JEFF edition)
- → It serves to reveal the sensitivity of fission observables to basic nuclear properties (e.g. shell at Z=44)

...and perspectives

- → Inclusion of ternary fission
- → Include proton-, electron- and photon-induced fission
- → Improve nuclear structure information of the fission fragments
- → Perform a quantitative assessment of the deviations between GEF and experimental and evaluated data
- → etc…

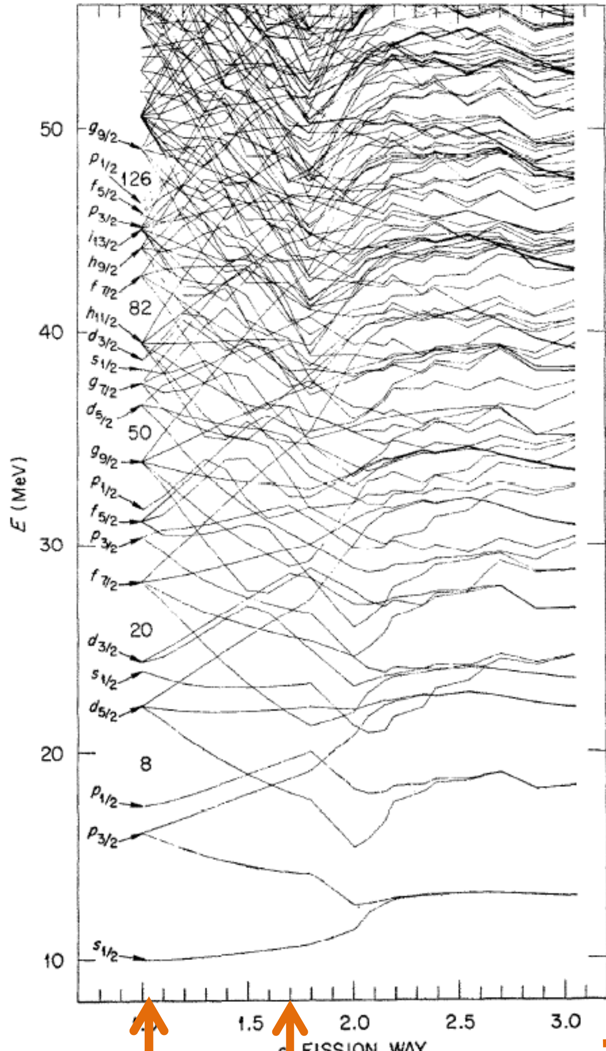
Download and further information can be found in :

www.khs-erzhausen.de or www.cenbg.in2p3.fr/GEF

Influence of fragment properties on the fission process

Neutron shell-model states of 236U

(U. Mosel, H. W. Schmitt, Nucl. Phys. A 165 (1971) 73)

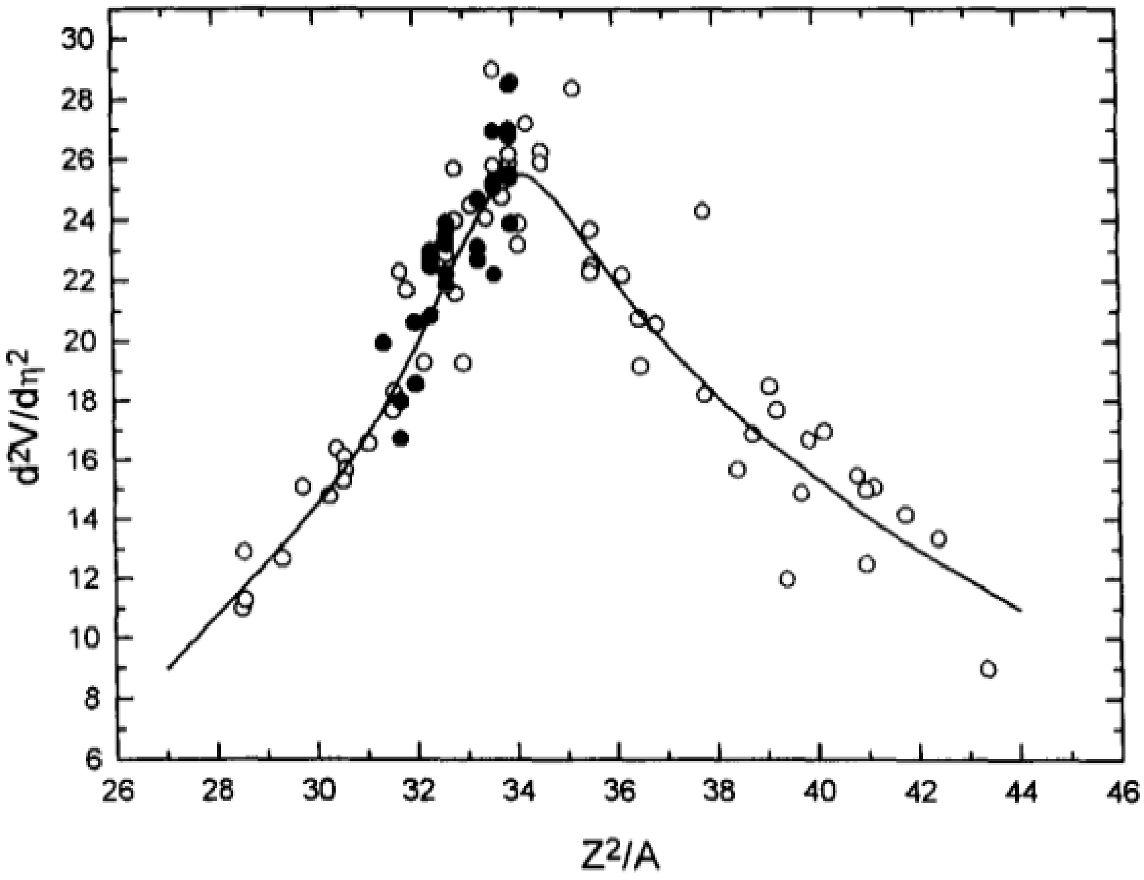


Ground state — Second barrier → → … Scission

- **Fragments acquire their individual properties near the second barrier**
  - --> Shell-effects
  - --> Pairing
  - (H.J. Krappe et al., NPA 690 (2001) 431)
  - --> Congruence energy
  - (W.D. Myers et al. NPA 612 (1997) 249)
- **Level crossing considerably reduced after second barrier**

  Most of the energy is dissipated near the second barrier

Macroscopic potential



From measured σA of symmetric fission mode.

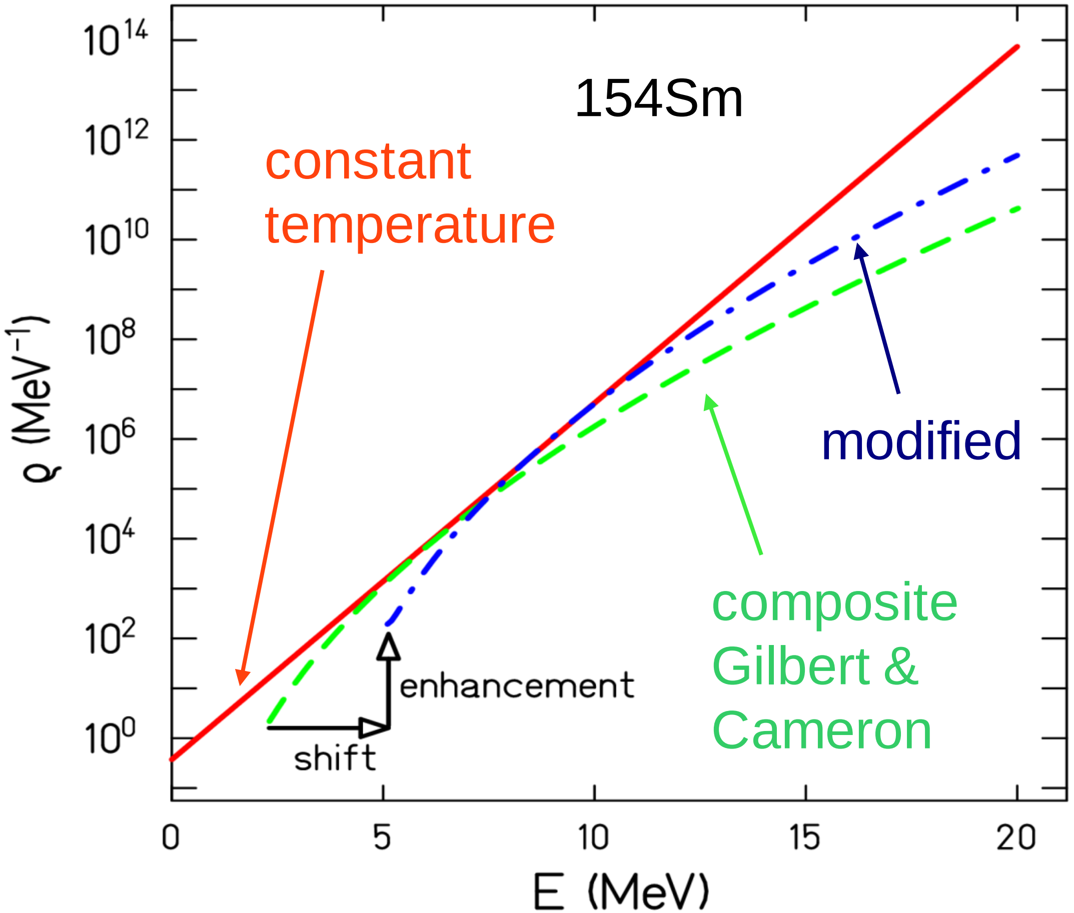
$$\sigma^2 = \frac{temperature}{stiffness}$$

(Harmonic oscillator in a heat bath.)

Mulgin et al., NPA 640 (1998) 375

Stiffness vs. mass asymmetry of the macroscopic potential.
A unique function of fissility.

Improved level-density description



Benefit of composite formula:

1. Constant temperature reflects large heat capacity due to pairing correlations. Empirical systematics can be used.

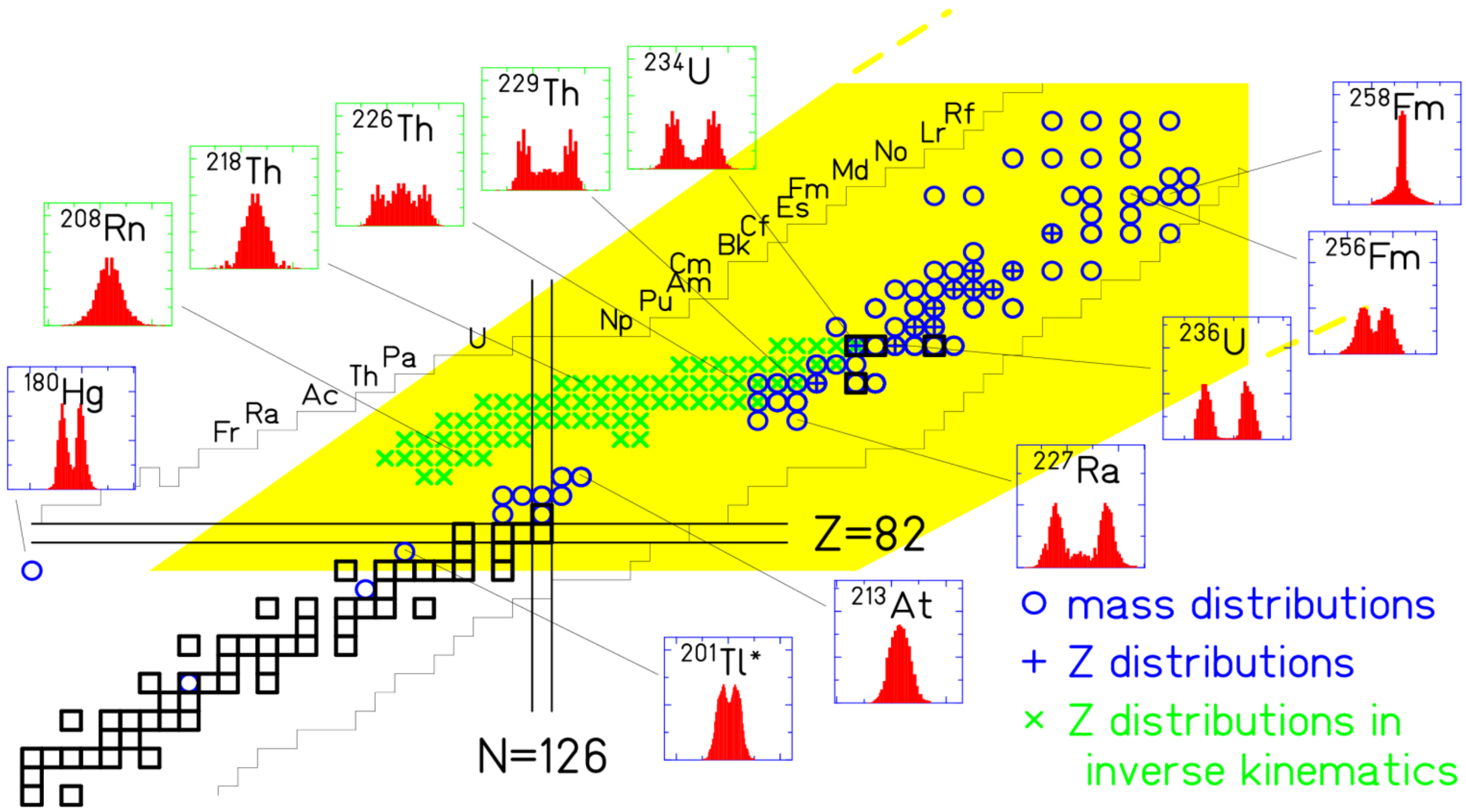
2. Fermi gas above the critical pairing energy (Independent-particle)

Proposed modifications:

1. Increased shift parameter required for stability of pairing. (Condensation must enhance binding energy!)

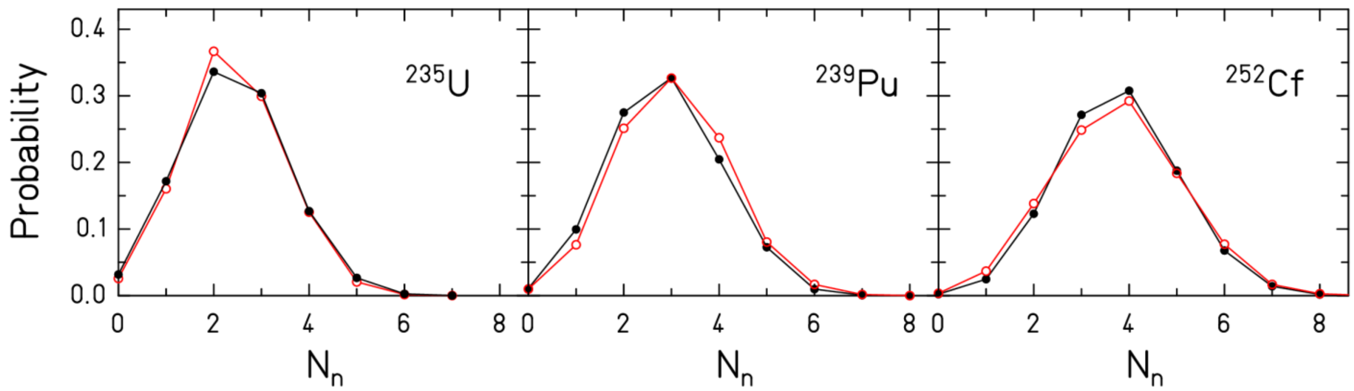
2. Enhancement factor reflects contribution of collective excitations.

K.-H. Schmidt, B. Jurado, Phys. Rev. C 86 (2012) 044322



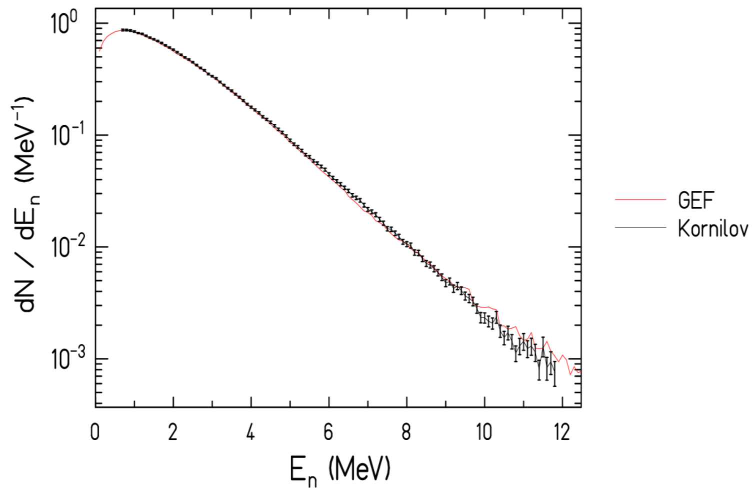
^{180}Hg
^{208}Rn
^{218}Th
^{226}Th
^{229}Th
^{234}U
^{258}Fm
^{256}Fm
^{236}U
^{227}Ra
^{213}At
^{201}Tl*
Fr
Ra
Ac
Th
Pa
U
Np
Pu
Am
Cm
Bk
Cf
Es
Fm
Md
No
Lr
Rf
Z=82
N=126
○ mass distributions
+ Z distributions
× Z distributions in inverse kinematics

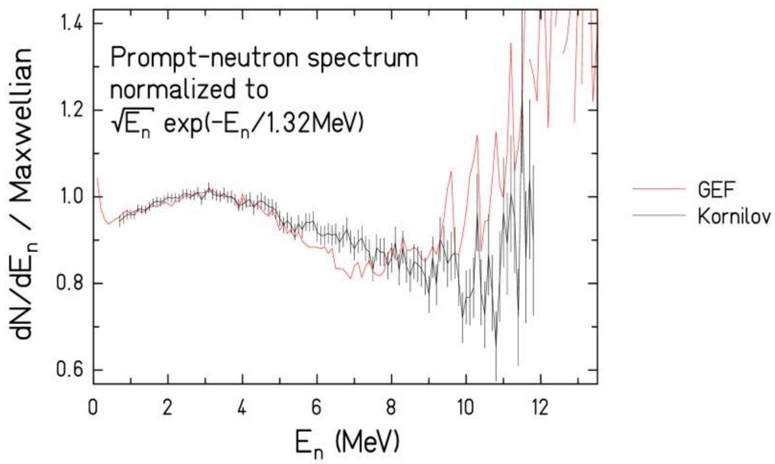
GEF: Prompt-neutron multiplicity



Fluctuations of the prompt-neutron multiplicities are attributed to shape fluctuations of the nascent fragments

GEF: Prompt-neutron spectra





235U(nth,f)

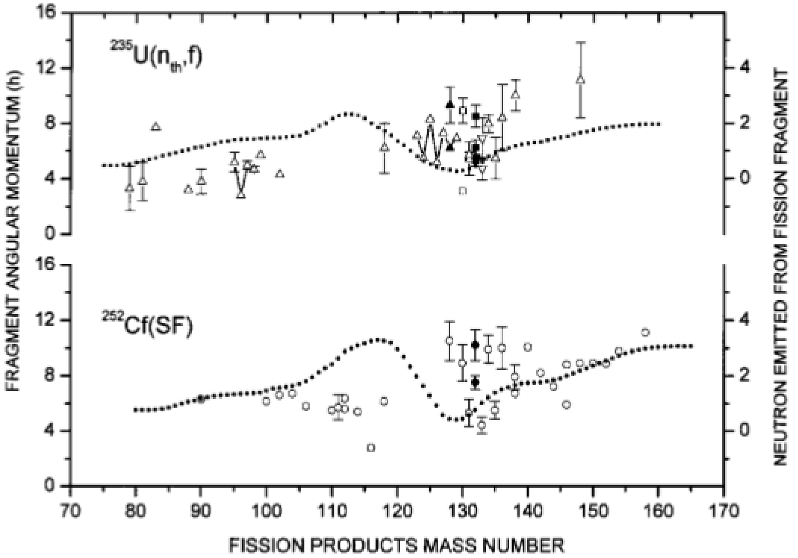
Very good reproduction for all measured systems.
Predictions for other systems without need for any experimental information or specific adjustments.

Initial conditions: angular momentum

- Angular momentum "pumping" of orbital angular momentum by quantum-mechanical uncertainty principle
  - S. G. Kadmensky, Phys. Atom. Nuclei 70 (2007) 1628

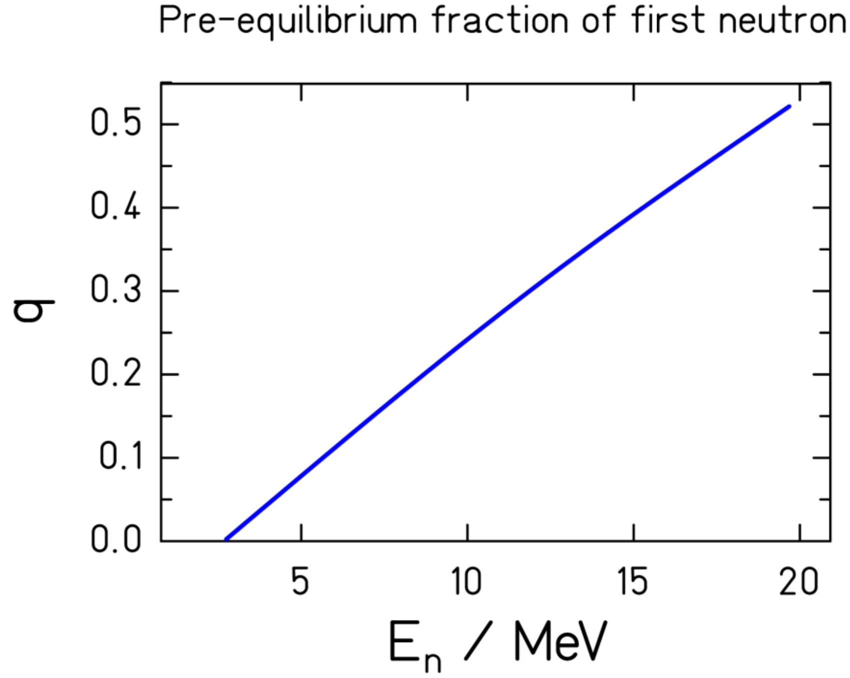
- Enhanced spin by unpaired nucleons
  - B. S. Tomar, R. Tripathi, A. Goswami, Pramana 68 (2007) 111

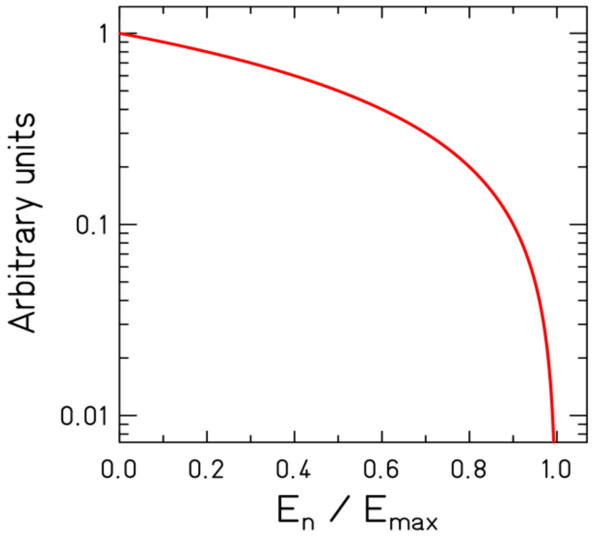
- Empirical scaling
  - H. Naik et al, Eur. Phys. J. A 31 (2007) 195



1. step: formation of the CN

- Neutron-induced fission: Pre-equilibrium emission





Shape of first-step neutron spectrum

Ignatyuk et al., Sov. J. Nucl. Phys. 47 (1988) 224

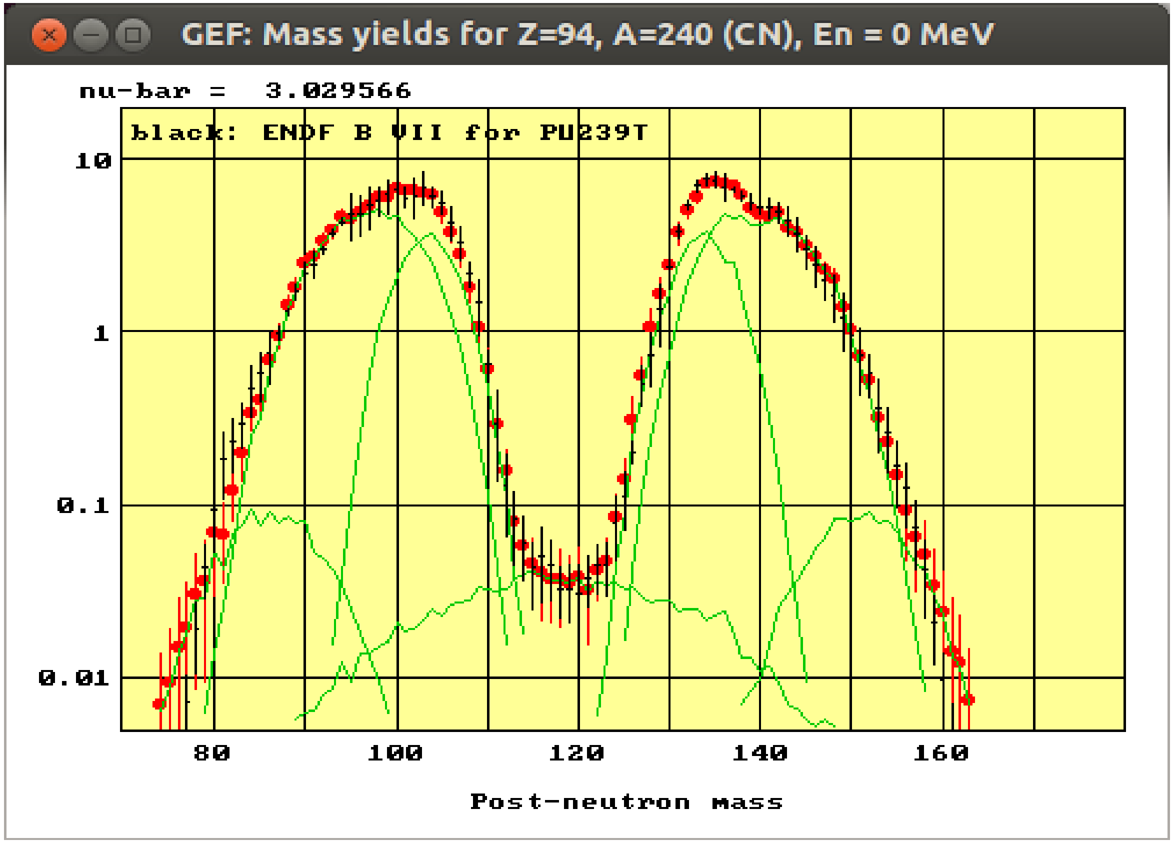
(Exciton model, Griffin, Blann)

Fission barriers (global description)

- Topographic theorem:
  $B_{max} = B_{ld} - Shell_{GS}$ [1]
- B_{ld} from Thomas-Fermi model [2]
- $Shell_{GS}$ from $BE_{exp} – BE_{ld}$ (Thomas-F.) [1]
- Correction for systematic deviation of B_{ld} as $f(Z)$
- Correction for nuclei with $B_A \approx B_B$
  (Position of liquid-drop barrier at 2nd minimum)
- Lower barrier from fit B_A-B_B

[1] W. D. Myers, W. J. Swiatecki, Nucl. Phys. A 601 (1996) 141
[2] W. D. Myers, W. J. Swiatecki, Phys. Rev. C 60 (1999) 014606

Uncertainty estimates from perturbed-parameter calculations



red: Error bars of the model calculation.
black: Error bars of the evaluated data.

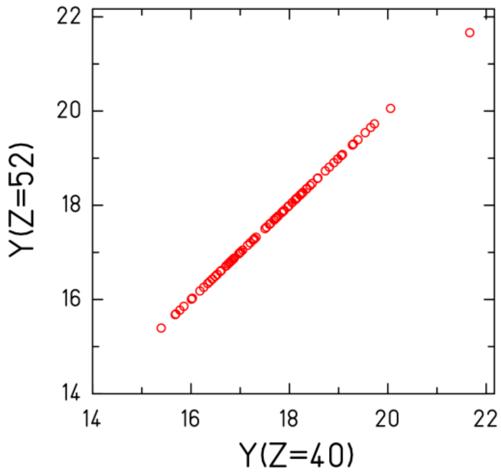
Model parameters fluctuate inside their uncertainty range (deduced from the fit procedure).

Fluctuations of the results → uncertainties of the fission observables. (Used for GEFY.)

Applicable to any of the fission properties.

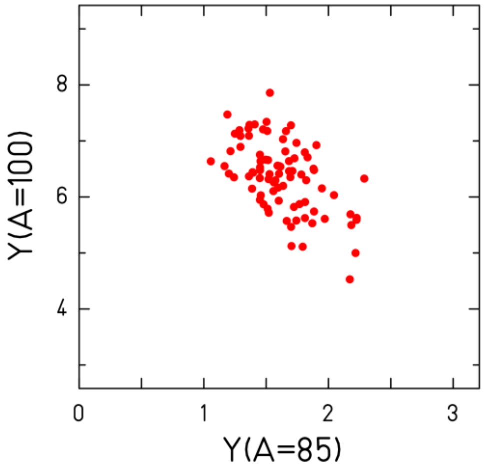
GEF calculations provide a covariance matrix

- relations required by physics



Two complementary elements (Strictly correlated)

- relations required by the model



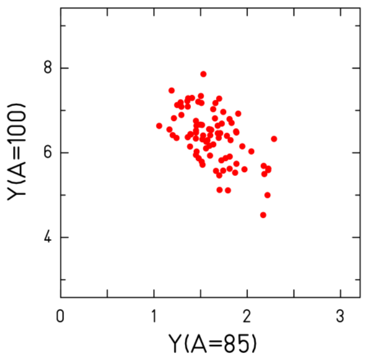
Two masses from different modes. (Slightly anti-correlated)

Result of perturbed GEF calculations for

Establishing the covariance matrix

The covariance between two variables *x* and y is defined by:

$$\mathrm{cov}(x,y)=\sum_{i=1}^{N}\frac{(x_i-\bar{x})(y_i-\bar{y})}{N}$$

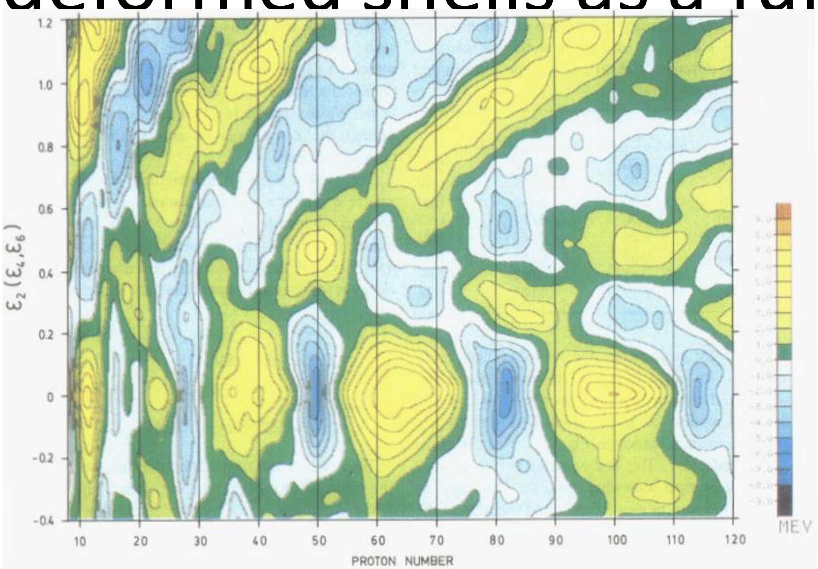


GEF result: Calculation with perturbed parameter values.

The covariance values between any two yield values *Ya* and *Yb* can be determined from the GEF calculation with perturbed parameters.
All covariance values form the covariance matrix.
The covariance matrix represents the internal logic dependences (trivial ones and model-specific ones) of GEF.

Aspects of statistical mechanics in fission dynamics

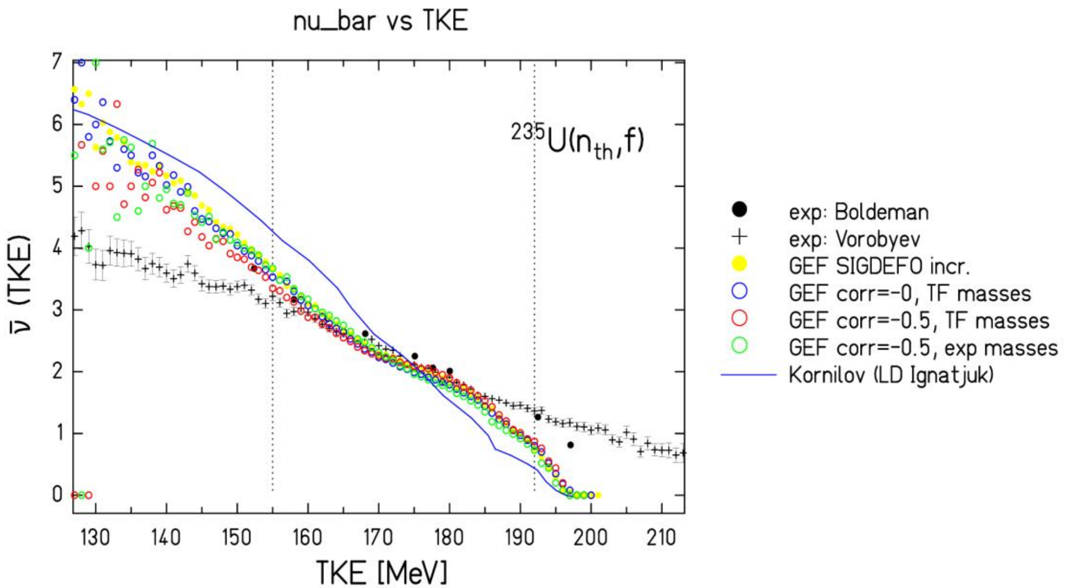
- Deformation energy at scission from deformed shells as a function of *Z* (saw-tooth

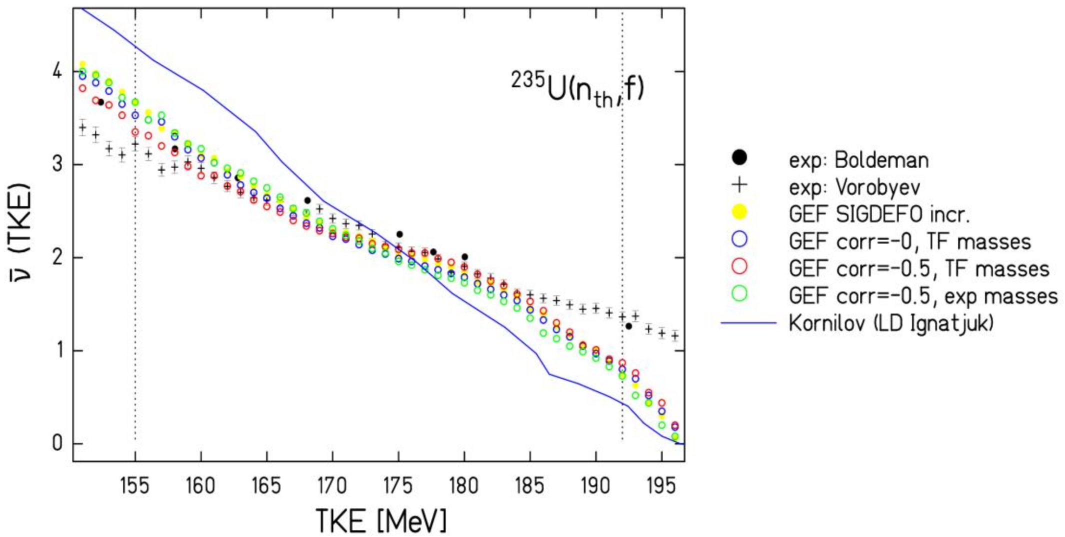


I. Ragnarsson,
R. K. Sheline,
Phys. Scr. 29 (1984) 38

- Energy sorting of thermal energy at scission ($\nu(A)= f(E^*)$, even-odd effect in *Z* yields)

Other correlations of fission observables





Prompt-neutron yield vs. TKE, quoted as an indication for scission neutrons.

GEF result differs from analytical estimations.
GEF considers all (also hidden) correlations.

Level densities of deformed nuclei:

a = 0.073 A / MeV + 0.095 Bs A^(2/3) / MeV (A. V. Ignatyuk et al., Sov. J. Nucl. Phys. 21 (1975) 612.)

Bs = 1 + 2/5 * alpha_2^2 - ...

beta = 3/2 * alpha_2

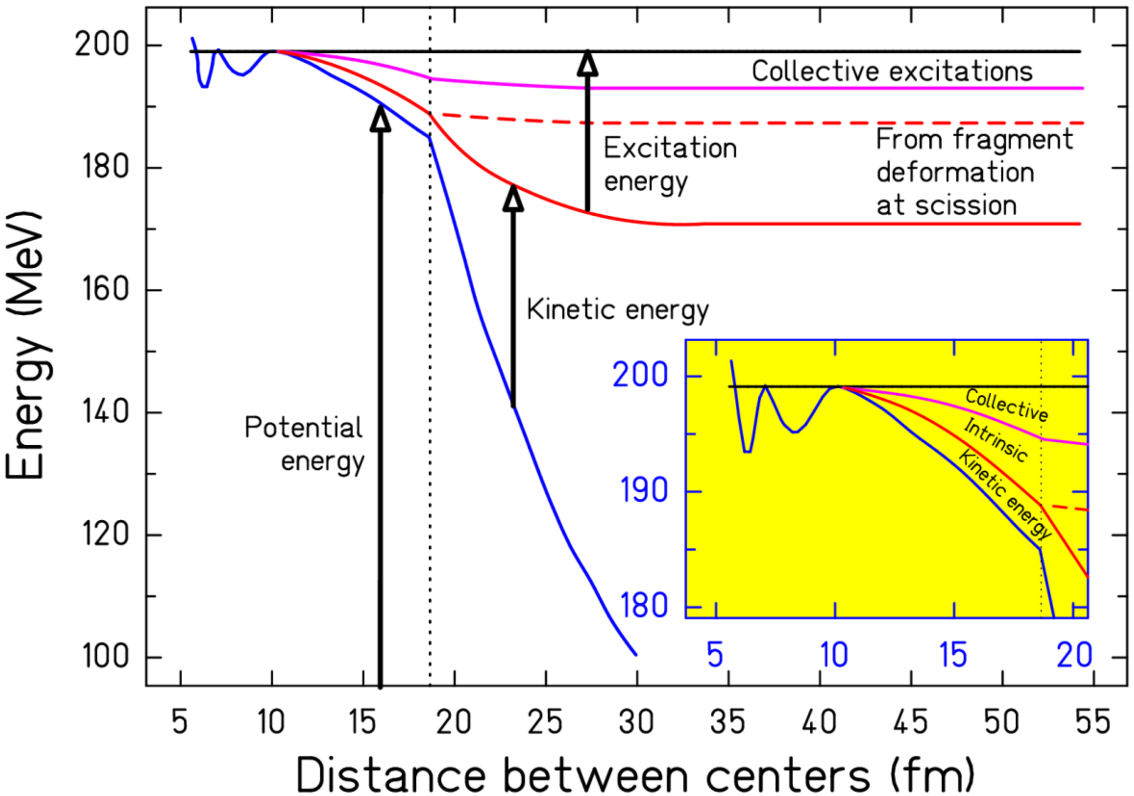
A=96, beta=0.2 to 0.6 → increase of level density of 13%
A=140, beta =0.2 to 0.6 → increase of level density of 14%
a increases by 1%

For SL and S2 there is no net effect because both fragments are deformed.
For S1 this influence is minor compared to the difference in the slopes of the level densities of the two nascent fragments in asymmetric fission.

T and a are closely related [D. Bucurescu, T. von Egidy, Phys. Rev. C 72 (2005) 067304]-->
T decreases only by 1%, --> Negligible compared to the difference in log slopes for asymetry

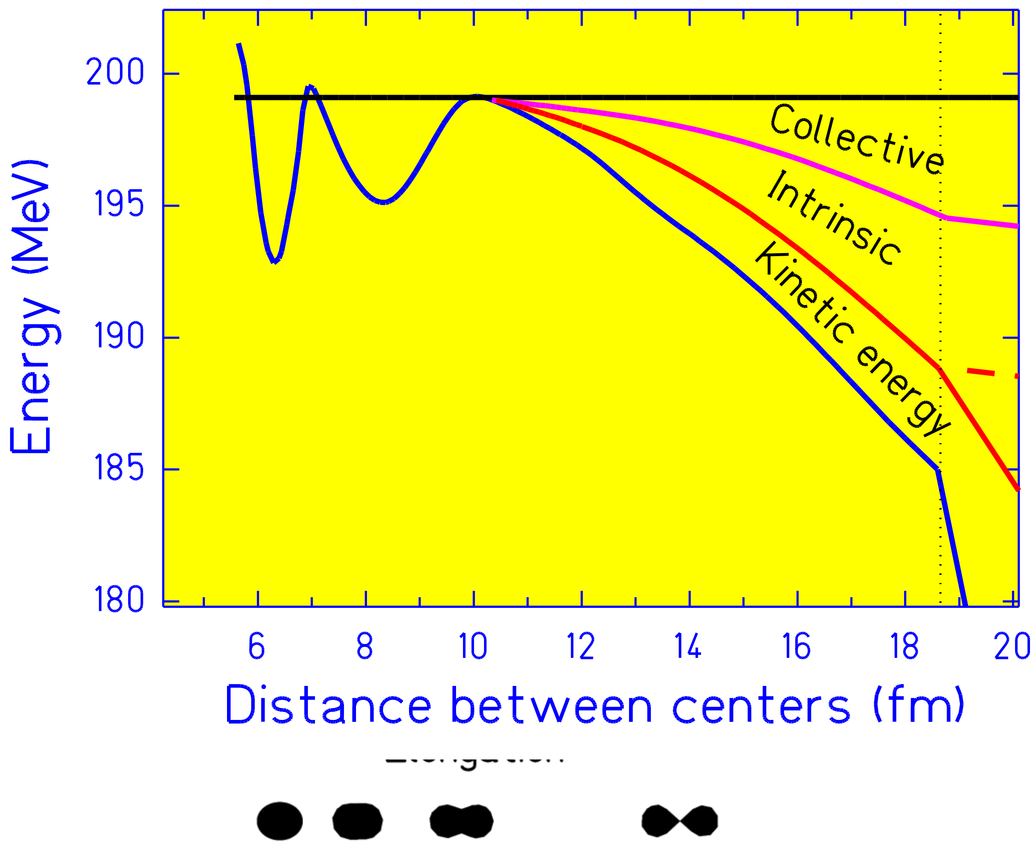
Note however that:
A shell effect of a few MeV causes a modifcation of the level density by a factor 10!!

Initial conditions: Energies



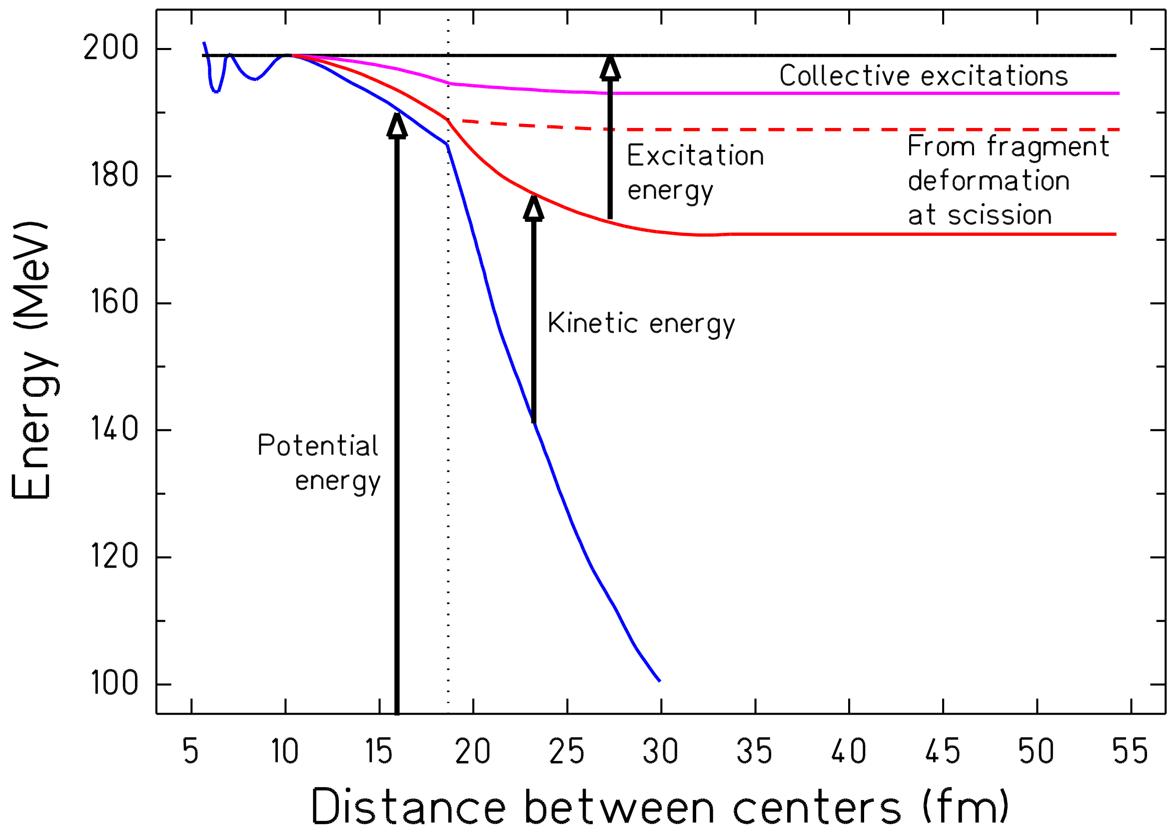
•Energy transformations

Energy considerations: situation at scission



Energy at saddle $E^*_{sad}=E^*_{CN}-FB$
Intrinsic E*, "heat"
(We consider E^*_{CN} < 15 MeV)
Increase in Ebeam mainly goes to intrinsic E*

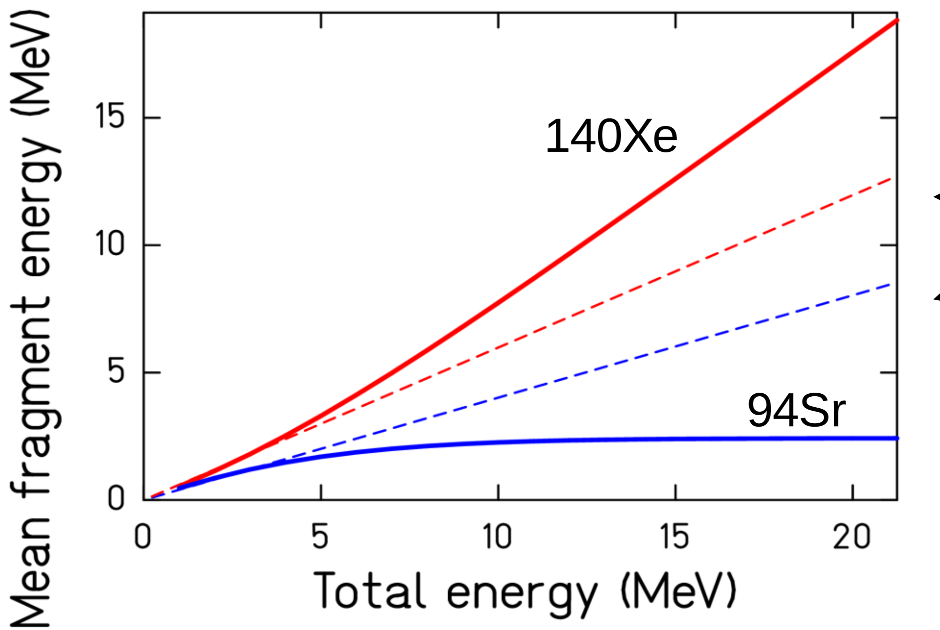
Energy considerations: fully accelerated fragments



Total E* (TXE)

Total Ekin (TKE)

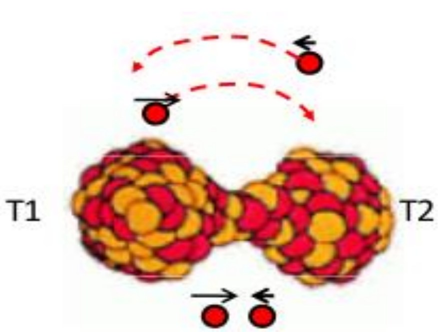
Initial conditions: Energy sorting



94Sr and 140Xe

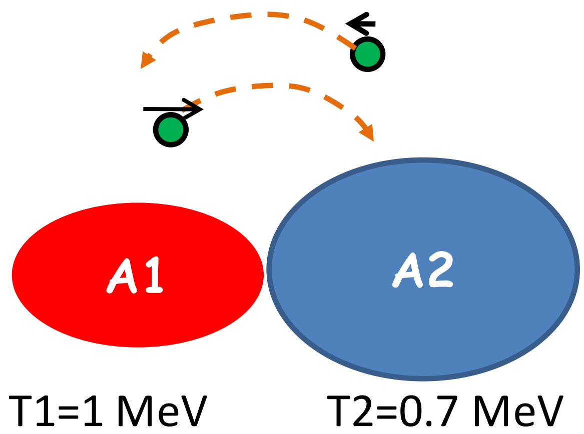
Fermi gas

K.-H. Schmidt,
B. Jurado,
PRC 83 (2011) 061601



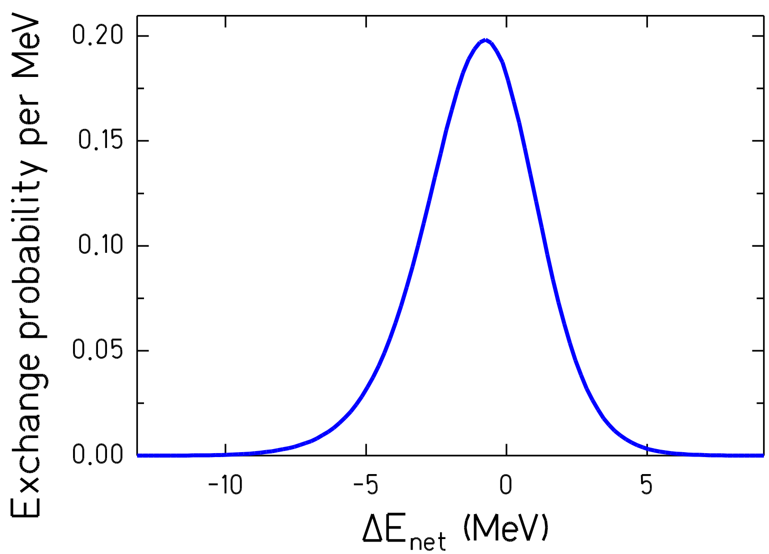
•Sorting of *E** at scission caused by constant nuclear temperature. (Data from “Oslo group”.)

Microscopic view of energy transfer



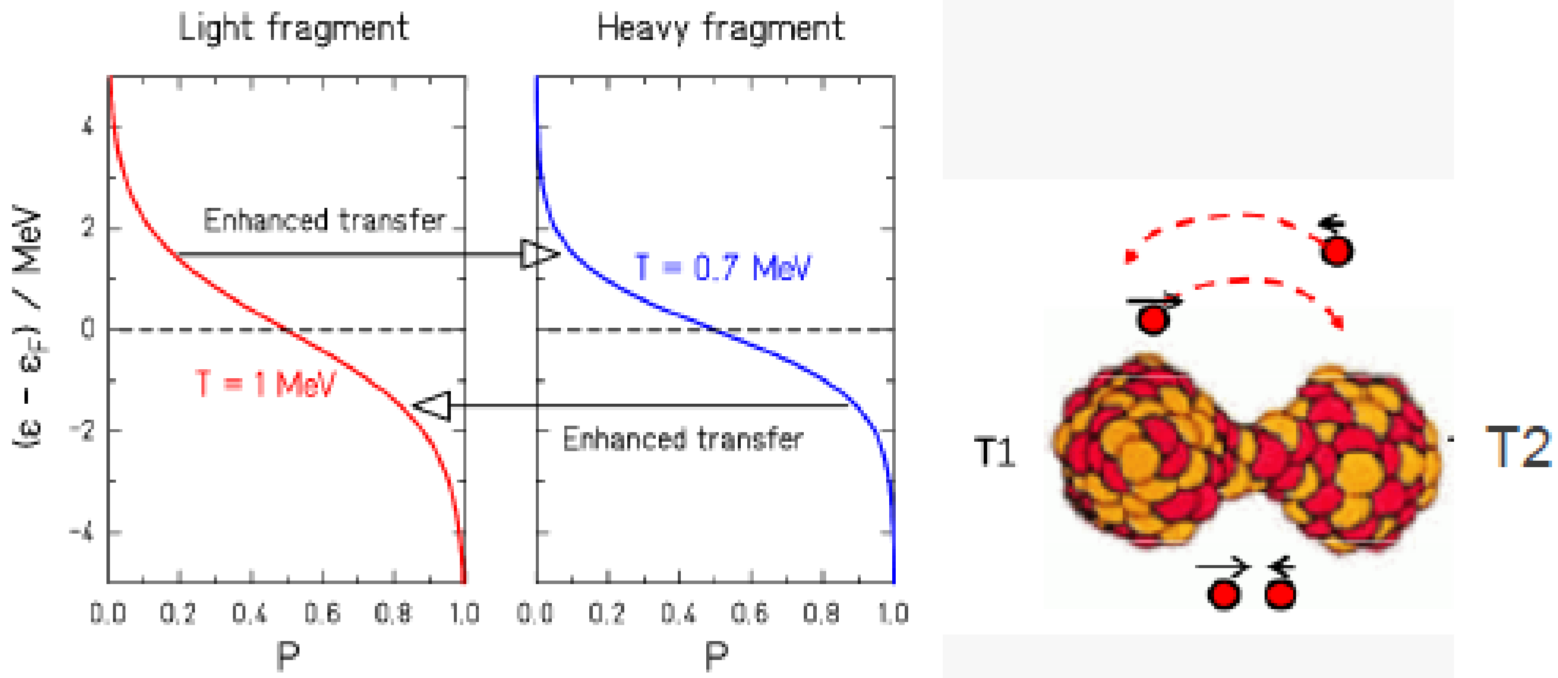
Heat is mainly transferred via nucleon exchange through the neck region

Simple model calculation



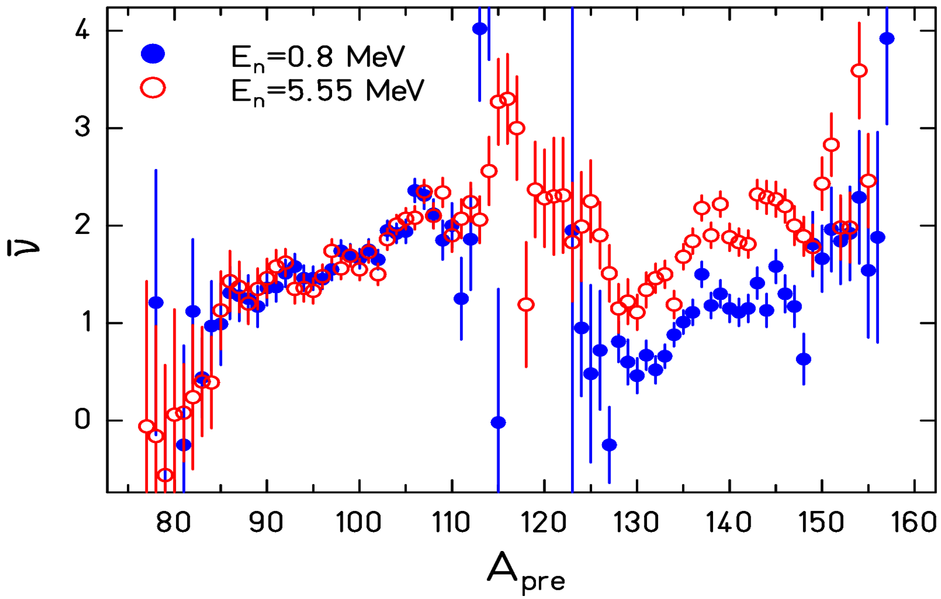
Probability distribution of the change ΔE of the excitation energy of the light nucleus after one nucleon exchange.

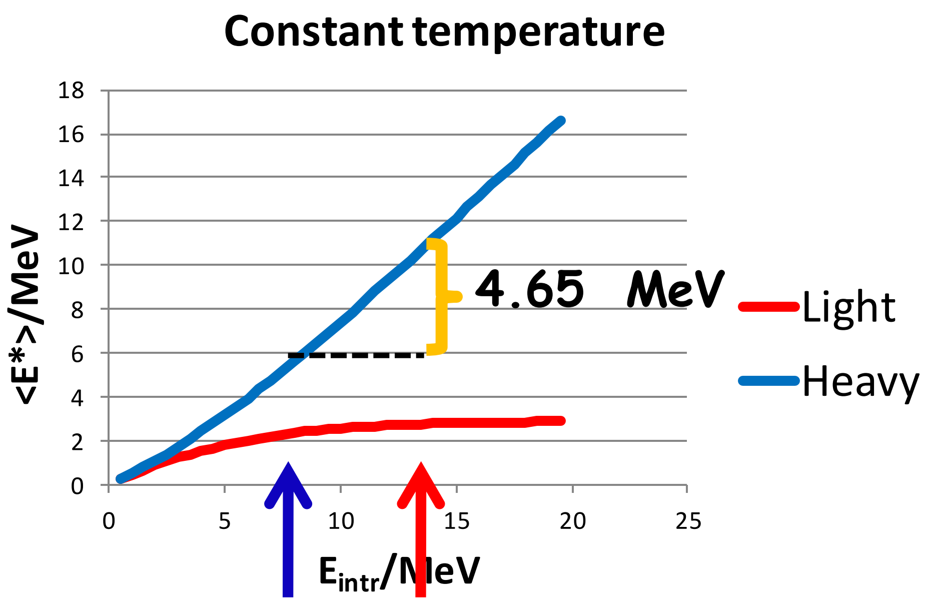
Energy transfer occurs in large steps of about 0.96 MeV and is subject to strong fluctuations σ ~ 3 MeV!!



Heat transport (Randrup NPA 327 (1979) 490

ν(A) en fonction de l'énergie : Signature du tri d'énergie d'excitation





L'augmentation du nombre de neutrons correspond à une augmentation d'E^*_{lourd} de 4.8 ± 0.2 MeV

→Peut être seulement expliqué avec le tri d'énergie d'excitation!!!