The Abdus Salam
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Educational, Scientific and
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IAEA
International Atomic Energy Agency

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Introduction to Nuclear Model Code TALYS

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Introduction to the nuclear model code TALYS

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&

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www.talys.eu

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Why do we need nuclear data ?

Nuclear data needed for

Understanding basic reaction mechanism between particles and nuclei

Astrophysical applications (Age of the Galaxy, element abundances …)

Existing or future nuclear reactor simulations

Medical applications, oil well logging, waste transmutation …

But

Finite number of experimental data (price, safety or counting rates)

Complete measurements restricted to low energies (< 1 MeV)

→ **Predictive & Robust Nuclear models (codes) are essential**

Contents

- General features of TALYS
- Models implemented in TALYS
- Some TALYS results
- Conclusions and prospects

General features of TALYS

The TALYS team

Authors

Arjan Koning, NRG Petten
Stéphane Hilaire, CEA-DIF
Marieke Duijvestijn, NRG Petten

Computational & Theoretical support, validation

Several members of CEA-DIF
Stéphane Goriely, ULB
Emmeric Dupont, CEA Cadarache
Jura Kopecky, JUKO Research
Robin Forrest, UKAEA

Current version

***TALYS-1.2 at* www.talys.eu**

TALYS in numbers

- Date of birth : 1998
- Fortran 77
- 50000 lines (+ 20000 lines of ECIS)
- Modern programming
  - modular (270 subroutines)
  - descriptive variable names & well commented (45% of lines are comments)
  - transparent programming
- Very extensive input handling and checking
  - Flexible (from default to multi-parameter adjustment : > 200 keywords)
  - Random input to check stability
  - Drip-line to drip-line calculations
- > 380 pages manual
- Compiled and tested with f77, f90, f95, … over several OS
- Externally driven for :
  - ENDF formatting
  - Random input to check stability

Other codes

ALICE – LLNL – 1974 – Blann

(Mc-)GNASH – LANL – 1977 – Young, Arthur & Chadwick

TNG – ORNL – 1980 – Fu

STAPRE – Univ. Vienna – 1980 – Uhl

UNF,MEND – CIAE, Nanking Univ. – 1985 – Cai, Zhang

EXIFON – Univ. Dresden – 1989 – Kalka

EMPIRE – ENEA/IAEA/BNL – 1980 – Herman

TALYS – NRG/CEA – 1998 – Koning, Hilaire & Duijvestijn

Modern computers (i.e. High speed & Big memory) already available when TALYS development started

What TALYS does !

- Simulates a nuclear reaction between a projectile and a target

projectiles : n,p,d,t,^{3}he, ^{4}he
target : 3 ≤ Z ≤ 110 or 5 ≤ A ≤ 339

- Projectile energy from 1keV up to 200 MeV

- TALYS mantra : “ Completeness then quality ”

- **Optical, pre-equilibrium and statistical model implemented with sets of default parameters**
- **All opened channels smoothly described**
- **Possibilities for future improvements anticipated**
  - Level densities (stored and interpolated)
  - Parity dependence
- **Still under development (improvement)**

How TALYS works !

INPUT
- projectile n
- element Fe
- mass 56
- energy 14.

Loop over energies and isotopes

OPTICAL MODEL (ECIS)
- **Phenomenologic**
  - Local or global
- **Semi-Microscopic**
- **Tabulated**

STRUCTURE
- Abundances
- Discrete levels
- Deformations
- Masses
- Level densities
- Resonances
- Fission parameters
- Radial matter dens.

DIRECT REACTION
- **Spherical / DWBA**
- **Deformed / Coupled channel**
  - Rotational
  - Vibrational
- **Giant Resonances**
- **Pickup, stripping, exchange**

PRE-EQUILIBRIUM
- **Exciton model**
- **Partial densities**
- **Kalbach systematic**
  - Angular distributions
  - Cluster emissions
- **γ emission**
- **Approx DSD**

COMPOUND
- **Hauser-Feshbach**
- **Fluctuations**
- **Fission**
- **γ Emission**
- **Level densities**
  - GC + Ignatyuk
  - Tabulated
  - Superfluid Model

MULTIPLE EMISSION
- **Exciton model**
- **Hauser-Feshbach**
- **Fission**
- **γ cascade**
- **Exclusive channels**
- **Recoils**

OUTPUT
- XS
- Spectra
- Astro-rates
- Fission yields
- FF decay
- ENDF

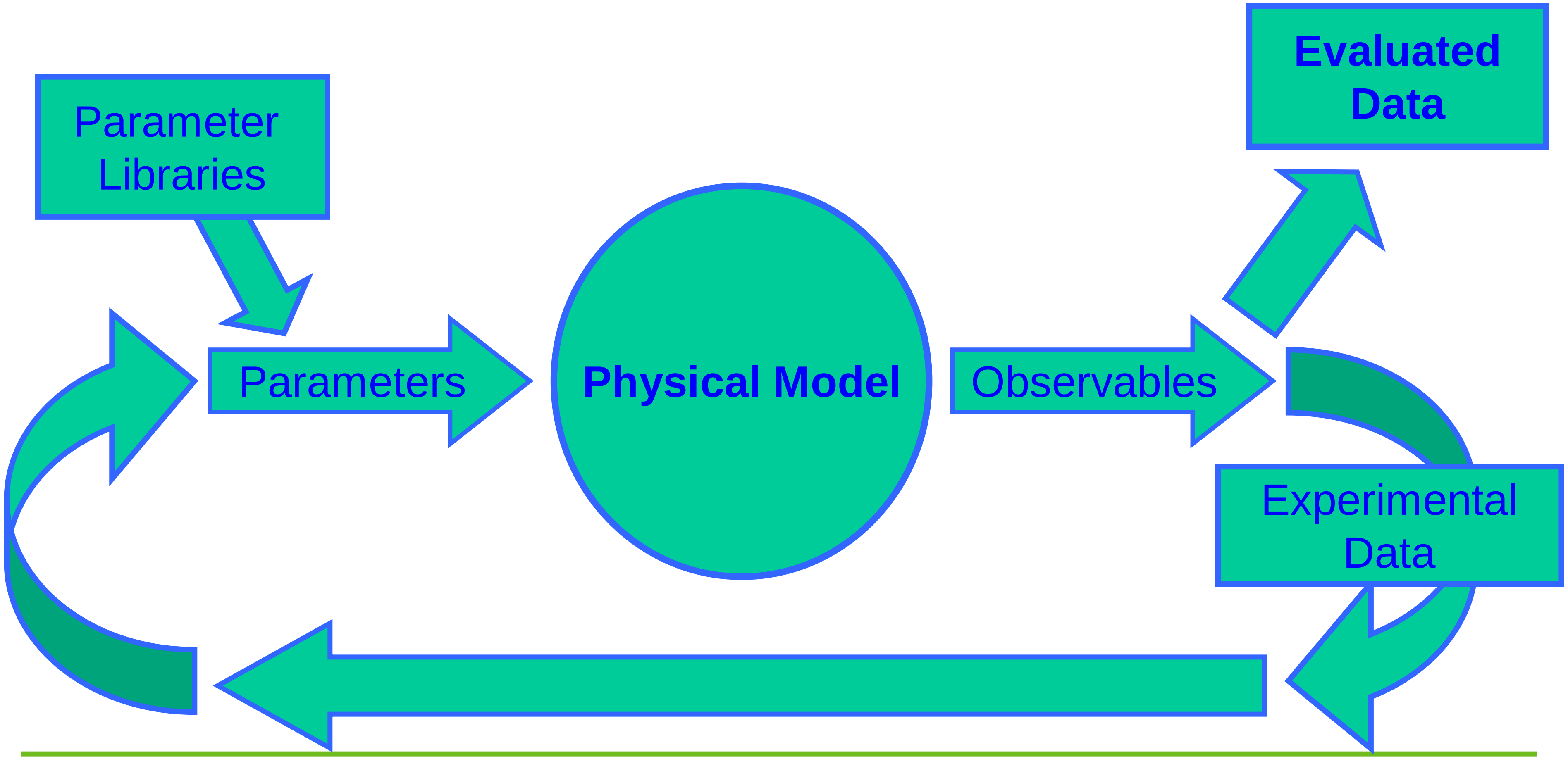
What TALYS yields !

-Cross sections : total, reaction, elastic (shape & compound), inelastic (per level & total) and all opened channels.

- Elastic and inelastic angular distribution
- Exclusive reaction channels : xs, spectra & ddx
- Exclusive discrete and continuum γ-ray production
- Photonuclear reactions & reactions on isomeric targets
- Fission cross sections and fission yields
- Residuals production and recoils
- Total particle production : xs, spectra & ddx
- Extrapolation down to thermal energy
- Stellar reaction rates
- Fission fragment decay
- Level density tables

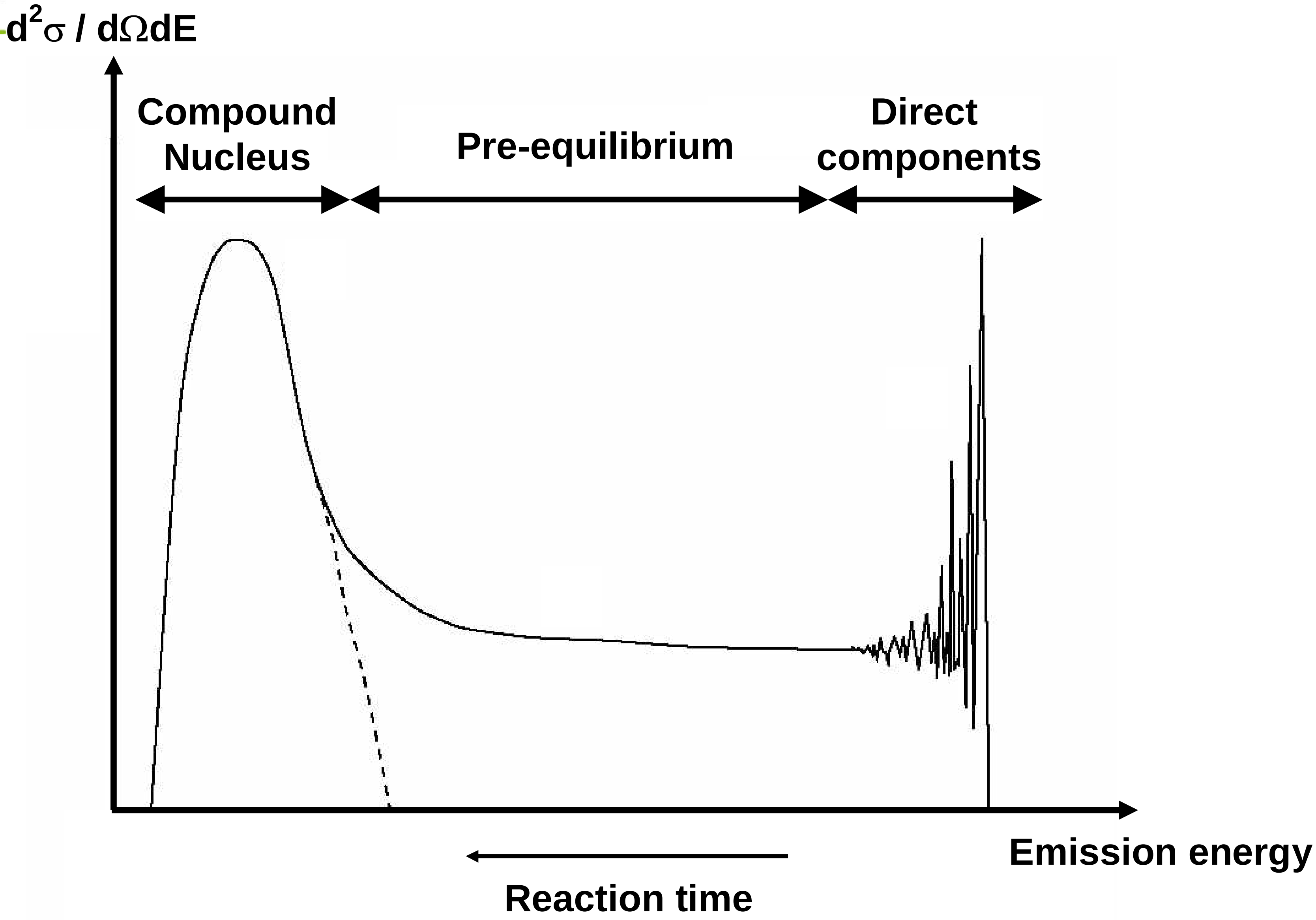
Nuclear reaction modeling

Method which consists in using a physical model (together with sets of parameters) to calculate evaluated data.

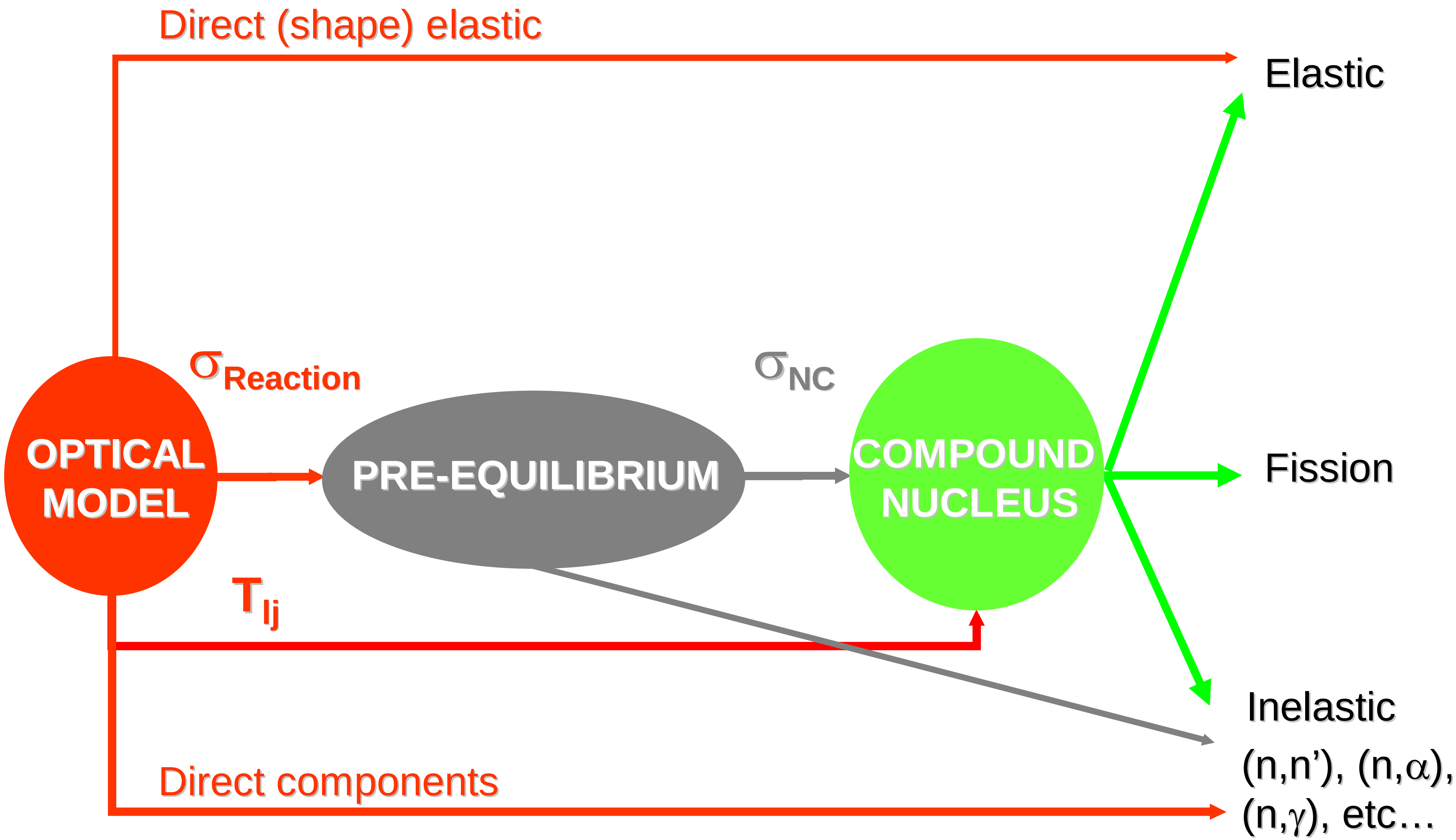


Models implemented in TALYS

Models sequence



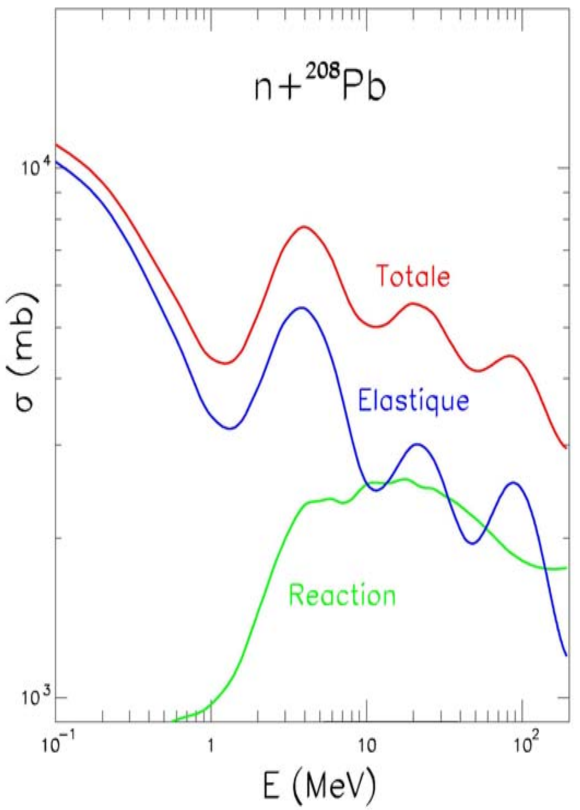
Models sequence



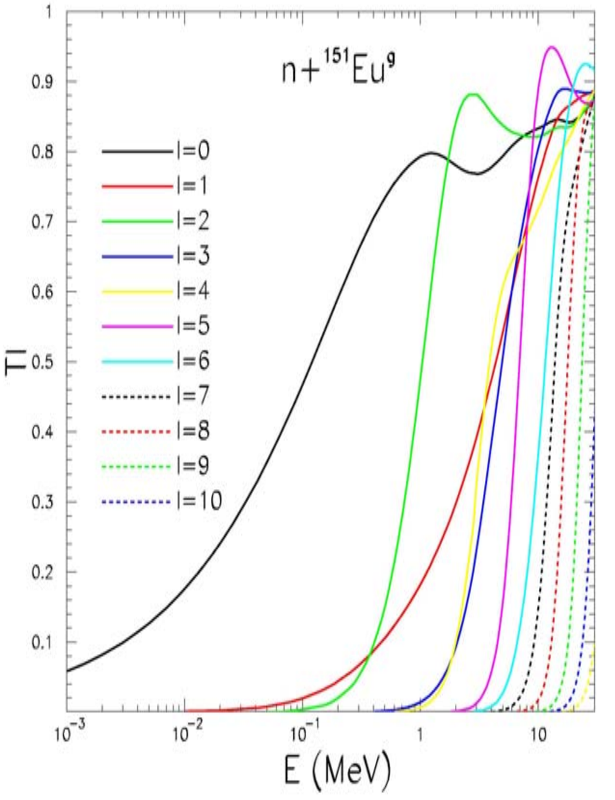
The Optical model

This model yields :

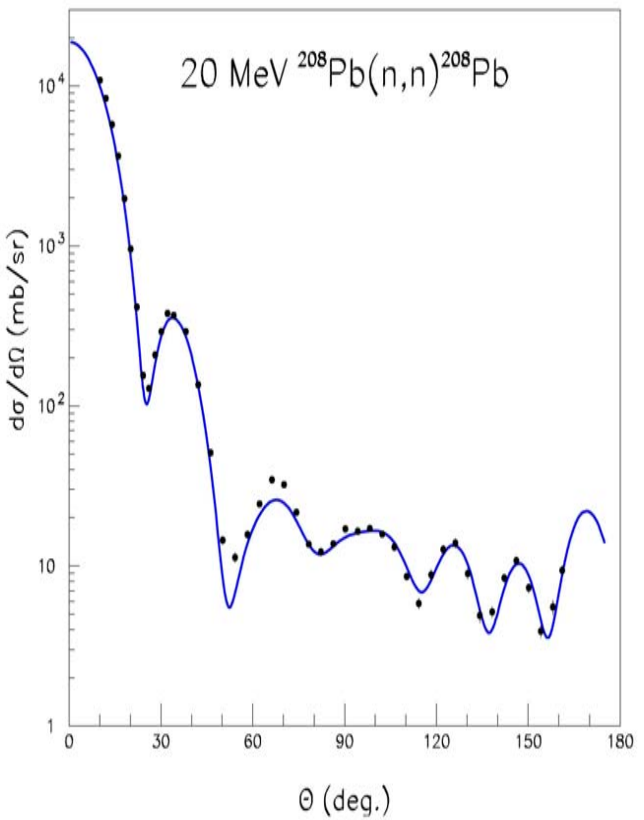
Integrated cross sections



Transmission coefficients



Angular distributions



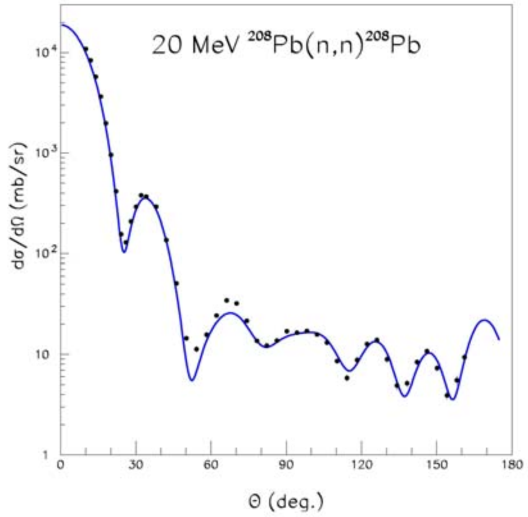
The Optical model

Direct interaction of a projectile with a target nucleus considered as a whole

Quantum model → Schrödinger equation

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + U - E\right)\Psi = 0$$

Fig.1

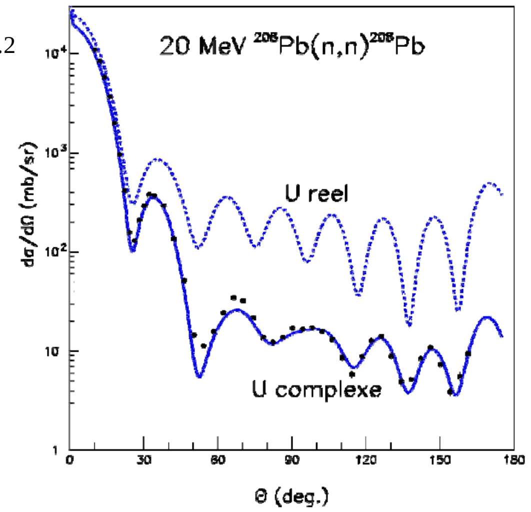


Complex potential:

$$U = V + iW$$

Refraction (V) — Absorption (iW)

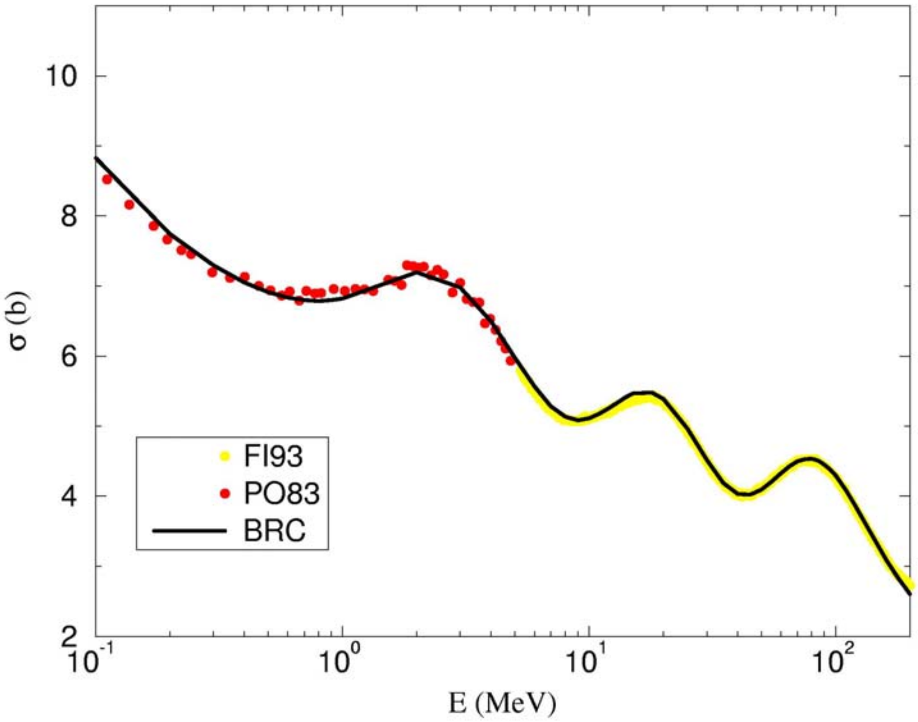
Fig.2



Approaches implemented in TALYS

Phenomenologic

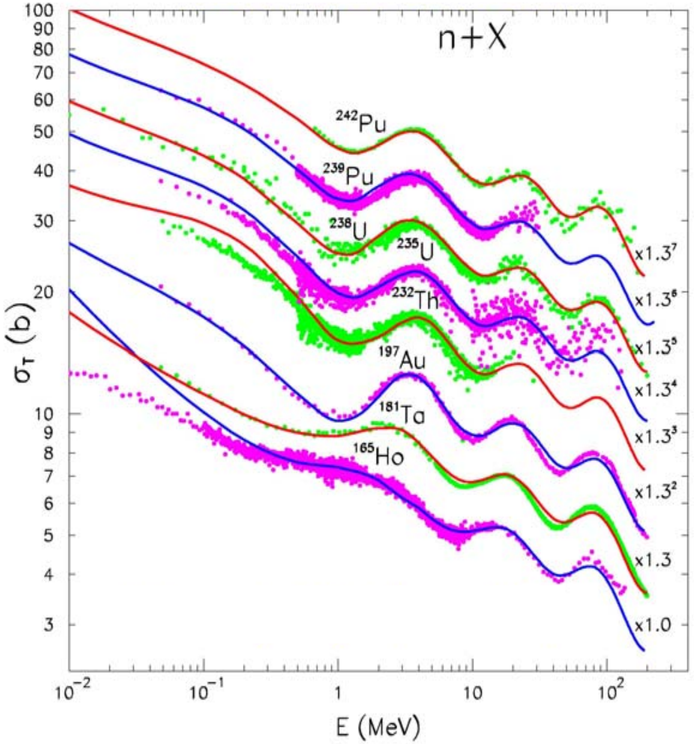
Adjusted parameters
Weak predictive power
Very precise (≈ 1%)
Important work



Semi-microscopic

No adjustable parameters
Usable without exp. data
Less precise (≈ 5-10 %)
Quasi-automated

Total cross sections



Approaches implemented in TALYS

Phenomenologic :

- Koning-Delaroche for non-fissile nuclei
- Soukhovitsky for fissile nuclei
- Other implementations easy (e.g. α)
- Tabulation possible

Semi-microscopic

- JLM approach based on matter densities

  $\Rightarrow$ any type of matter density can be used

  (Skyrme and Gogny already available)

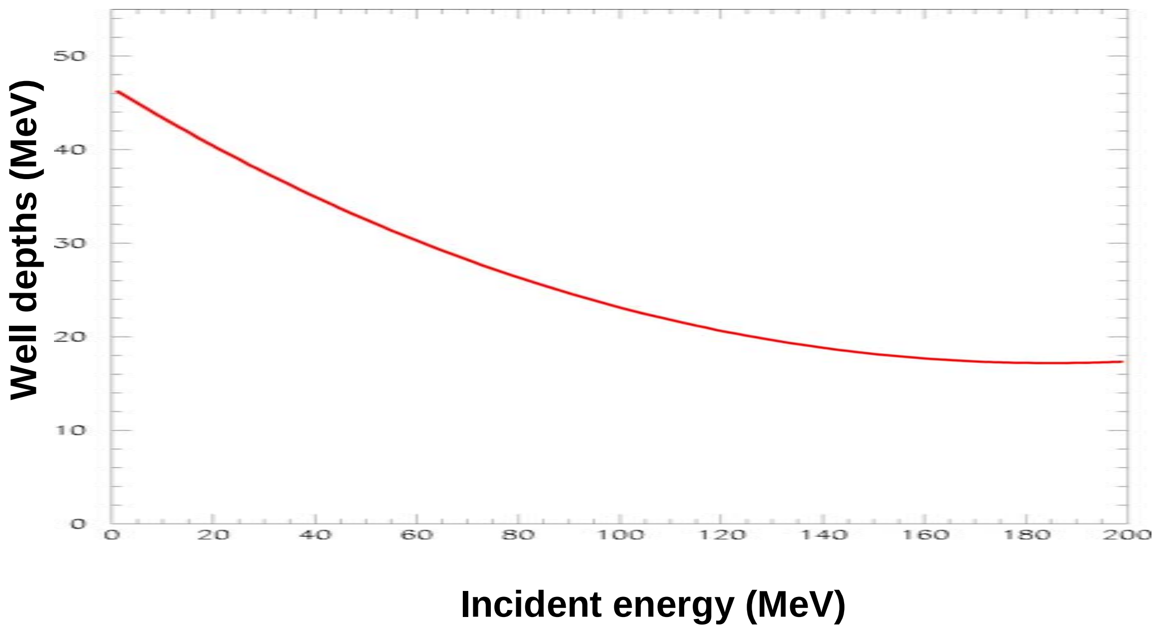
$\Rightarrow$ OMP calculations essentially performed with ECIS

Phenomenological OMP

$$U(r,E) = V(E,r) + i\,W(E,r)$$

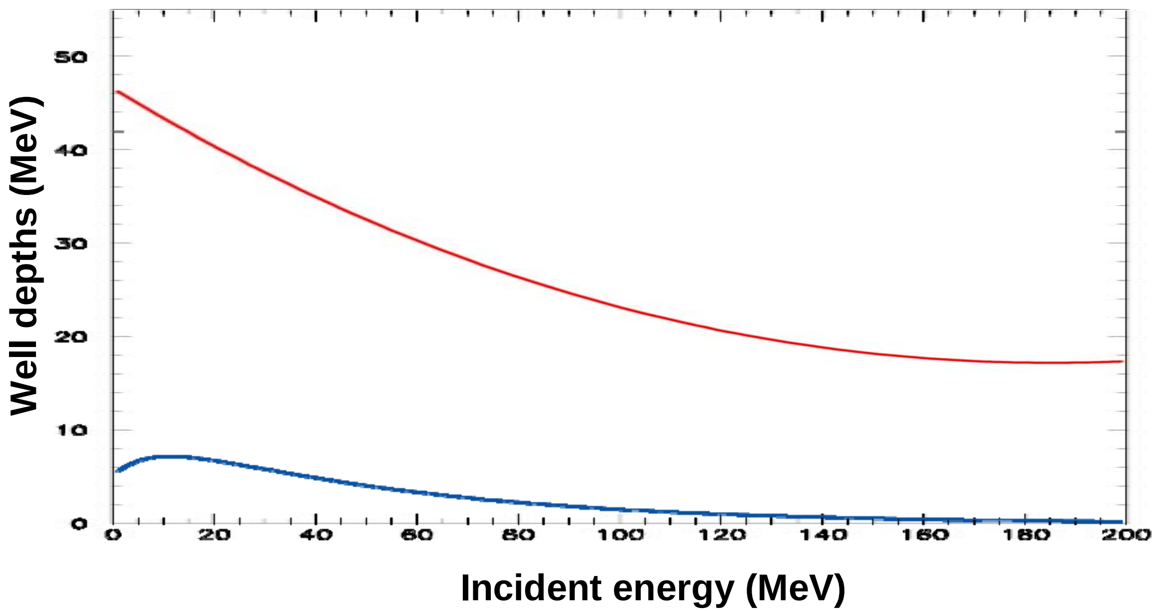
Phenomenological OMP

$$U(r,E) = \left[V_V(E)\, f(r, R_V, a_V) + V_S(E)\, g(r, R_S, a_S) \right]$$
$$+\, i \left[W_V(E)\, f(r, R_V, a_V) + W_S(E)\, g(r, R_S, a_S) \right]$$



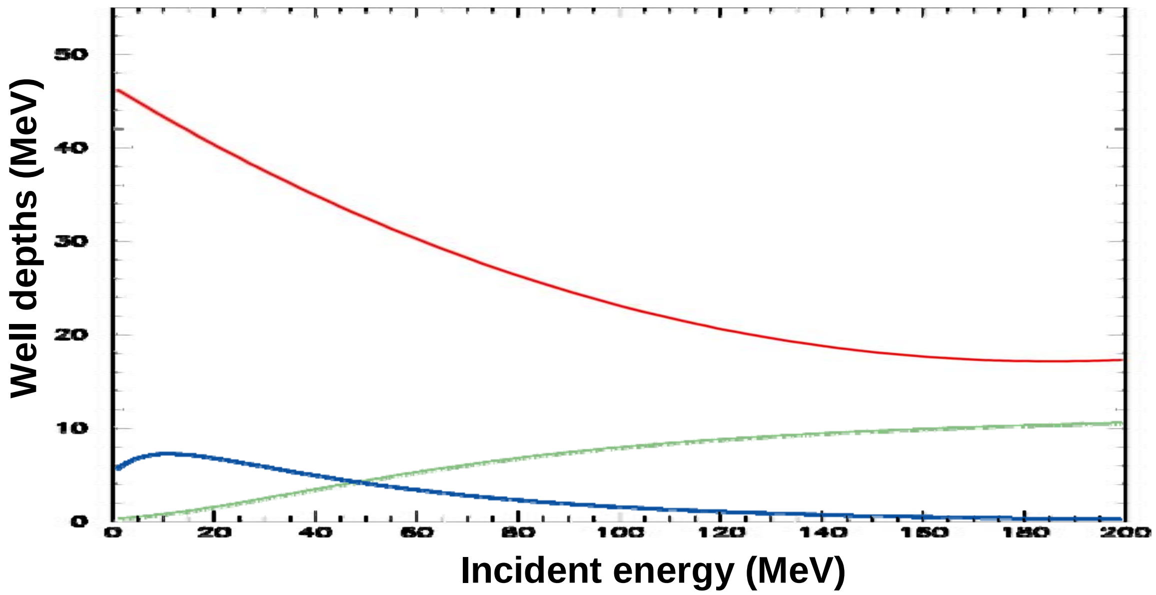
Phenomenological OMP

$$U(r,E) = \left[V_V(E)\, f(r, \mathbf{R}_V, a_V) + V_S(E)\, g(r, R_S, a_S) \right]$$
$$+\, i \left[W_V(E)\, f(r, R_V, a_V) + W_S(E)\, g(r, R_S, a_S) \right]$$



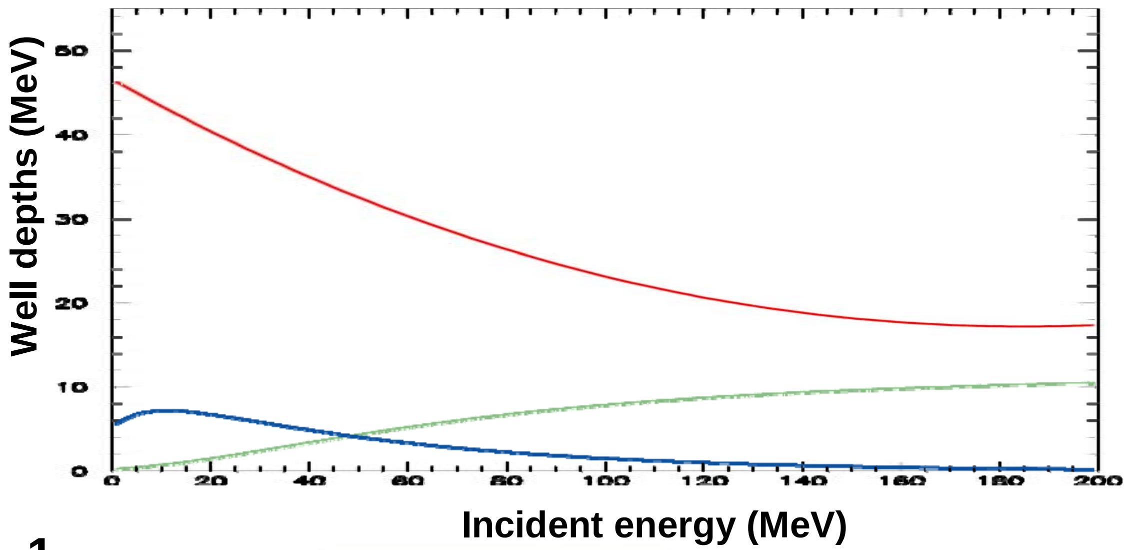
Phenomenological OMP

$$U(r,E) = \Big[V_V(E)\, f(r, \mathbf{R}_V, a_V) + V_S(E)\, g(r, R_S, a_S) \Big]$$
$$+\, i \Big[W_V(E)\, f(r, R_V, a_V) + W_S(E)\, g(r, R_S, a_S) \Big]$$

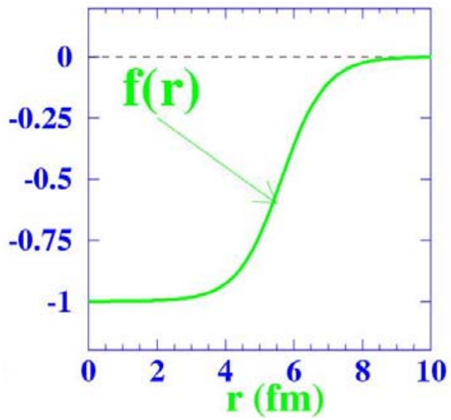


Phenomenological OMP

$$U(r,E) = \left[V_V(E)\, f(r, R_V, a_V) + V_S(E)\, g(r, R_S, a_S) \right]$$
$$+\, i \left[W_V(E)\, f(r, R_V, a_V) + W_S(E)\, g(r, R_S, a_S) \right]$$

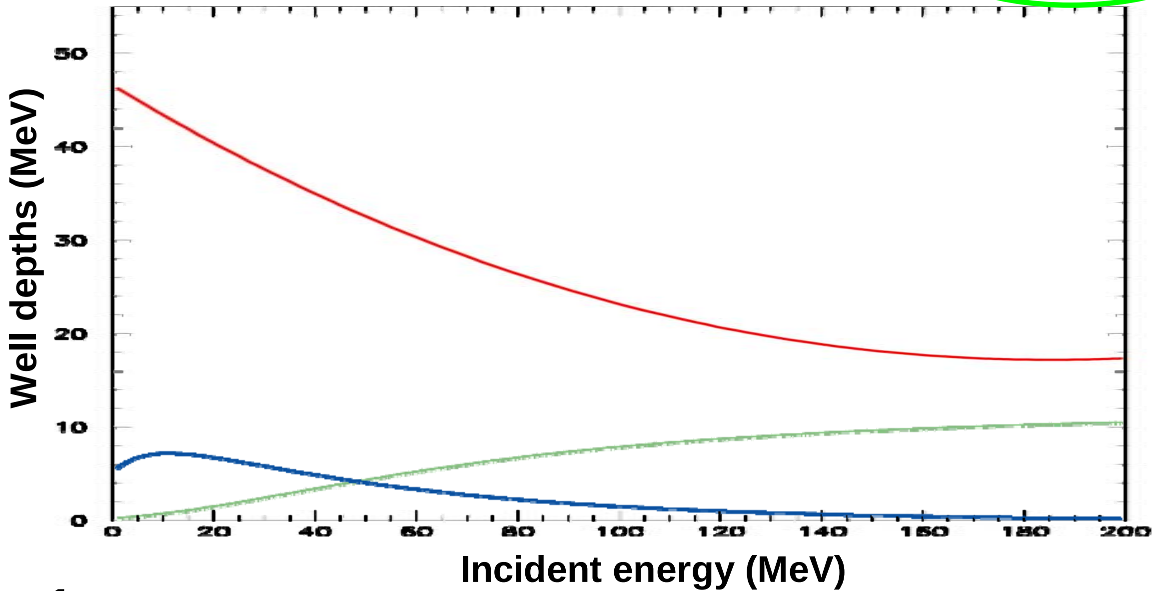


$$f(r,R,a) = \frac{-1}{1+\exp((r-R)/a)}$$

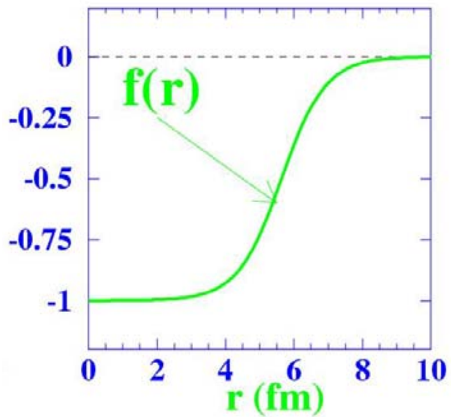


Phenomenological OMP

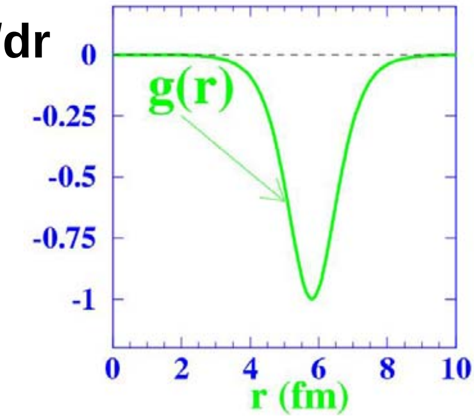
$$U(r,E) = \left[V_V(E)\, f(r, \mathbf{R}_V, a_V) + V_S(E)\, g(r, R_S, a_S) \right]$$
$$+\, i \left[W_V(E)\, f(r, R_V, a_V) + W_S(E)\, g(r, R_S, a_S) \right]$$



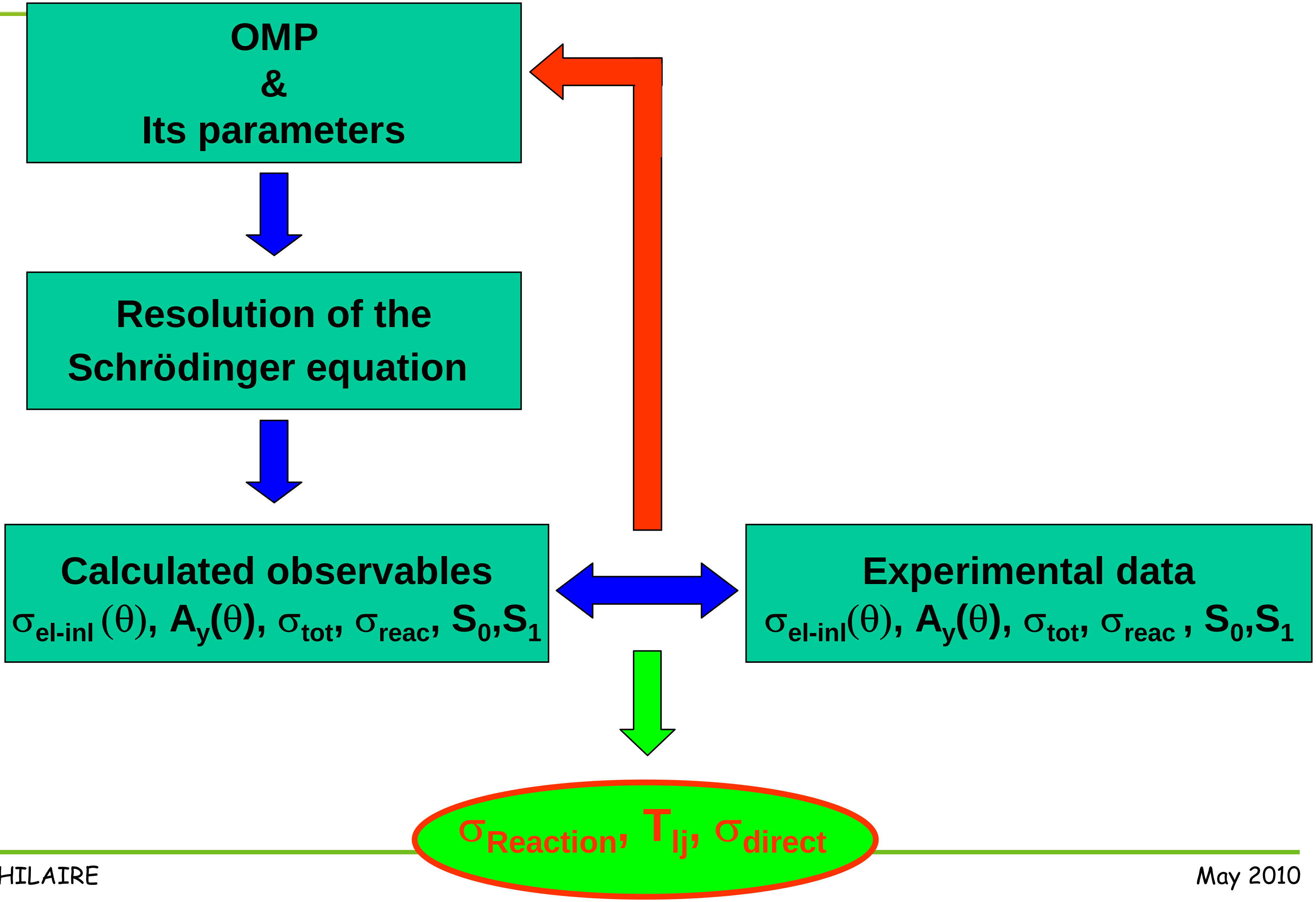
$$f(r,R,a) = \frac{-1}{1+\exp((r-R)/a)}$$



$$g(r,R,a) = -\,df/dr$$

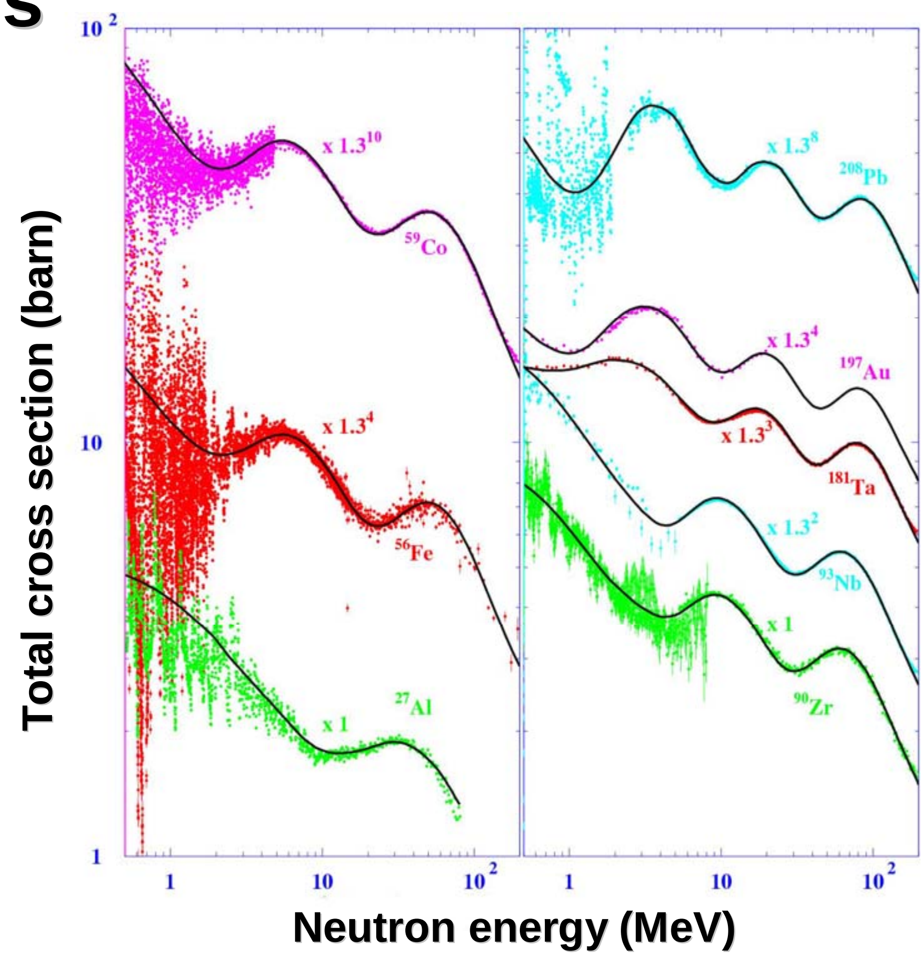


Phenomenological OMP



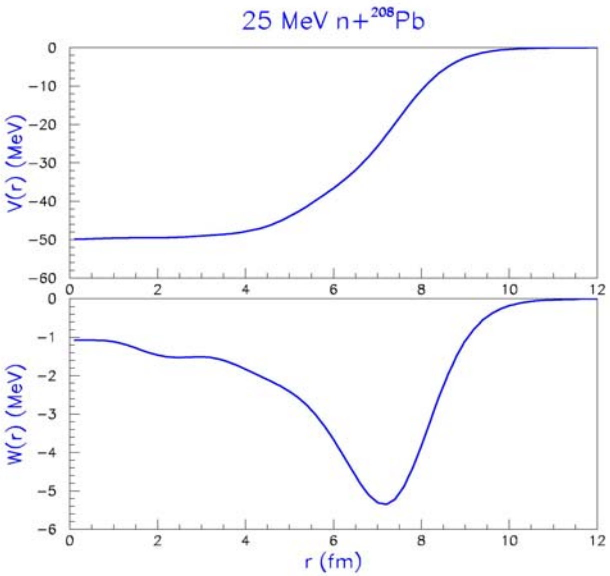
Phenomenological OMP

- $\approx$ 20 adjusted parameters
- Very precise (1%)
- Relatively weak predictive power far away from stability



Semi-microscopic OMP

Optical potential = Effective Interaction ⊗ Radial densities



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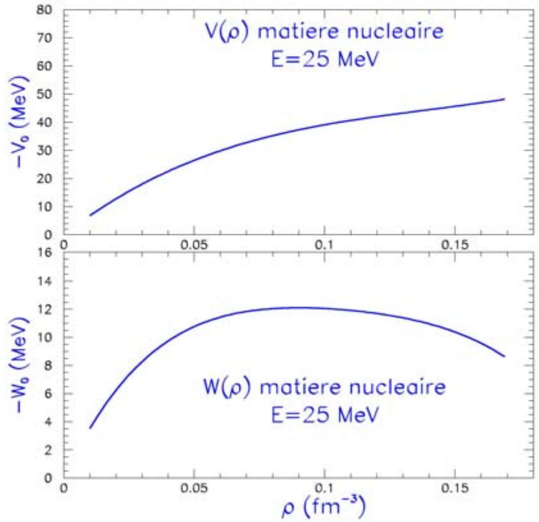
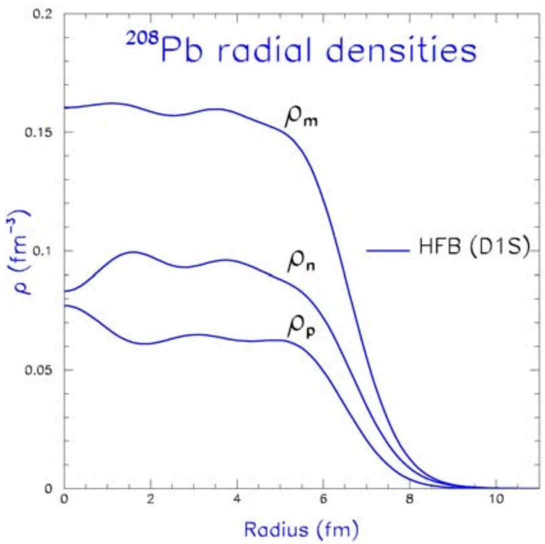


⊗



$$U(r,E) = \frac{U(\rho(r'),E)}{\rho(r')} \otimes \rho(r)$$

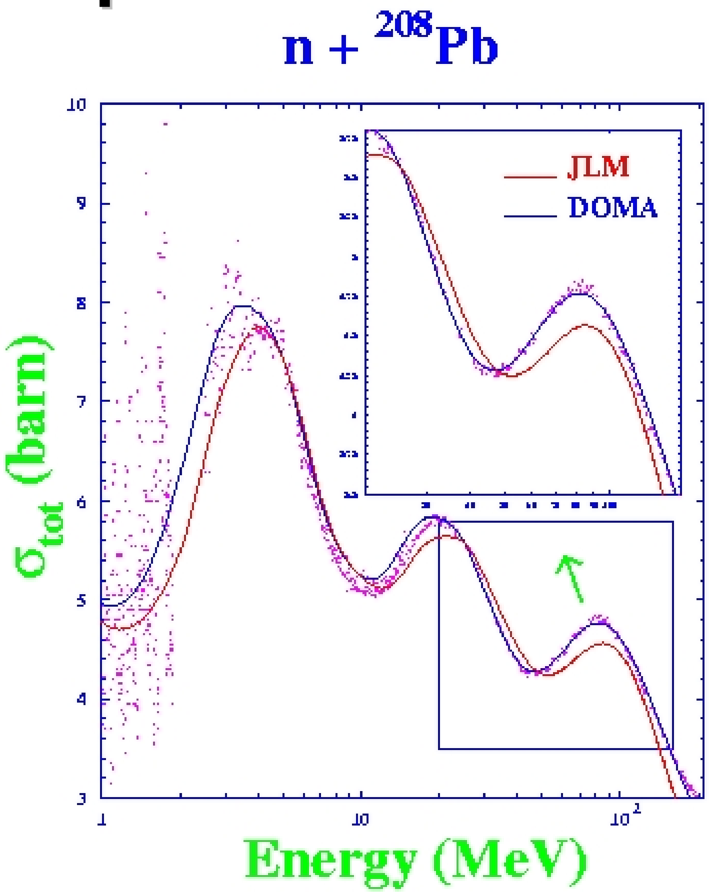
Depends on the nucleus | Independent of the nucleus | Depends on the nucleus

Semi-microscopic OMP

- **No adjustable parameters**
- **Based on nuclear structure properties**

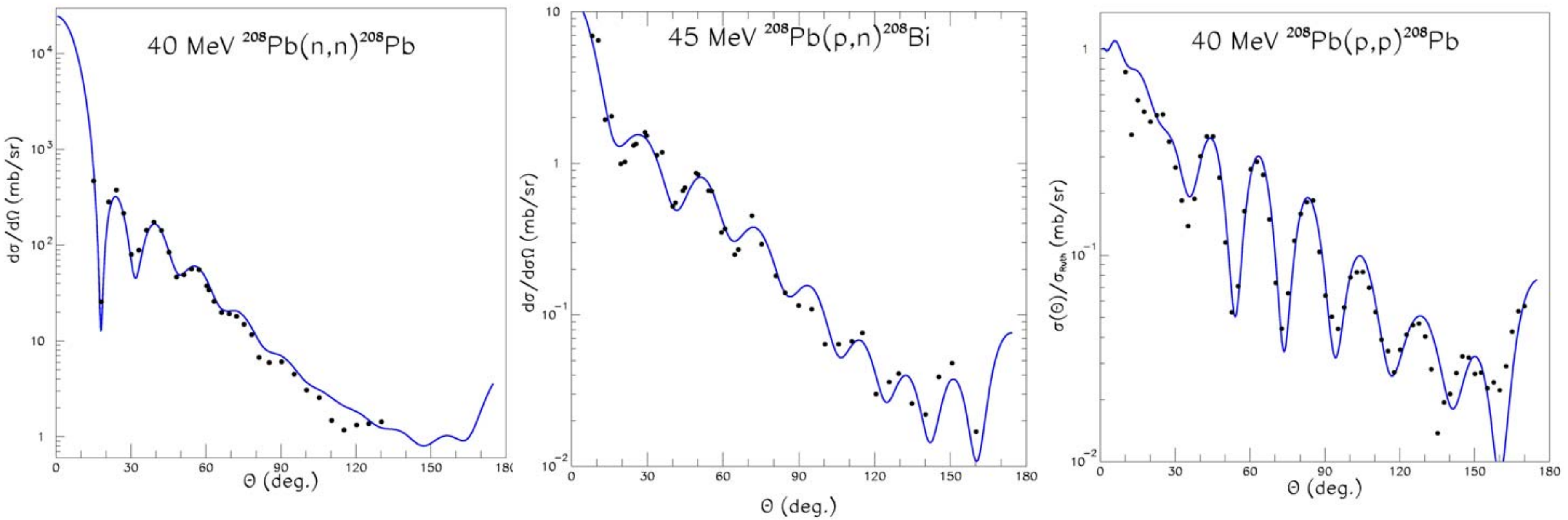
⇒ usable for any nucleus

- **Less precise than the phenomenological approach**



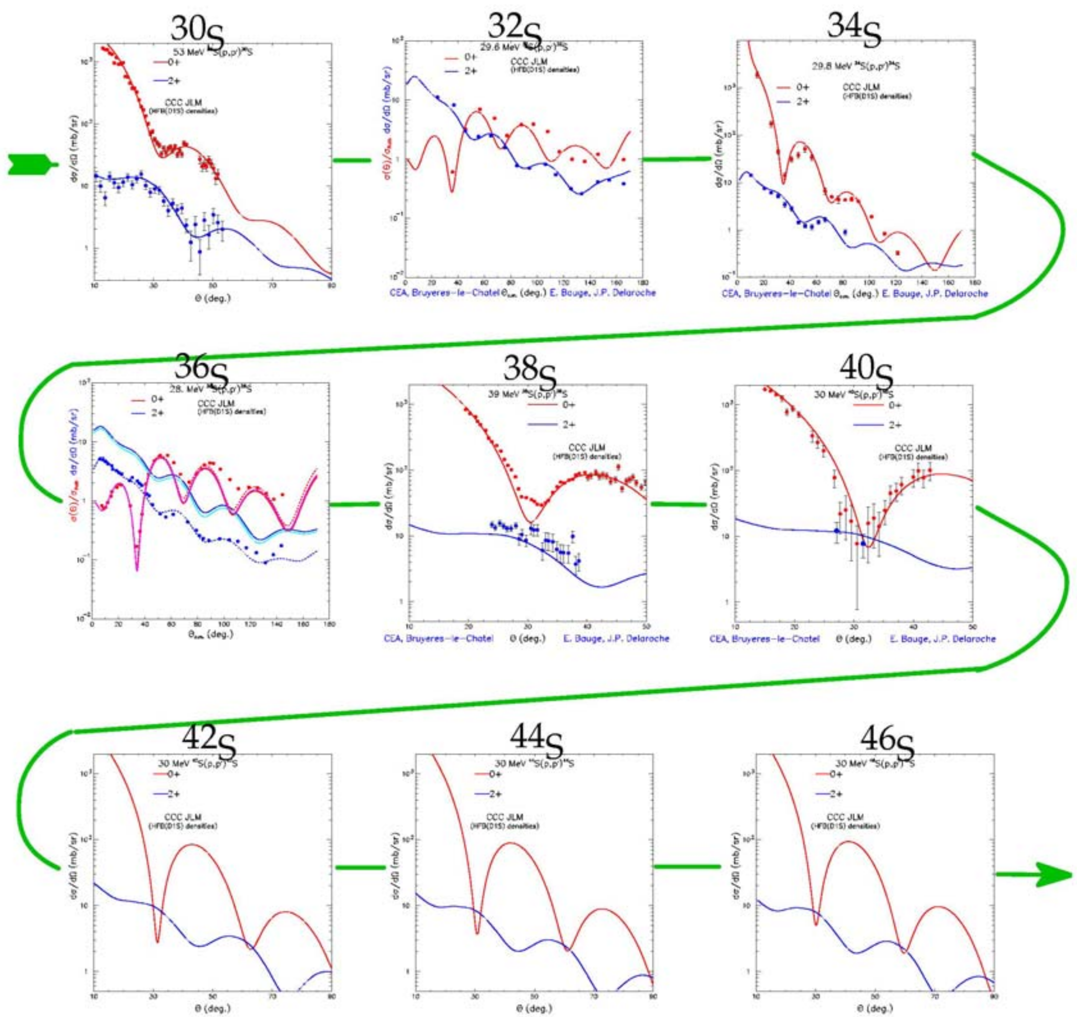
Semi-microscopic OMP

Unique description of elastic scattering (n,n), (p,p) et (p,n)

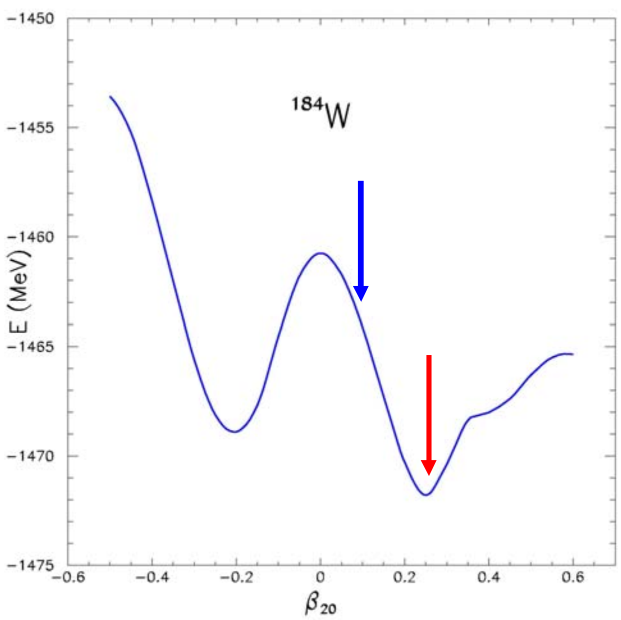


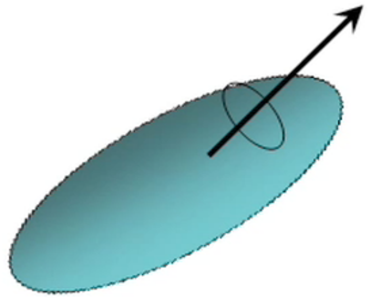
Semi-microscopic OMP

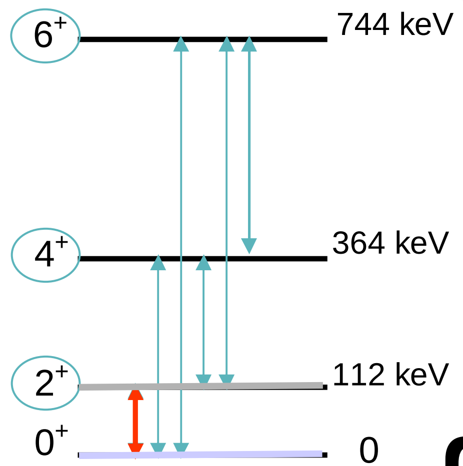
Enables to perform predictions for very exotic nuclei for which There exist no experimental data



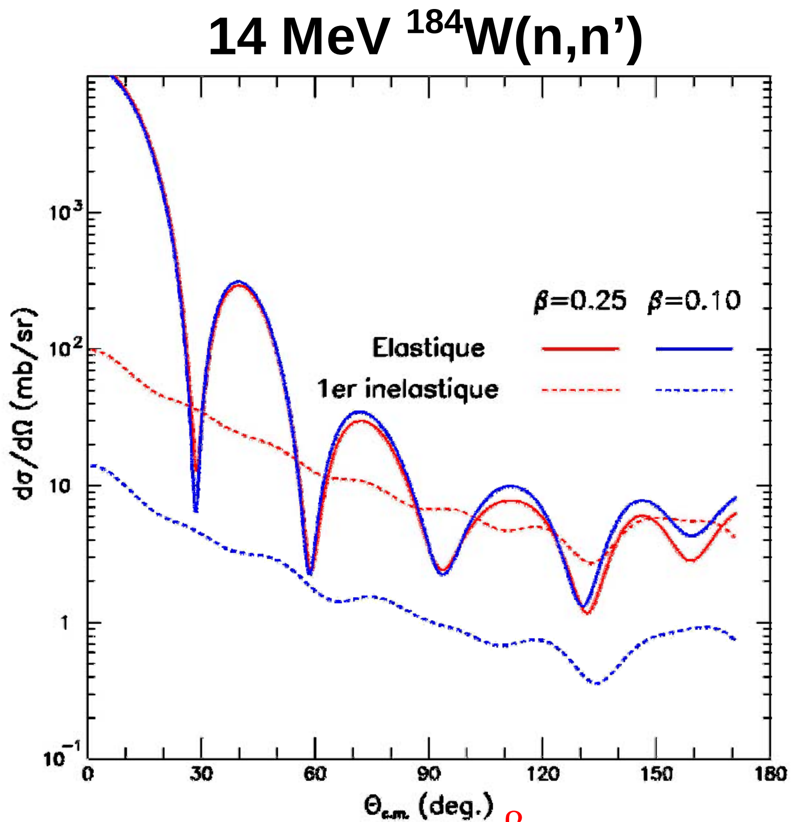
Coupled channels in OMP







^{184}W

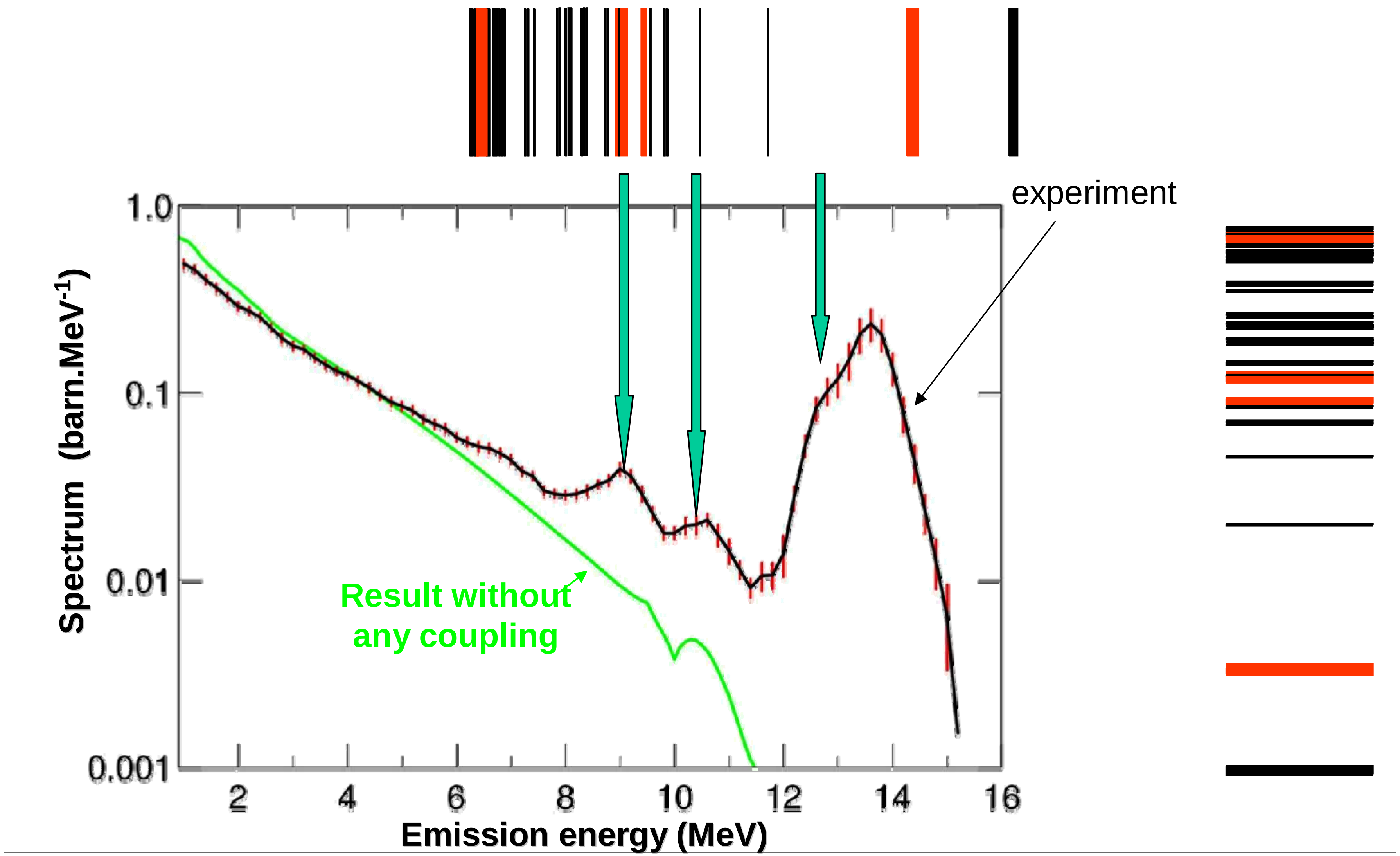


β

$$\begin{cases}(T+V_{00}-E)\,\Psi_0 = V_{02}\,\Psi_2\\ (T+V_{22}-E)\,\Psi_2 = V_{20}\,\Psi_0\end{cases}$$

movie

Coupled channels in OMP



movie

Coupled channels in TALYS

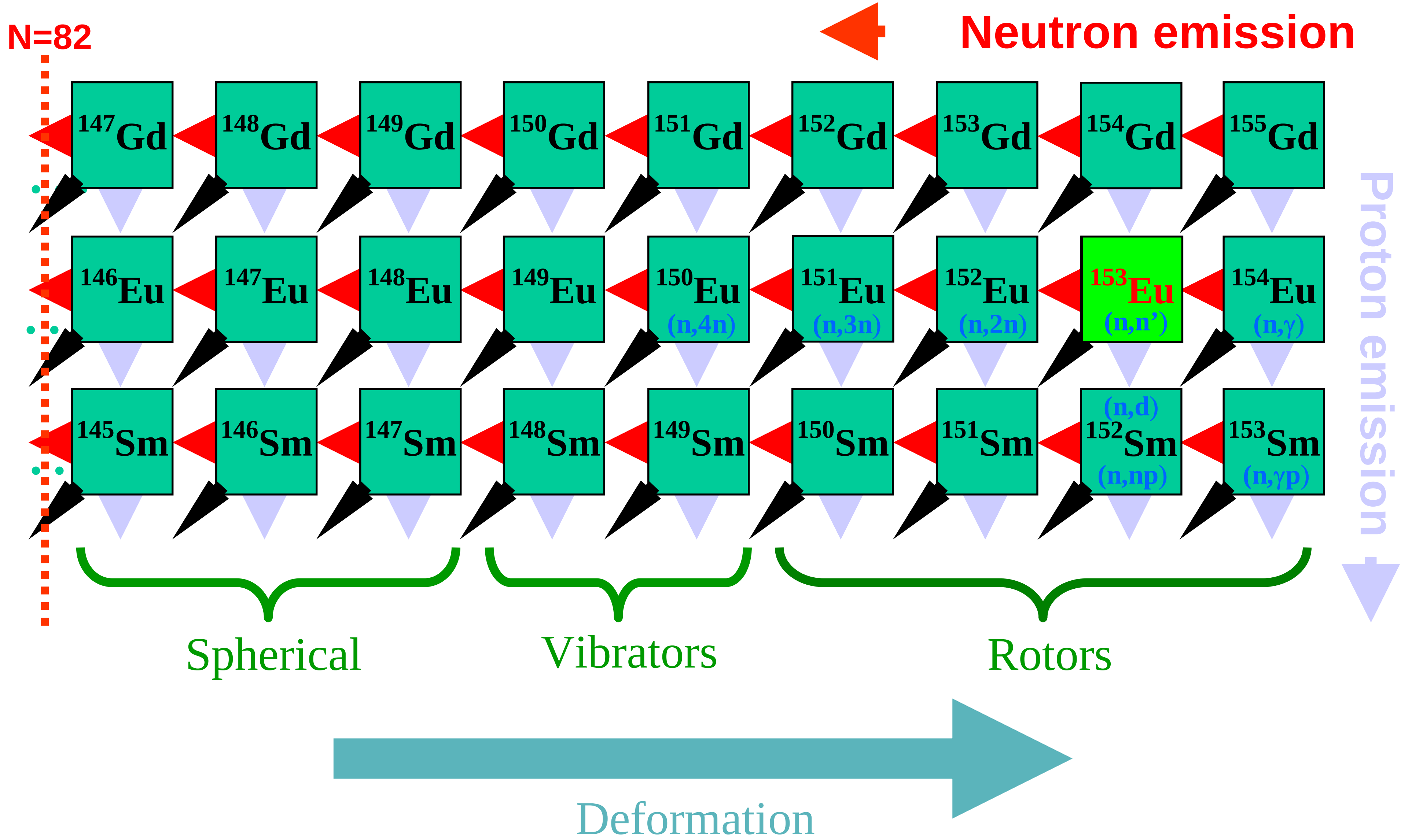
deformation file z092

```
92 237   5   R   D
 0   R   0              1.75000  0.65000
 1   R   0
 2   R   0
 3   R   0
 5   R   0
92 238  23   R   D
 0   R   0              1.54606  0.44508
 1   R   0
 2   R   0
 3   R   0
 4   R   0
 5   V   1   3   0      0.90000
 6   V   1
 7   R   0
 8   V   1
 9   V   2   4   0      0.20000
10   V   3   3   1      0.10000
11   V   3
12   V   2
13   V   1
14   V   4   2   0      0.10000
15   V   3
16   V   4
17   V   2
21   V   5   2   2      0.10000
22   R   0
23   V   5
25   V   4
31   V   5
```

level file z092

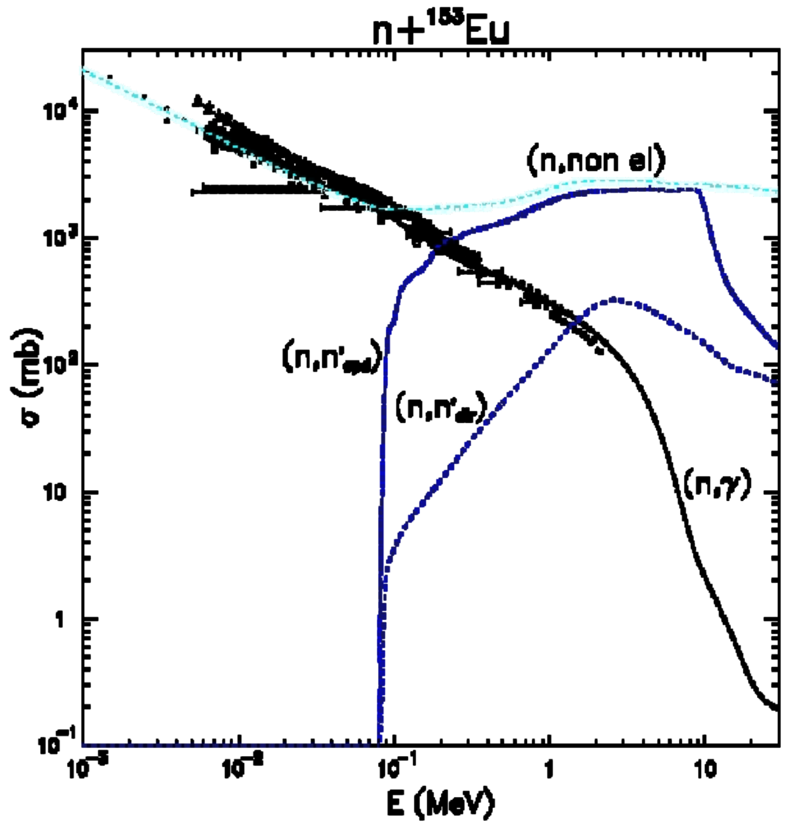
```
 92 238  501  152                                                238U
  0   0.000000   0.0    1  0                   1.410E+17         0+
  1   0.044916   2.0    1  1                   2.060E-10         2+
                           0  1.000000 6.090E+02
  2   0.148380   4.0    1  1                                     4+
                           1  1.000000 1.160E+01
  3   0.307180   6.0    1  1                                     6+
                           2  1.000000 1.870E+00
  4   0.518100   8.0    1  1                   2.300E-11         8+
                           3  1.000000 6.260E-01
  5   0.680110   1.0   -1  2                   3.500E-14         1-
                           1  0.558700 2.000E-02
                           0  0.441300 2.000E-02
  6   0.731930   3.0   -1  3                                     3-
                           5  0.000000 3.123E+02
                           2  0.450225 1.000E-02
                           1  0.549775 7.045E-03
  7   0.775900  10.0    1  1                   9.000E-12        10+
                           4  1.000000 3.130E-01
  8   0.826640   5.0   -1  2                                     5-
                           3  0.335445 1.195E-02
                           2  0.664555 7.213E-03
  9   0.927210   0.0    1  1                                     0+
                           1  1.000000 1.341E-02
 10   0.930550   1.0   -1  3                                   (1-)
                           5  0.157218 3.413E-01
                           1  0.673221 4.650E-03
                           0  0.169560 4.260E-03
 11   0.950120   2.0   -1  3                                     2-
                           6  0.419039 5.570E-01
                           5  0.251909 2.685E-01
                           1  0.329052 4.470E-03
 12   0.966130   2.0    1  5                   2.400E-12         2+
                           6  0.064358 6.890E-02
                           5  0.035757 4.380E-02
                           2  0.418755 1.660E-02
                           1  0.367863 2.300E-01
```

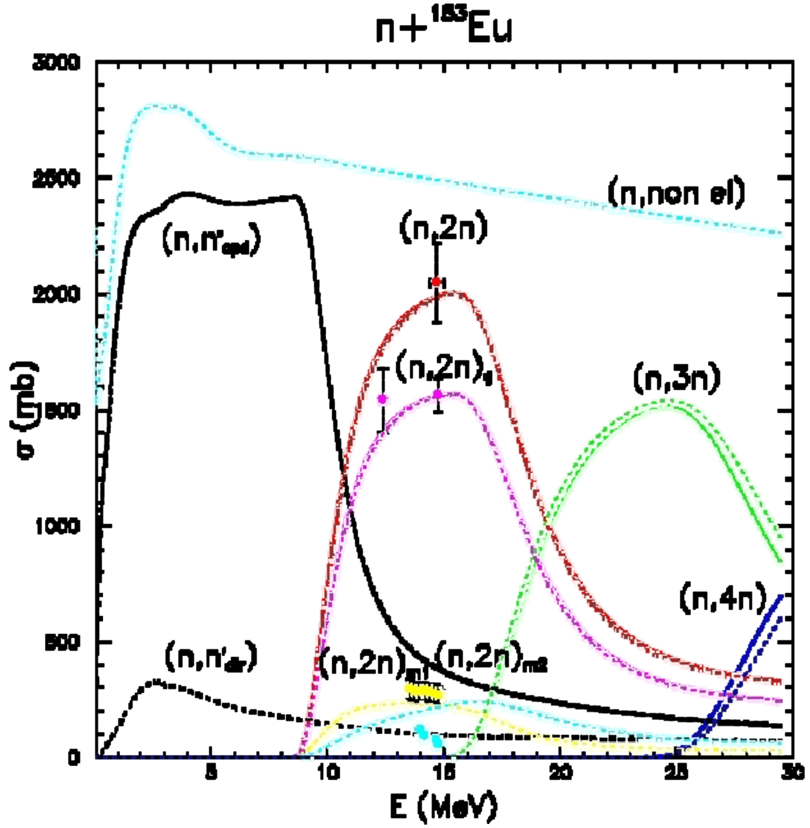
Decay-dependent OMPs in TALYS



movie

Decay-dependent OMPs in TALYS





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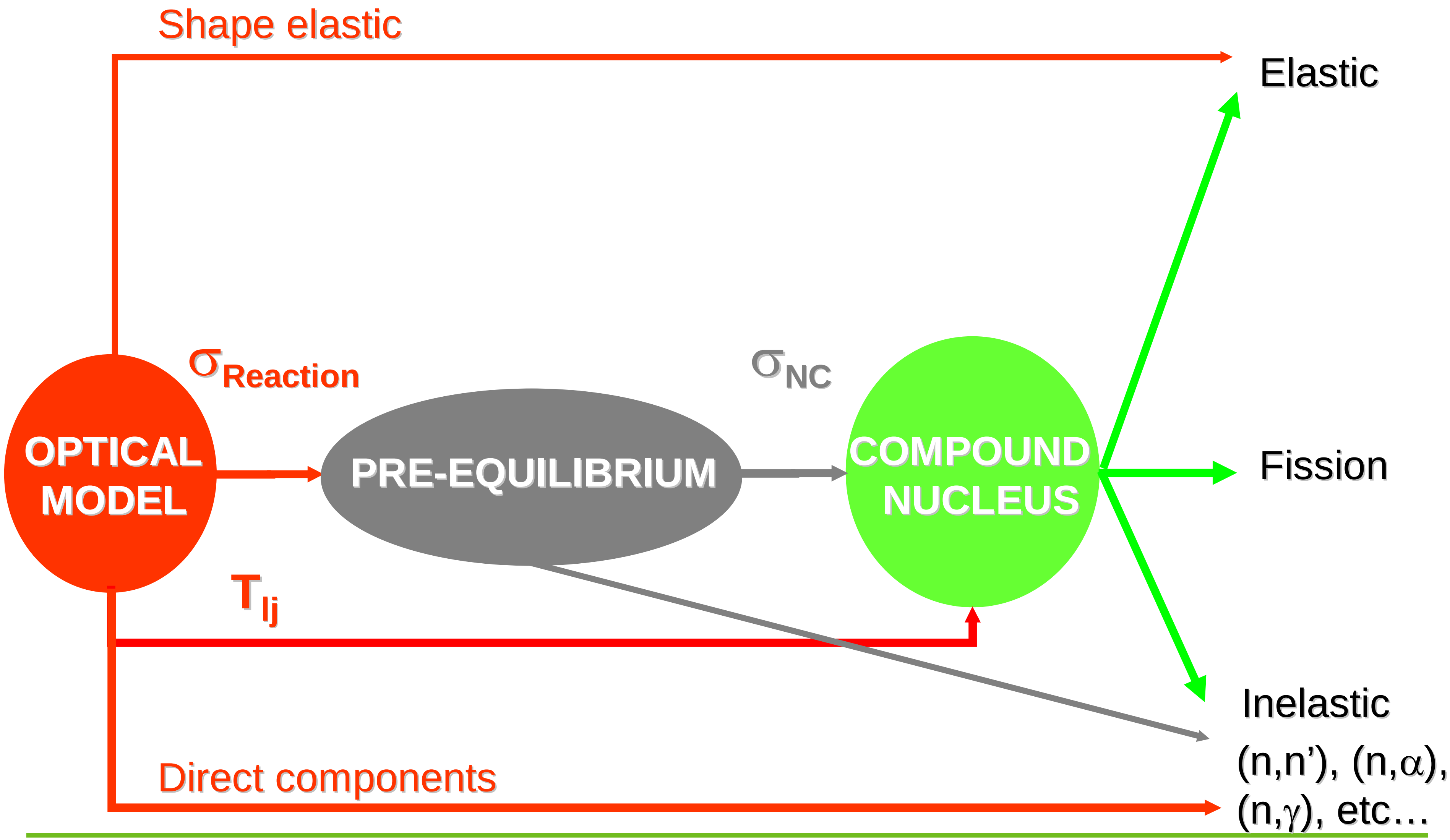
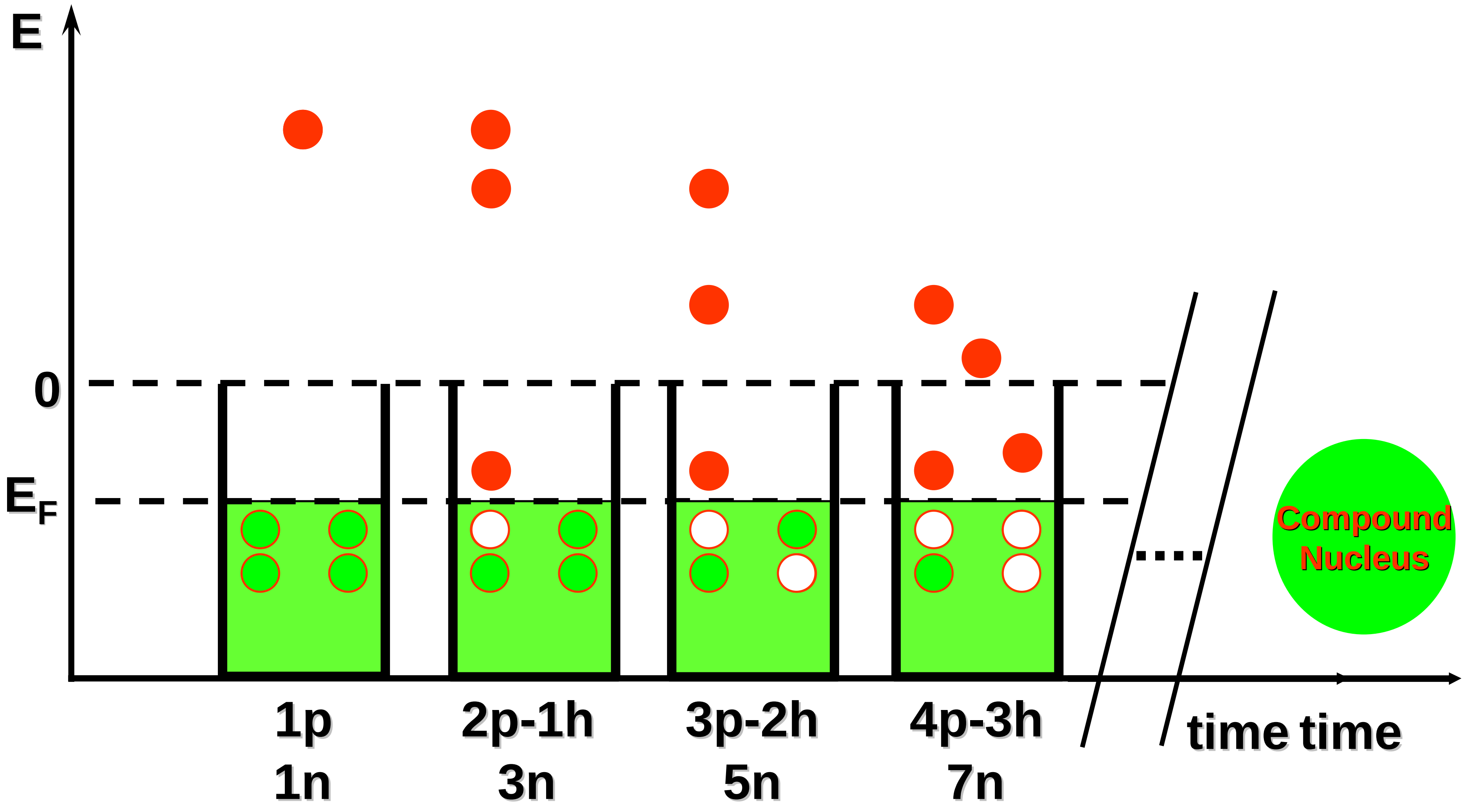
Models sequence



Pre-equilibrium model(s)



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Pre-equilibrium exciton model

P(n,E,t) = Probability to find for a given time t the composite system with an energy E and an excitons number n.

$\lambda_{a,b}(E)$ = Transition rate from an initial state a towards a state b for a given energy E.

Evolution equation

Apparition

Disparition

$$\frac{dP(n,E,t)}{dt} = P(n-2,E,t)\,\lambda_{n-2,n}(E) + P(n+2,E,t)\,\lambda_{n+2,n}(E) - P(n,E,t)\left[\lambda_{n,n+2}(E) + \lambda_{n,n-2}(E) + \lambda_{n,emiss}(E)\right]$$

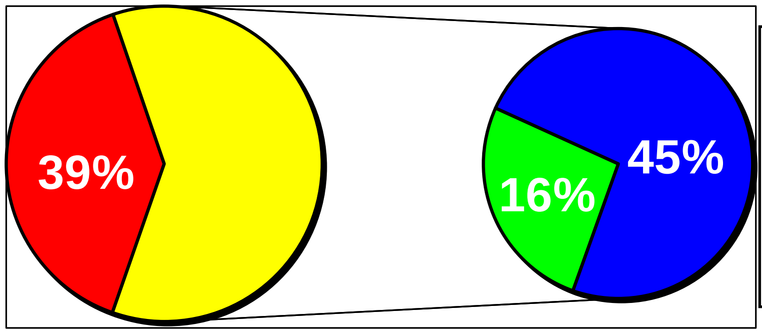
Emission cross section in channel c

$$\sigma_c(E,\varepsilon_c)\,d\varepsilon_c = \sigma_R \int_0^{t_{eq}} \sum_{n,\Delta n=2} P(n,E,t)\,\lambda_{n,c}(E)\,dt\;d\varepsilon_c$$

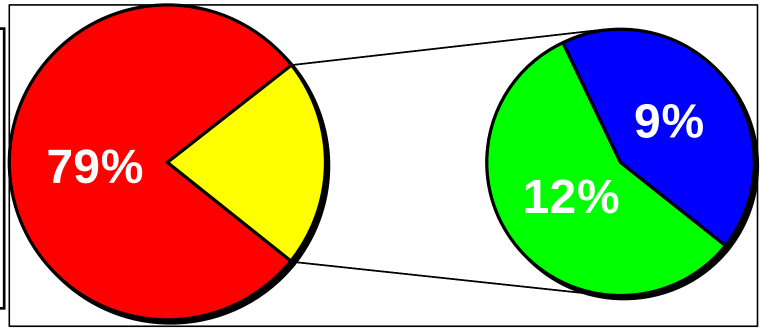
Pre-equilibrium model

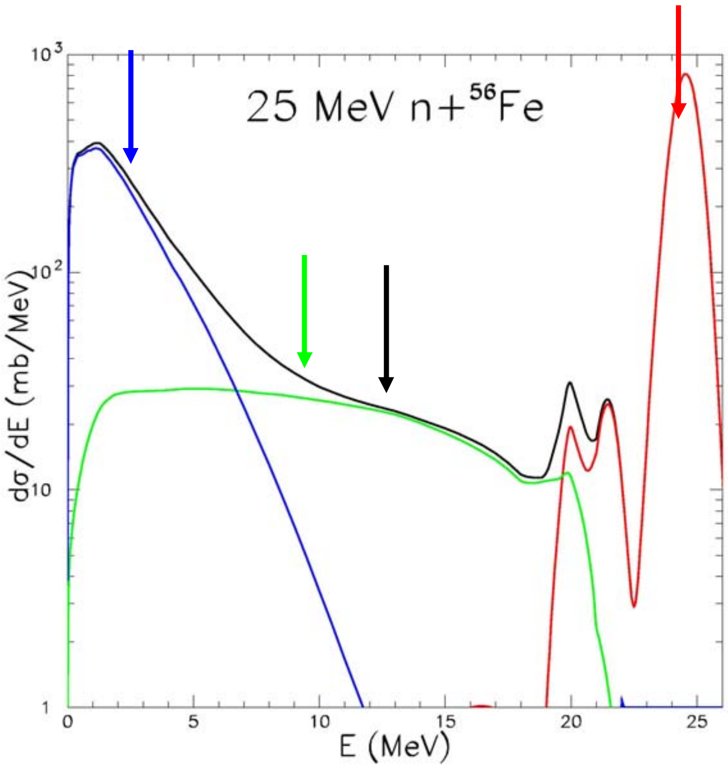
Cross section

Outgoing energy



Total
Direct
Pre-equilibrium
Statistical





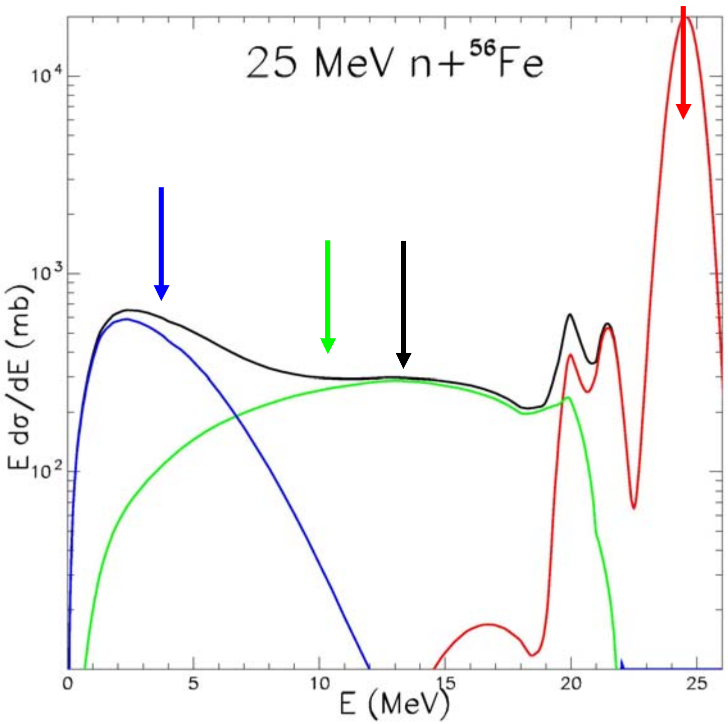
$\langle E_{Tot} \rangle = 12.1$

$\langle E_{Dir} \rangle = 24.3$

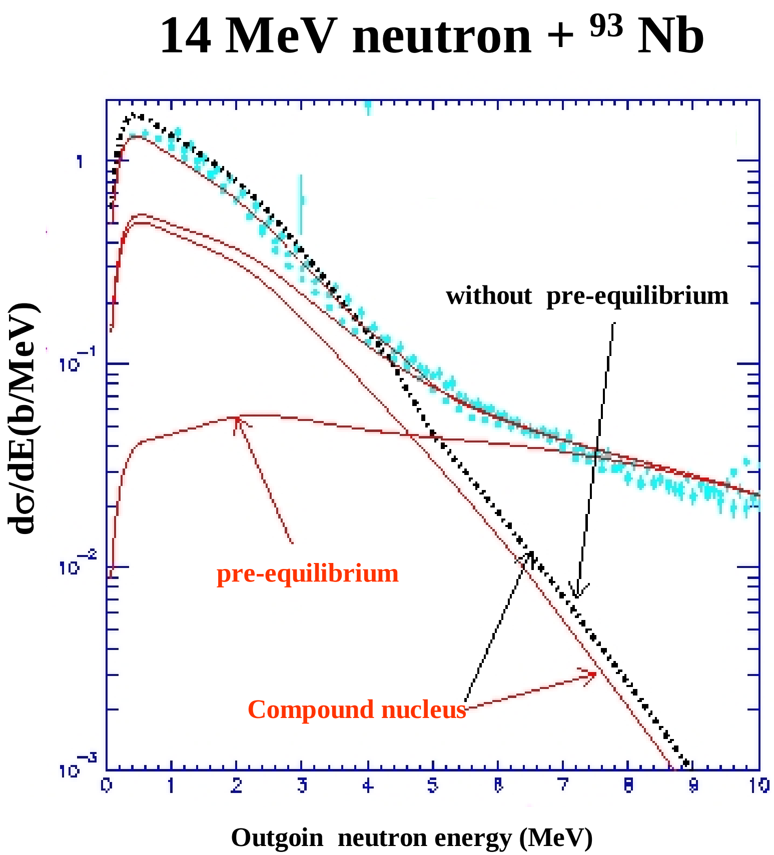
$\langle E_{PE} \rangle = 9.32$

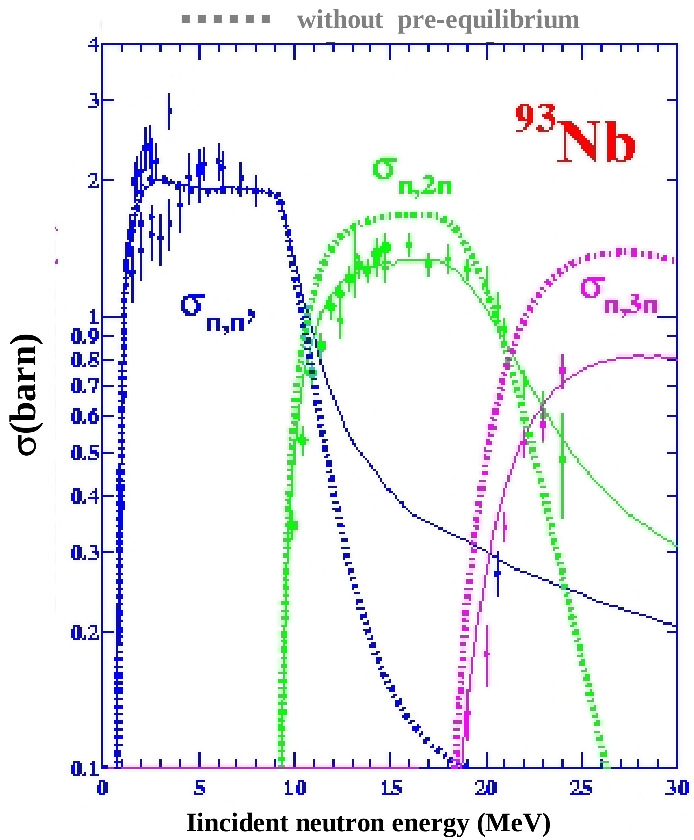
$\langle E_{Sta} \rangle = 2.5$

(MeV)

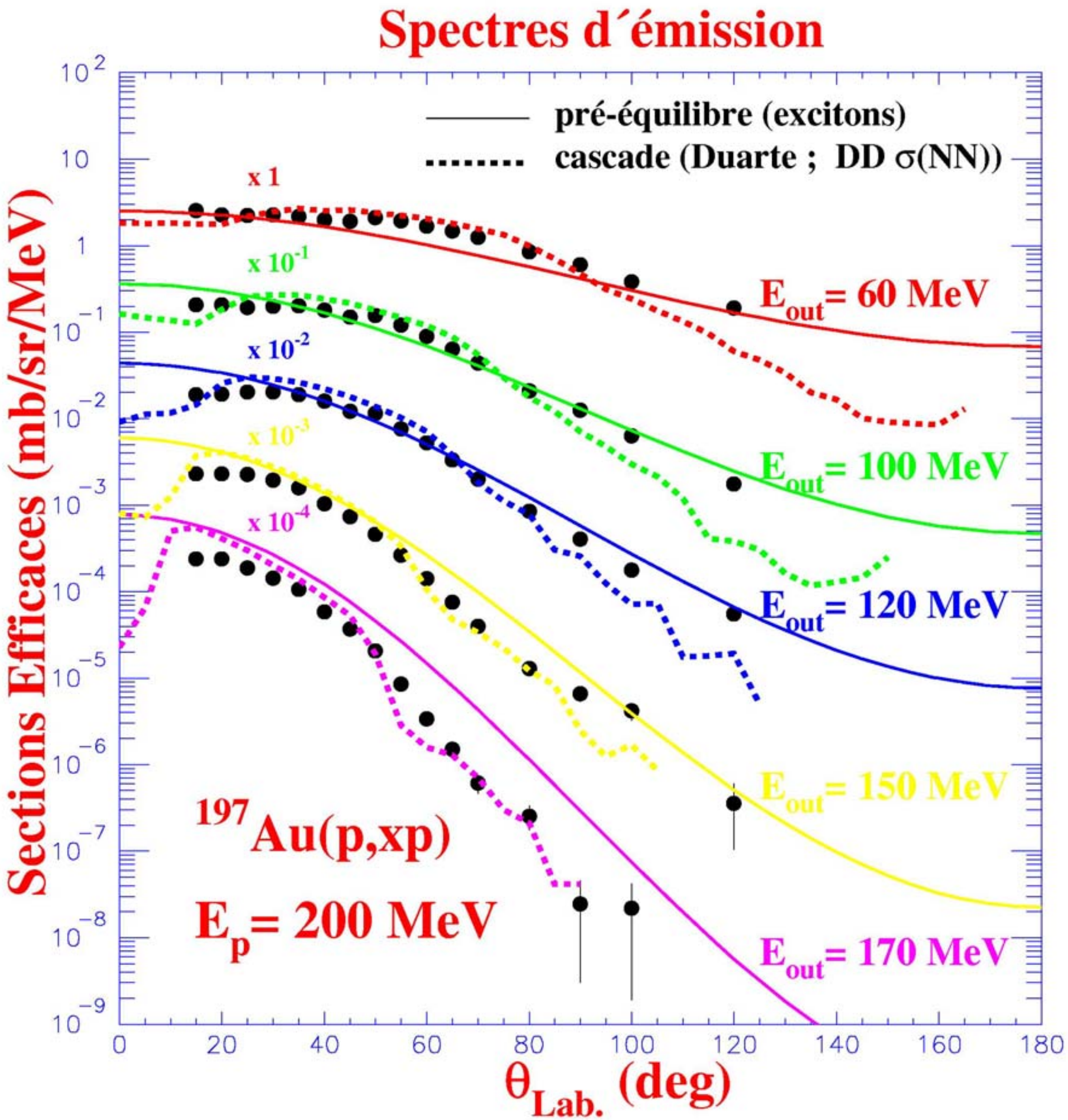


Pre-equilibrium model

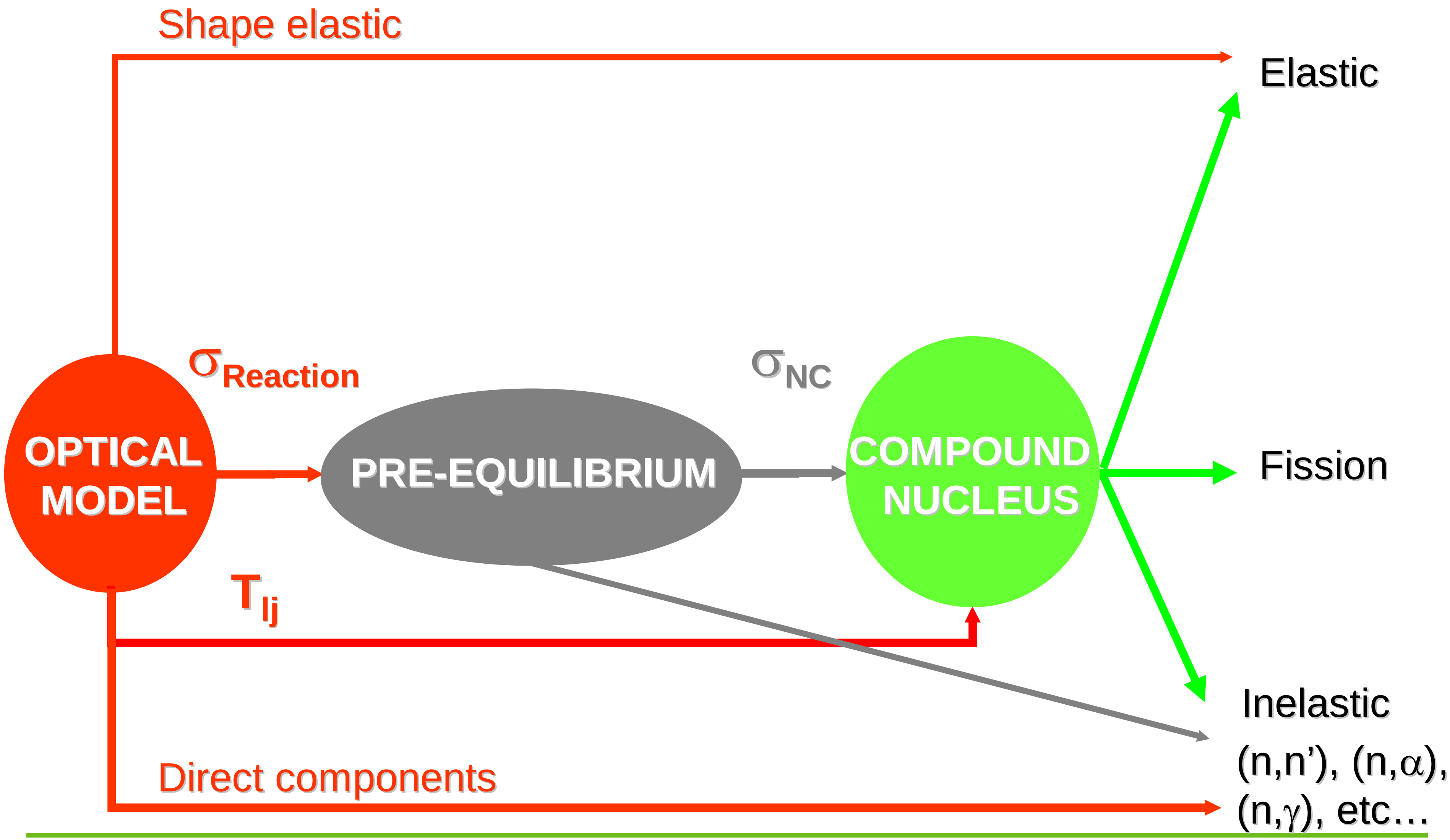




Link with high energy cascade



Models sequence



Compound Nucleus Model : Content

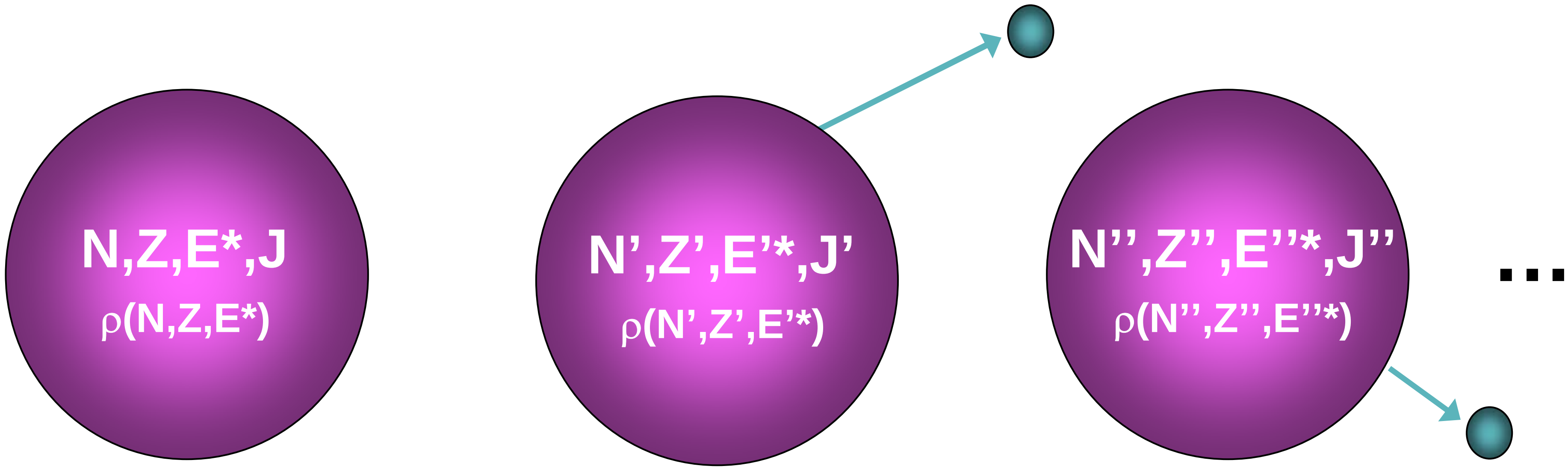
- Generalities and definitions
- Model ingredients
- Fission
- Level densities

Compound Nucleus model

After direct and pre-equilibrium emission

$$\sigma_{reaction} = \sigma_{dir} + \sigma_{pre-equ} + \sigma_{NC}$$

N_0	N_0-dN_D	$N_0-dN_D-dN_{PE}$	$= E$
Z_0	Z_0-dZ_D	$Z_0-dZ_D-dZ_{PE}$	$= Z$
E^*_0	$E^*_0-dE^*_D$	$E^*_0-dE^*_D-dE^*_{PE}$	$= E^*$
J_0	J_0-dJ_D	$J_0-dJ_D-dJ_{PE}$	$= J$



movie

Compound Nucleus model

Compound nucleus hypothesys

- **Continuum of excited levels**
- **Independence between incoming channel a and outgoing channel b**

$$\sigma_{ab} = \sigma_a^{(CN)} P_b$$

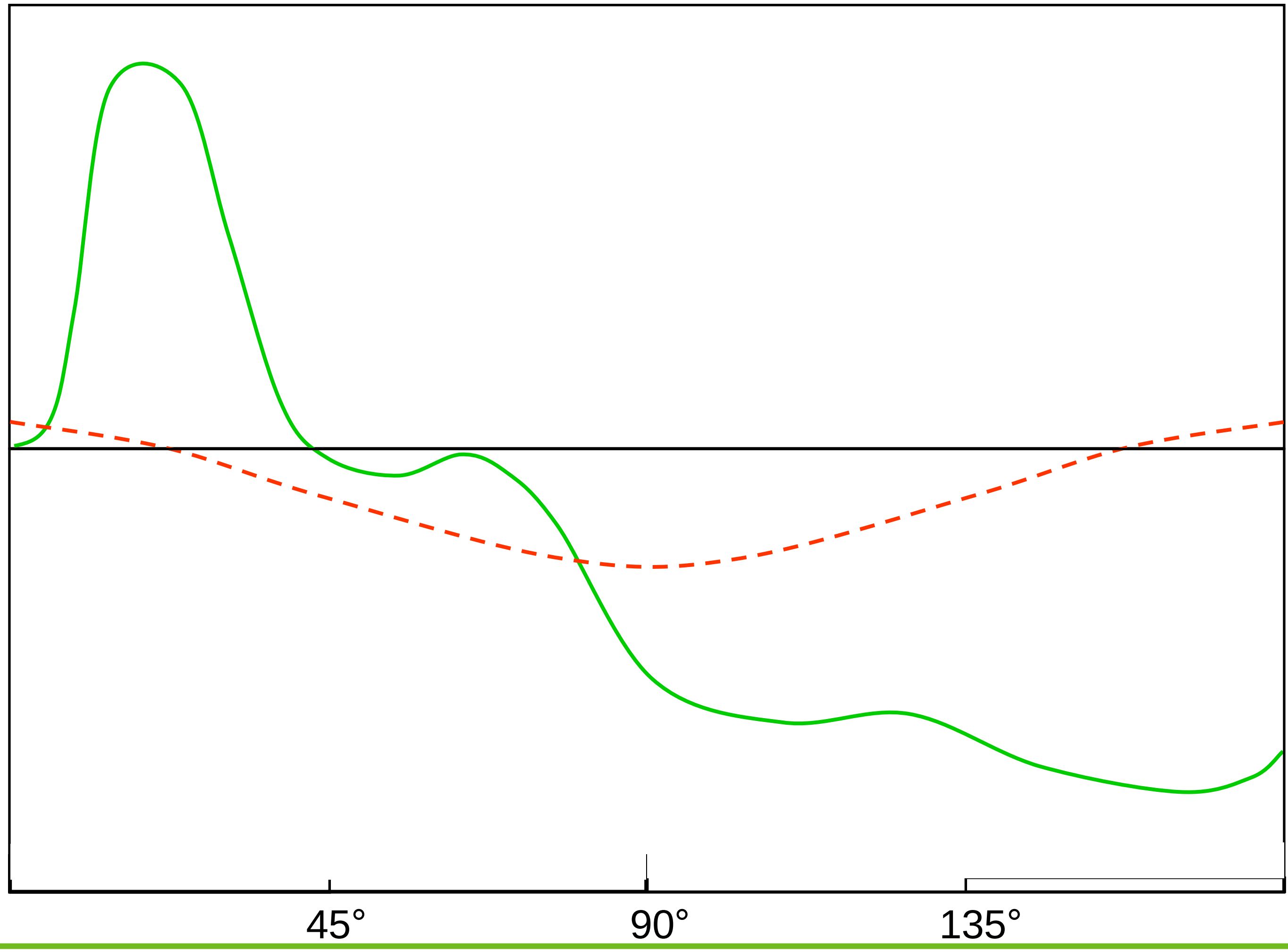
$$\sigma_a^{(CN)} = \frac{\pi}{k_a^2} T_a \qquad\qquad P_b = \frac{T_b}{\sum_c T_c}$$

⇒ **Hauser- Feshbach formula**

$$\sigma_{ab} = \frac{\pi}{k_a^2} \frac{T_a T_b}{\sum_c T_c}$$

Compound Nucleus model

Compound angular distribution & direct angular distributions



Compound Nucleus model

Channel Definition

$$a + A \rightarrow (CN)^* \rightarrow b+B$$

Incident channel $a = (\vec{l}_a, \vec{j}_a=\vec{l}_a+\vec{s}_a, \vec{J}_A, \pi_A, E_A, E_a)$

Conservation equations

- **Total energy :** $E_a + E_A = E_{CN} = E_b + E_B$
- **Total momentum :** $\vec{p}_a + \vec{p}_A = \vec{p}_{CN} = \vec{p}_b + \vec{p}_B$
- **Total angular momentum :** $\vec{l}_a + \vec{s}_a + \vec{J}_A = \vec{J}_{CN} = \vec{l}_b + \vec{s}_b + \vec{J}_B$
- **Total parity :** $\pi_A (-1)^{l_a} = \pi_{CN} = \pi_B (-1)^{l_b}$

Compound Nucleus model

In realistic calculations, all possible quantum number combinations have to be considered

$$\sigma_{ab} = \frac{\pi}{k_a^2} \sum_{J=|I_A - s_a|}^{I_A + s_a + l_a^{max}} \sum_{\pi=\pm} \frac{(2J+1)}{(2I_A+1)(2s_a+1)}$$

$$\sum_{j_a=|J-I_A|}^{J+I_A} \sum_{l_a=|j_a-s_a|}^{j_a+s_a} \sum_{j_b=|J-I_B|}^{J+I_B} \sum_{l_b=|j_b-s_b|}^{j_b+s_b}$$

$$\delta_\pi(a)\,\delta_\pi(b) \frac{T_{a,l_a,j_a}^{J\pi}\, T_{b,l_b,j_b}^{J\pi}}{\sum_c T_{c,l_c,j_c}^{J\pi}} W_{a,l_a,j_a,b,l_b,j_b}^{J\pi}$$

Width fluctuations

Breit-Wigner resonance integrated and averaged over an energy width Corresponding to the incident beam dispersion

$$<\sigma_{ab}> = \frac{\pi}{k_a^2}\frac{2\pi}{D}\left\langle\frac{\Gamma_a\Gamma_b}{\Gamma_{tot}}\right\rangle$$

Or $$T_\alpha \approx \frac{2\pi<\Gamma_\alpha>}{D}$$

$$\Rightarrow \begin{cases} <\sigma_{ab}> = \dfrac{\pi}{k_a^2}\dfrac{T_a T_b}{\sum_c T_c} W_{ab} \\ \text{with} \quad W_{ab} = \left\langle\dfrac{\Gamma_a\Gamma_b}{\Gamma_{tot}}\right\rangle \Big/ \dfrac{\langle\Gamma_a\rangle\langle\Gamma_b\rangle}{\langle\Gamma_{tot}\rangle} \end{cases}$$

Width fluctuations : models in TALYS

- Tepel method

  Simplified iterative method

- Moldauer method

  Simple integral

- GOE triple integral

  « exact » result

Elastic enhancement with respect to the other channels

The GOE triple integral

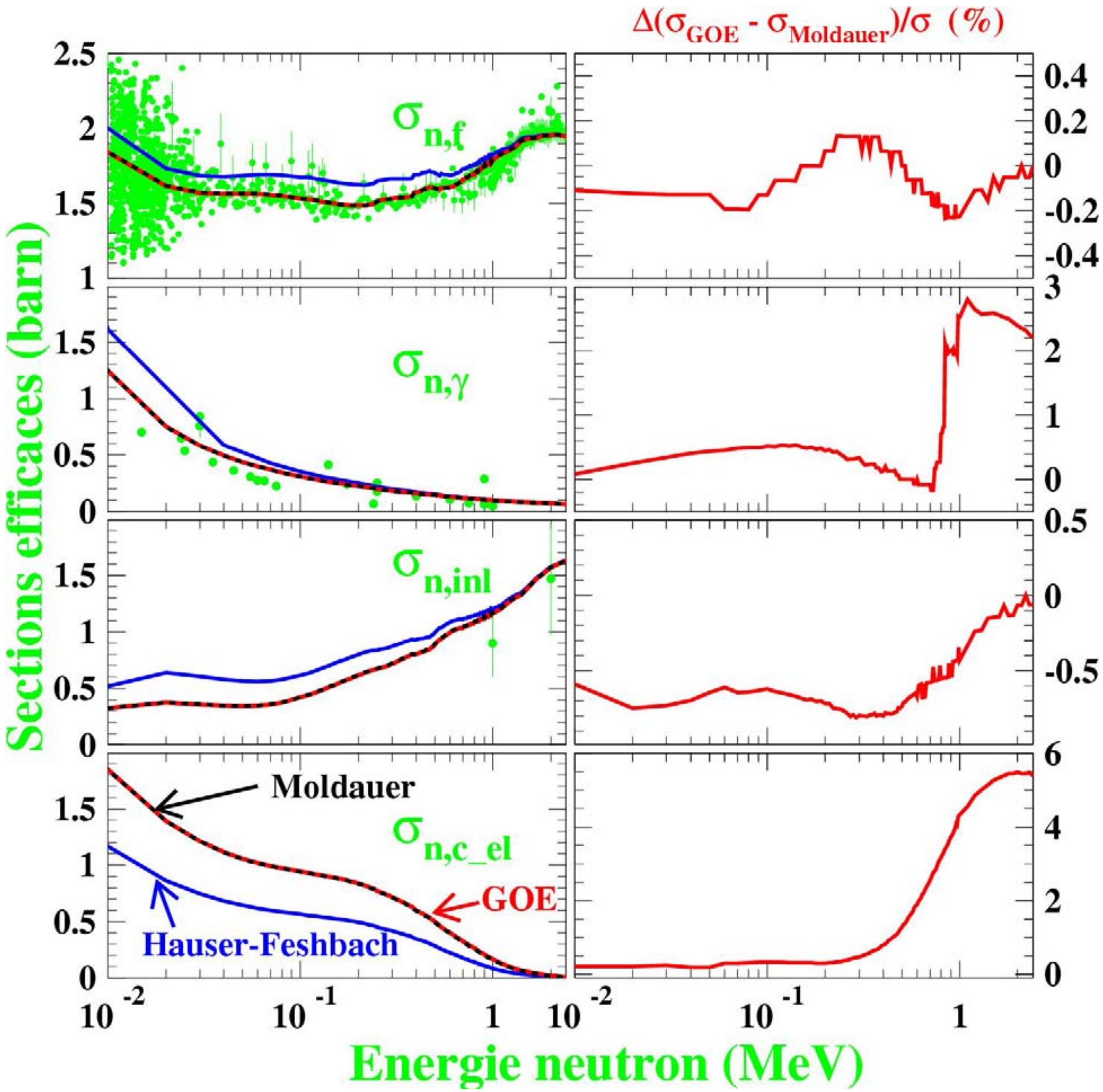
$$W_{a,l_a,j_a,b,l_b,j_b} = \int_0^{+\infty} d\lambda_1 \int_0^{+\infty} d\lambda_2 \int_0^{1} d\lambda \; \frac{\lambda(1-\lambda)|\lambda_1-\lambda_2|}{\sqrt{\lambda_1(1+\lambda_1)\lambda_2(1+\lambda_2)}(\lambda+\lambda_1)^2(\lambda+\lambda_2)^2}$$

$$\prod_c \frac{(1-\lambda\, T^J_{c,l_c,j_c})}{\sqrt{(1+\lambda_1\, T^J_{c,l_c,j_c})(1+\lambda_2\, T^J_{c,l_c,j_c})}} \quad \Bigg\{ \delta_{ab}(1-\; T^J_{a,l_a,j_a})$$

$$\left[\frac{\lambda_1}{1+\lambda_1\, T^J_{a,l_a,j_a}} + \frac{\lambda_2}{1+\lambda_2\, T^J_{a,l_a,j_a}} + \frac{2\lambda}{1-\lambda\, T^J_{a,l_a,j_a}}\right]^2 + (1+\delta_{ab})$$

$$\left[\frac{\lambda_1(1+\lambda_1)}{(1+\lambda_1\, T^J_{a,l_a,j_a})(1+\lambda_1\, T_{b,l_b,j_b})} + \frac{\lambda_2(1+\lambda_2)}{(1+\lambda_2\, T^J_{a,l_a,j_a})(1+\lambda_2\, T_{b,l_b,j_b})}\right.$$

$$\left. + \frac{2\lambda(1-\lambda)}{(1-\lambda\, T^J_{a,l_a,j_a})(1-\lambda\, T_{b,l_b,j_b})}\right]\Bigg\}$$


Δ(σGOE - σMoldauer)/σ (%)
σn,f
σn,γ
σn,inl
σn,c_el
Moldauer
GOE
Hauser-Feshbach
Sections efficaces (barn)
Energie neutron (MeV)

Compound Nucleus Model

$$\sigma_{NC} = \sum_b \sigma_{ab} \quad \text{où } b = \gamma\text{, n, p, d, t, …, fission}$$

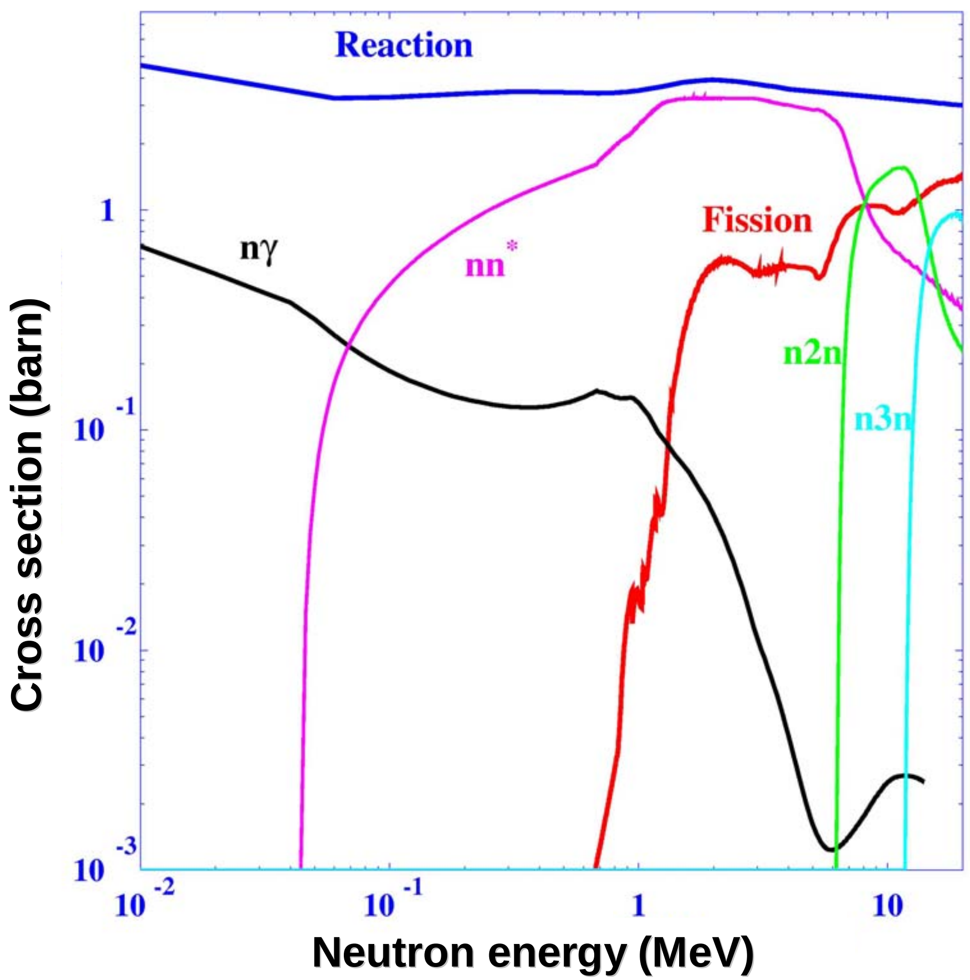
$$\sigma_{ab} = \frac{\pi}{k_a^2} \sum_{J,\pi} \sum_{\alpha,\beta} \frac{(2J+1)}{(2s+1)(2I+1)} T_{lj}^{J\pi}(\alpha) \frac{\langle T_b^{J\pi}(\beta) \rangle}{\sum_\delta \langle T_d^{J\pi}(\delta) \rangle} W_{\alpha\beta}$$

with $J = l_\alpha + s_\alpha + I_A = j_\alpha + I_A$ et $\pi = (-1)^{l_\alpha} \pi_A$

and $\langle T_b(\beta) \rangle$ = transmission coefficient for outgoing channel β associated with the outgoing particle b

Compound Nucleus Model

n + ^{238}U



Optical model

+

Statistical model

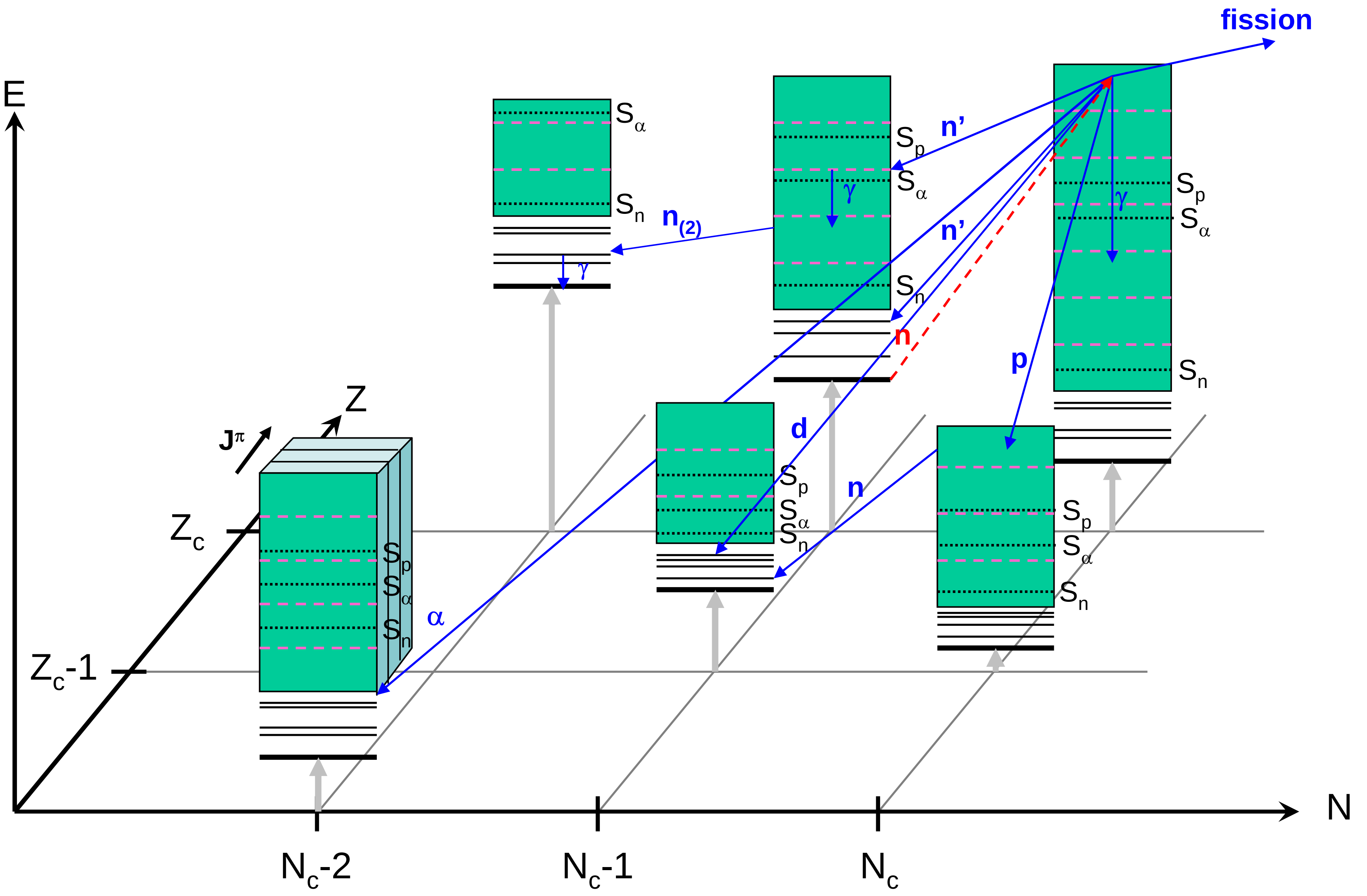
+

Pre-equilibrium model

$$\sigma_R = \sigma_d + \sigma_{PE} + \sigma_{CN}$$

$$= \sigma_{nn'} + \sigma_{nf} + \sigma_{n\gamma} + \ldots$$

Multiple Hauser-Feshbach



movie

Various decay channels

Possible decays

- Emission to a discrete level with energy E_d

$$\left\langle T_b(\beta) \right\rangle = T_{lj}^{J\pi}(\beta)$$ given by the O.M.P.

- Emission in the level continuum

$$\left\langle T_b(\beta) \right\rangle = \int_{E}^{E+\Delta E} T_{lj}^{J\pi}(\beta)\, \rho(E,J,\pi)\, dE$$

$\rho(E,J,\pi)$ density of residual nucleus' levels (J,π) with excitation energy E

- Emission of photons, fission

Specific treatment

Gamma decay

$$T^{k\lambda}(\varepsilon_\gamma) = 2\pi \int_{E}^{E+\Delta E} \Gamma^{k\lambda}(\varepsilon_\gamma)\, \rho(E)\, dE$$

$$= 2\pi\, f(k,\lambda,(\varepsilon_\gamma))\, \varepsilon_\gamma^{2\lambda+1}$$

k : transition type EM (E ou M)

λ : transition multipolarity

ε_γ : outgoing gamma energy

$f(k,\lambda,\varepsilon_\gamma)$: gamma strength function (several models)

Decay selection rules from a level $J_i^{\pi i}$ to a level $J_f^{\pi f}$:

Pour $E\lambda$: $\pi_f = (-1)^\lambda\, \pi_i$

Pour $M\lambda$: $\pi_f = (-1)^{\lambda+1}\, \pi_i$

$$|J_i - \lambda| \leq J_f \leq J_i + \lambda$$

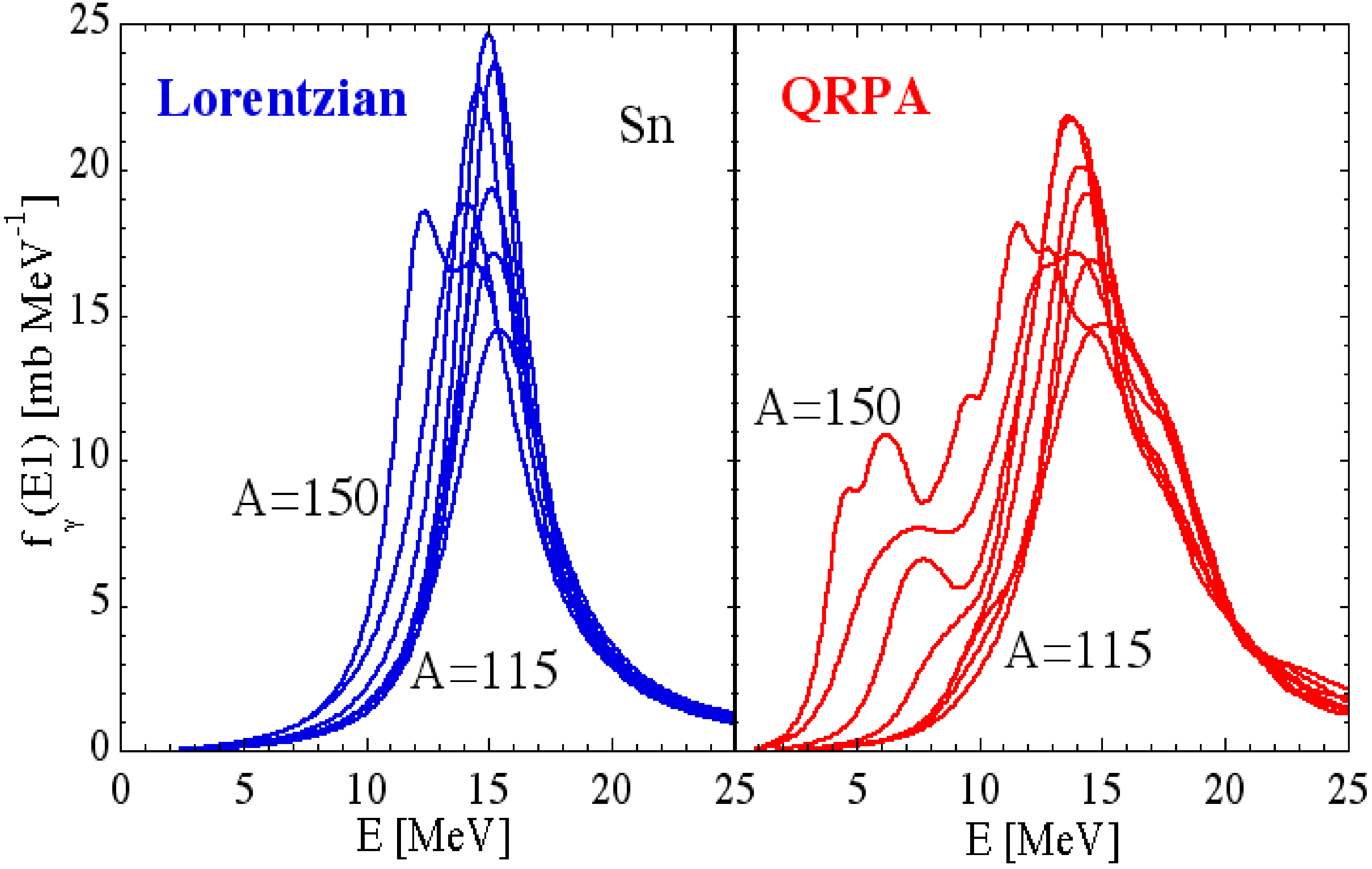
Renormalisation technique for thermal neutrons

$$\langle T_\gamma \rangle = \sum_{J_i,\pi_i} \sum_{k\lambda} \sum_{J_f,\pi_f} \int_0^{B_n} T^{k\lambda}(\varepsilon)\, \rho(B_n-\varepsilon, J_f, \pi_f)\, S(\lambda, J_i, \pi_i, J_i, \pi_f)\, d\varepsilon = 2\pi \langle \Gamma_\gamma \rangle\, \rho(B_n)$$

$$\langle T_\gamma \rangle = C \sum_{J_i,\pi_i} \sum_{k\lambda} \sum_{J_f,\pi_f} \int_0^{B_n} T^{k\lambda}(\varepsilon)\, \rho(B_n-\varepsilon, J_f, \pi_f)\, S(\lambda, J_i, \pi_i, J_i, \pi_f)\, d\varepsilon = 2\pi \langle \Gamma_\gamma \rangle \frac{1}{D_0}$$

experiment

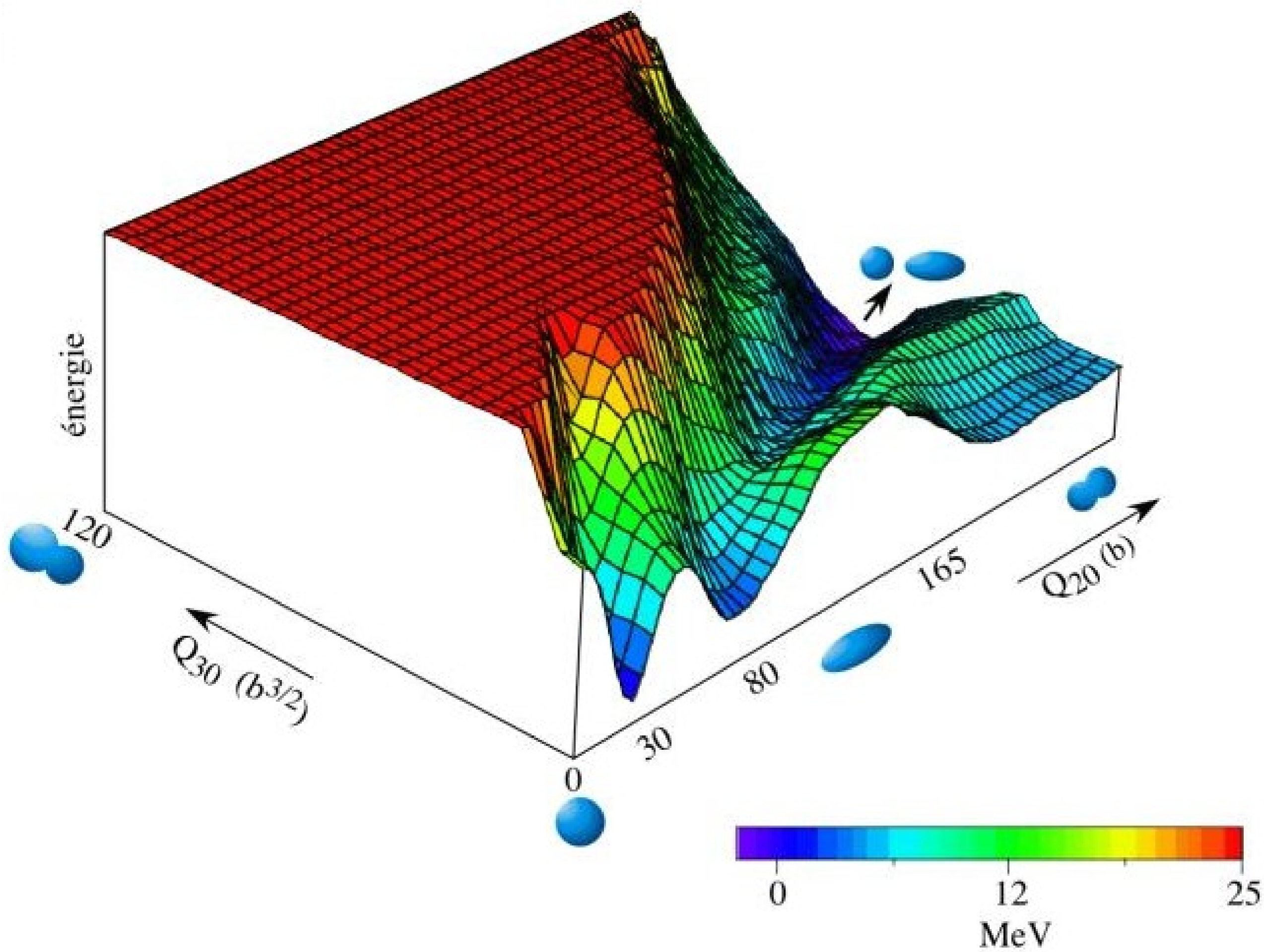
Gamma strength functions options



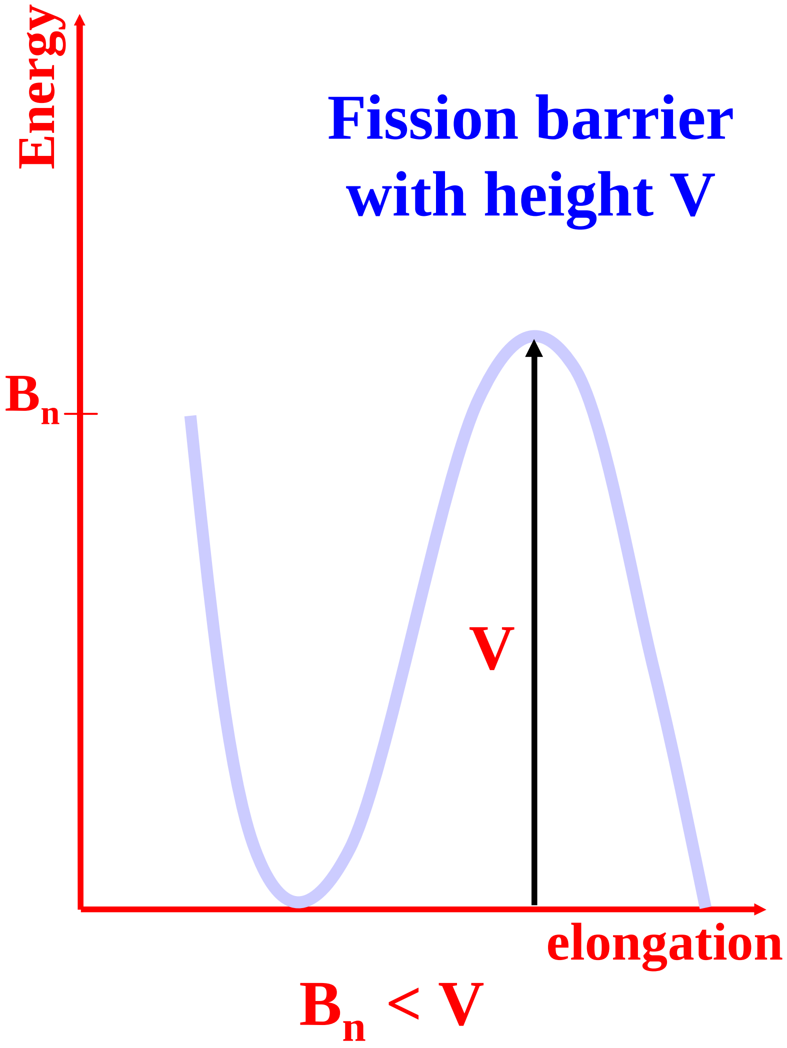
See S. Goriely & E. Khan, NPA 706 (2002) 217.
S. Goriely et al., NPA739 (2004) 331.

The fission process

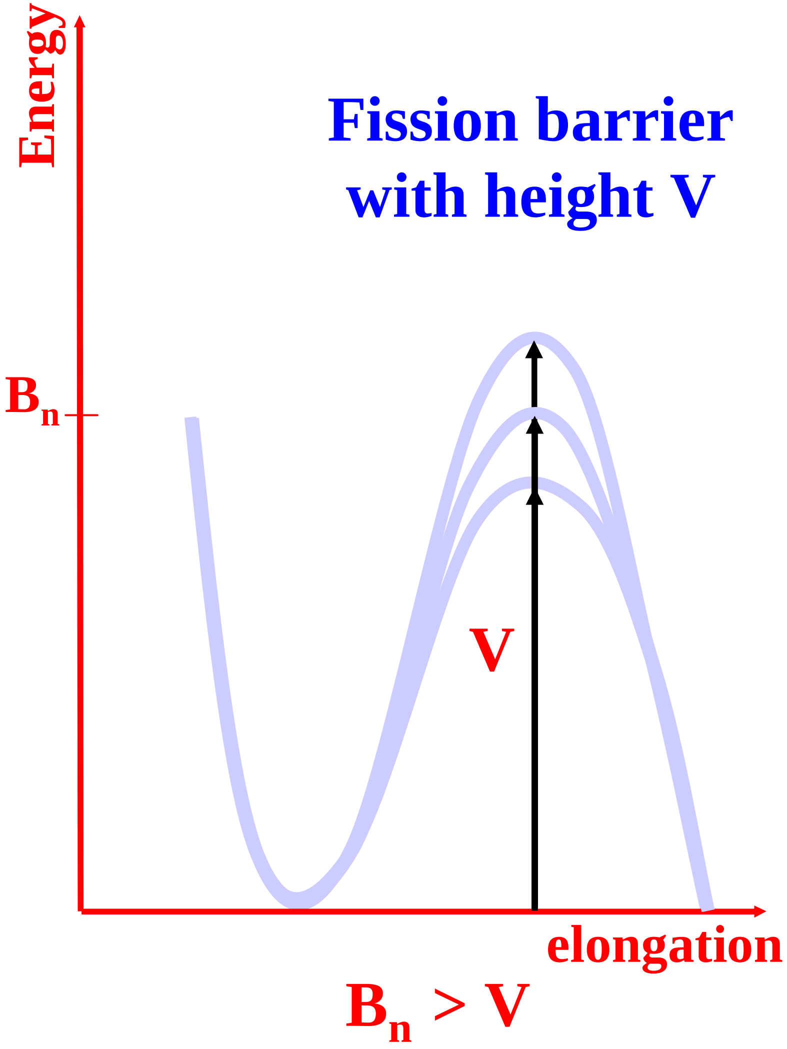
Surface ^{238}U



Fissile/Fertile



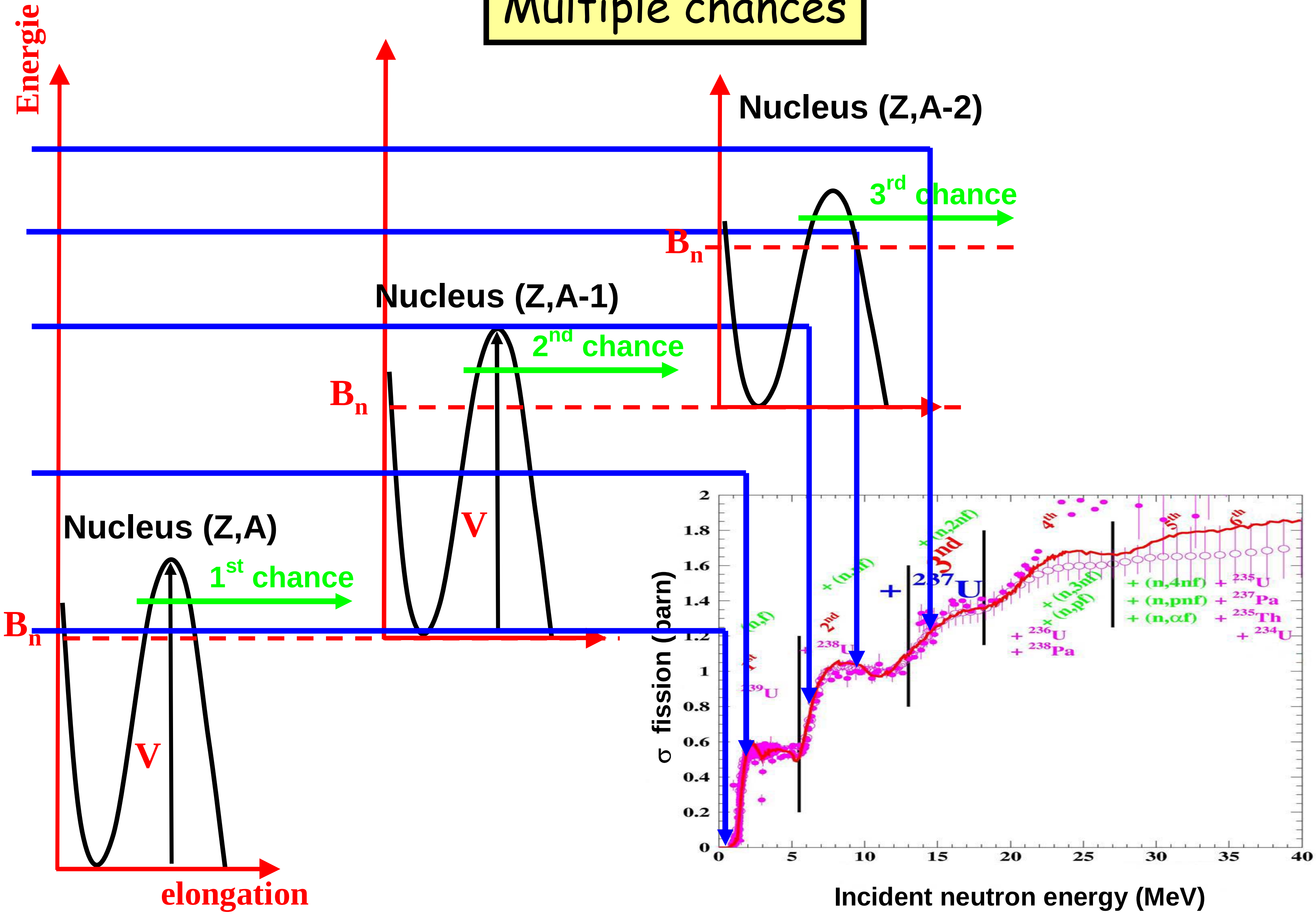
Fertile target (^{238}U)



Fissile target (^{235}U)

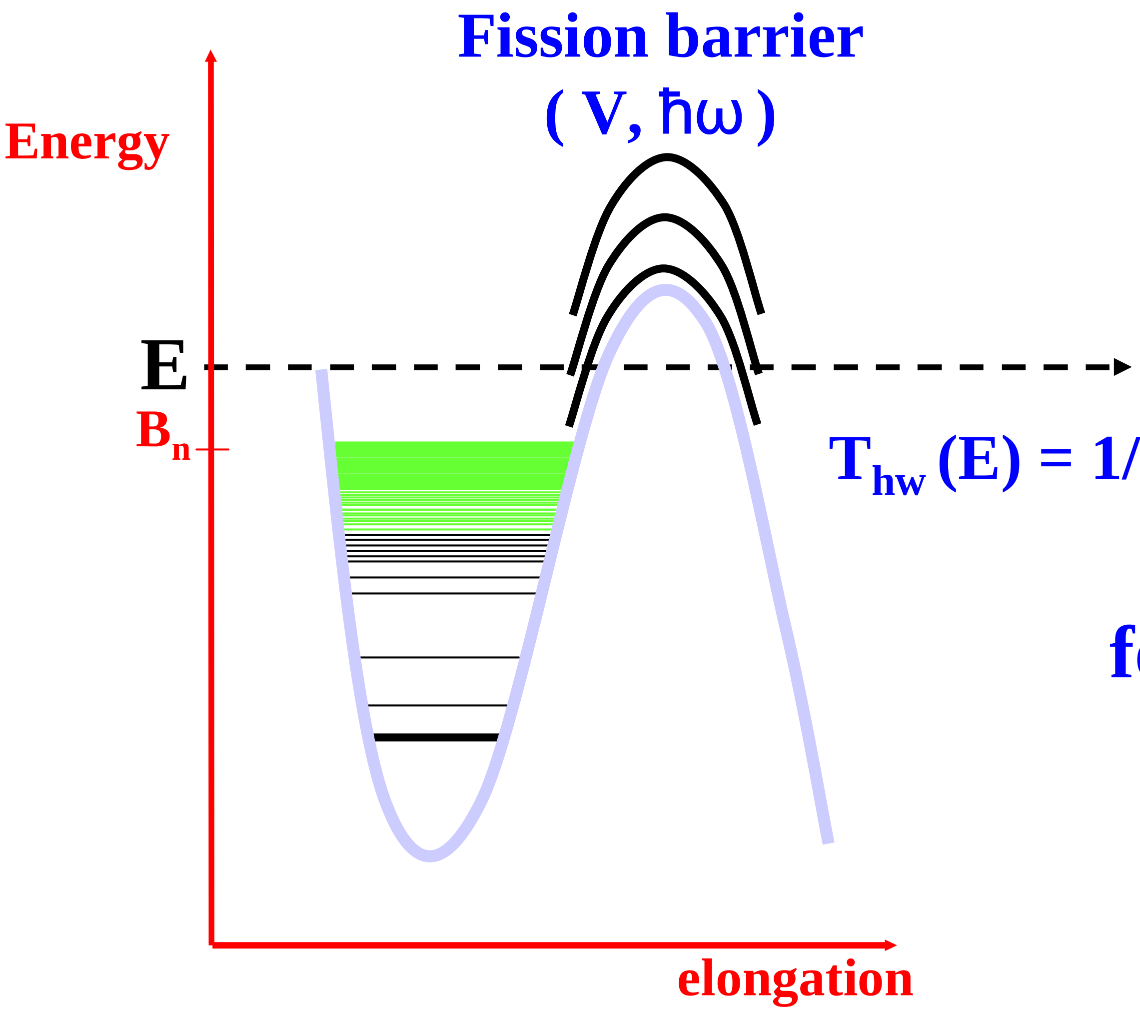
movie

Multiple chances



movie

Fission penetrability



$T_{hw}(E) = 1/[1 + \exp(2\pi(V-E)/\hbar\omega)]$

Hill-Wheeler

for one barrier !

+ transition state on top of the barrier !

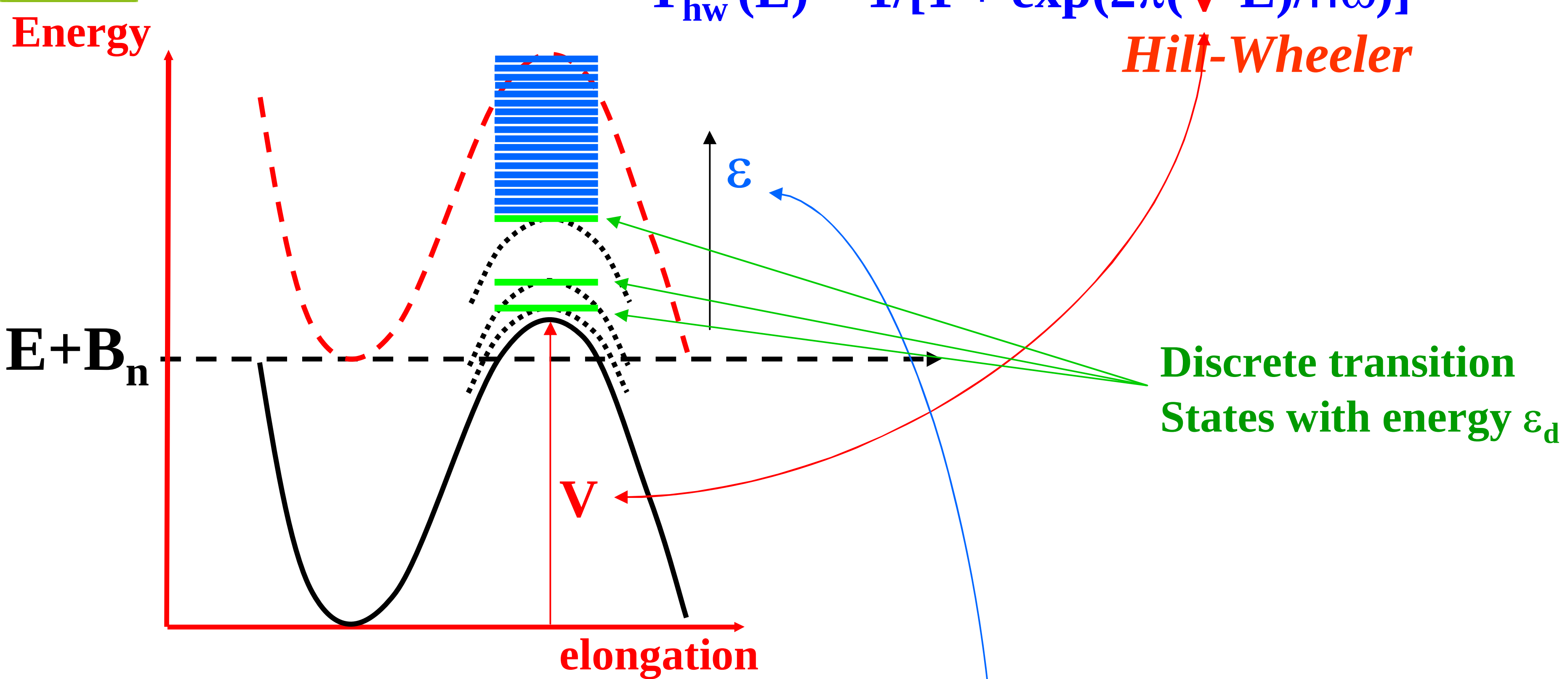
Bohr hypothesys

movie

Fission transmission coefficients

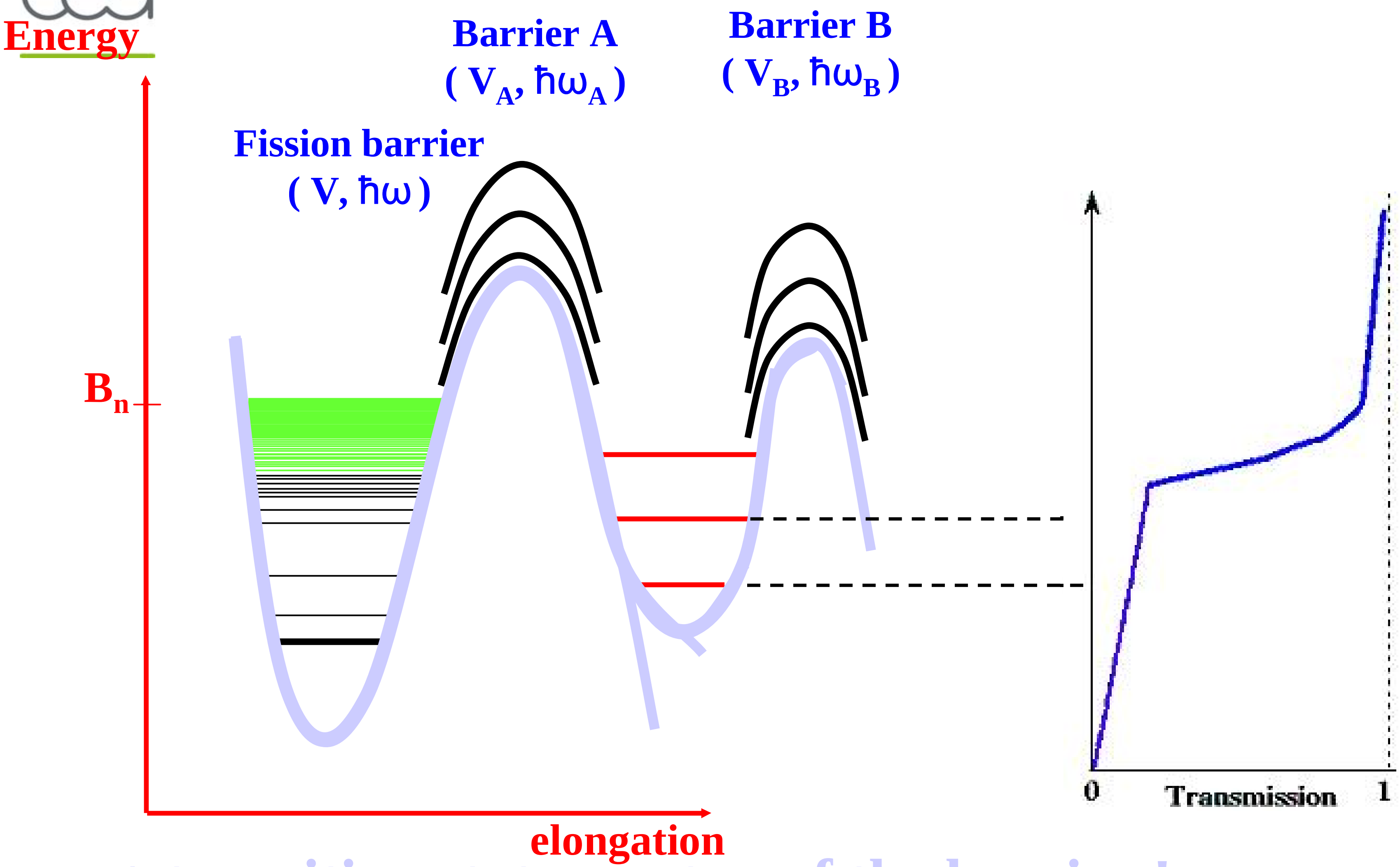
$$T_{hw}(E) = 1/[1 + \exp(2\pi(V-E)/\hbar\omega)]$$

Hill-Wheeler



$$T_f(E, J, \pi) = \sum_{\substack{\text{discrets}\\ J,\pi}} T_{hw}(E - \varepsilon_d) + \int_{E_s}^{E+B_n} \rho(\varepsilon, J, \pi)\, T_{hw}(E - \varepsilon)\, d\varepsilon$$

Multiple humped barriers



+ transition states on top of the barrier !

+ transition states on top of each barrier !
+ class II states in the intermediate well !

movie

Multiple humped barriers

Two barriers A and B

$$T_f = \frac{T_A \, T_B}{T_A + T_B}$$

Three barriers A, B et C

$$T_f = \frac{\dfrac{T_A \, T_B}{T_A + T_B} \times T_C}{\dfrac{T_A \, T_B}{T_A + T_B} + T_C}$$

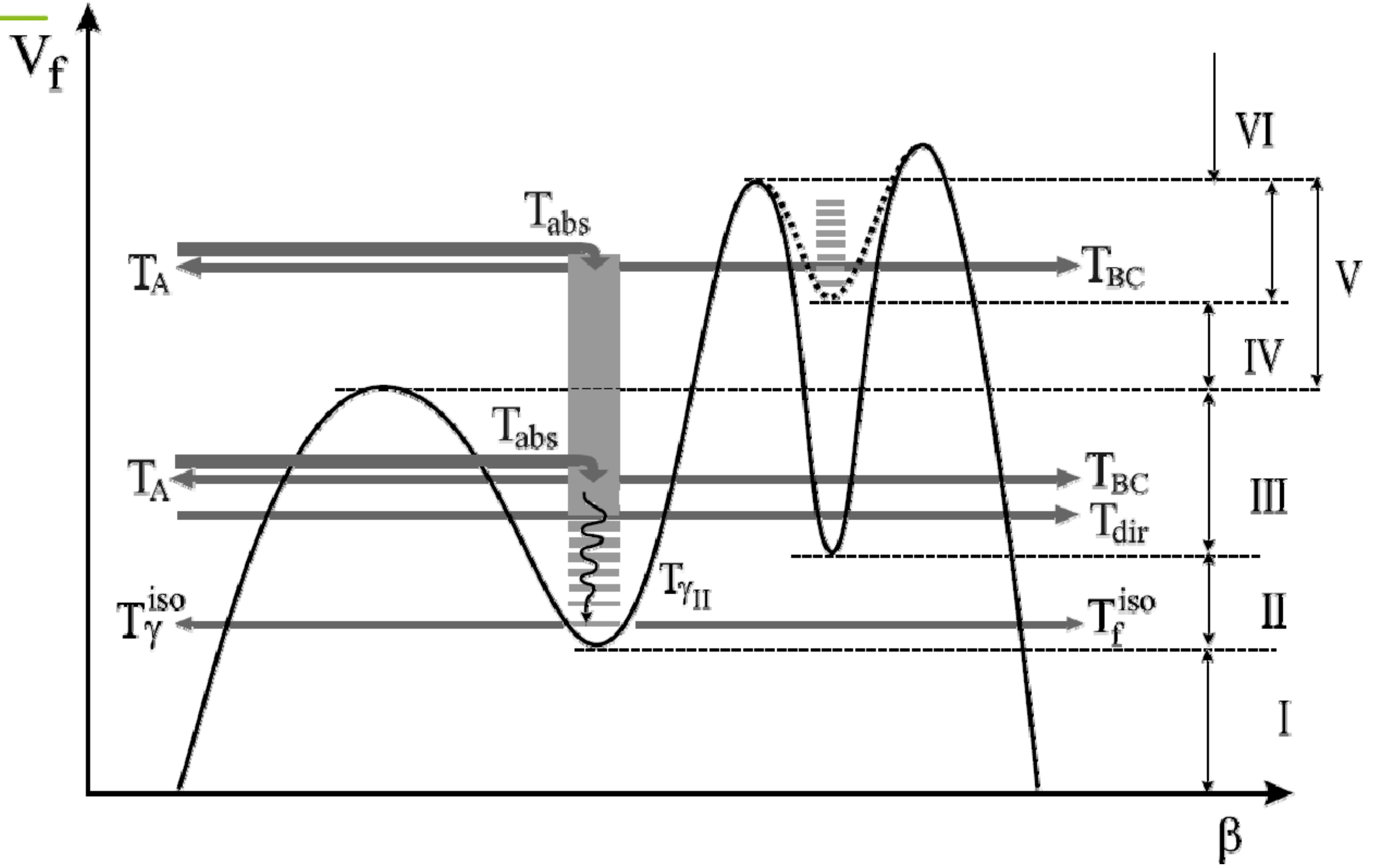
Resonant transmission

$$T_f = \frac{T_A \, T_B}{T_A + T_B} \qquad \frac{4}{T_A + T_B}$$

More exact expressions in Sin et al., PRC 74 (2006) 014608

movie

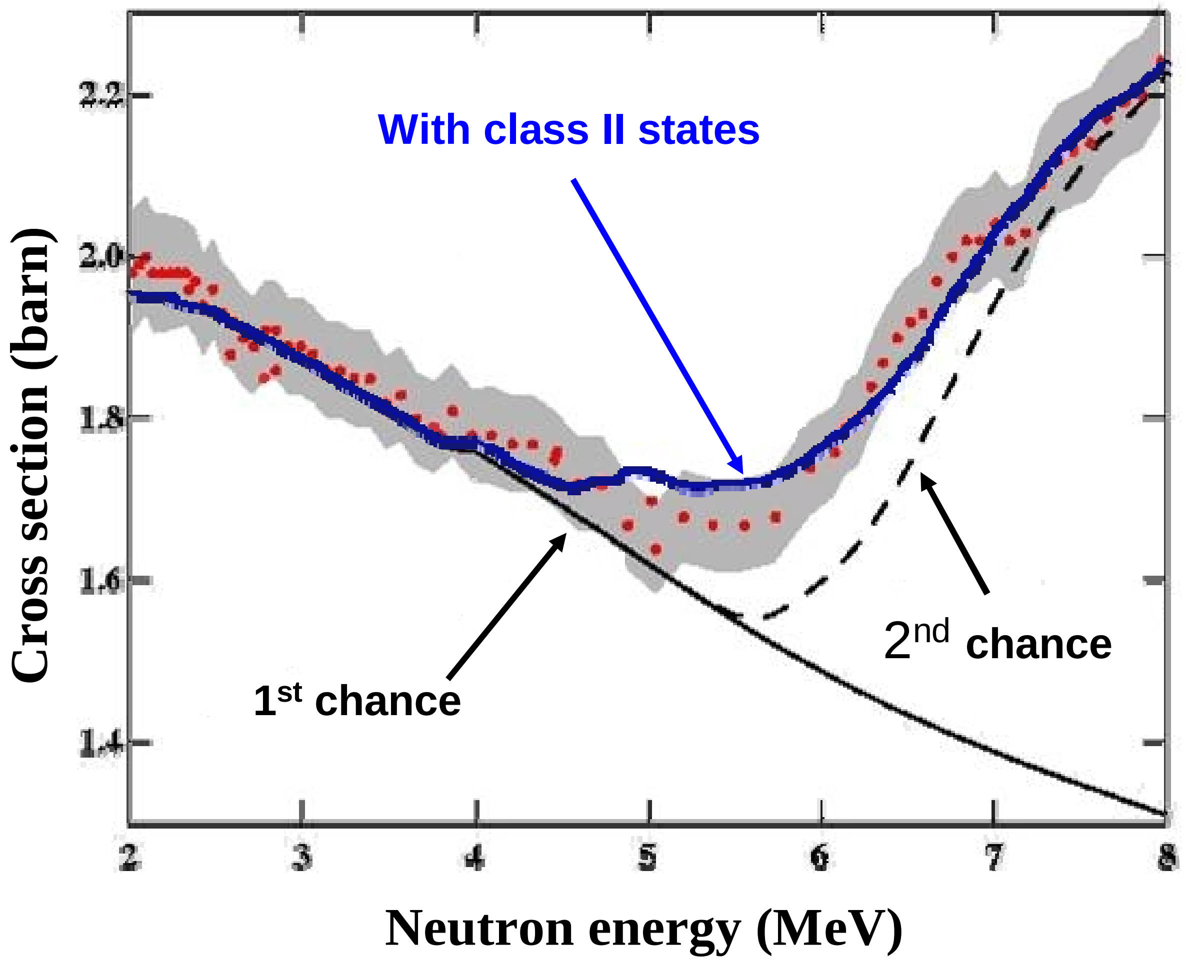
Multiple humped barriers with maximum complexity



See in Sin et al., PRC 74 (2006) 014608
Bjornholm and Lynn, Rev. Mod. Phys. 52 (1980) 725.

Impact of class II states

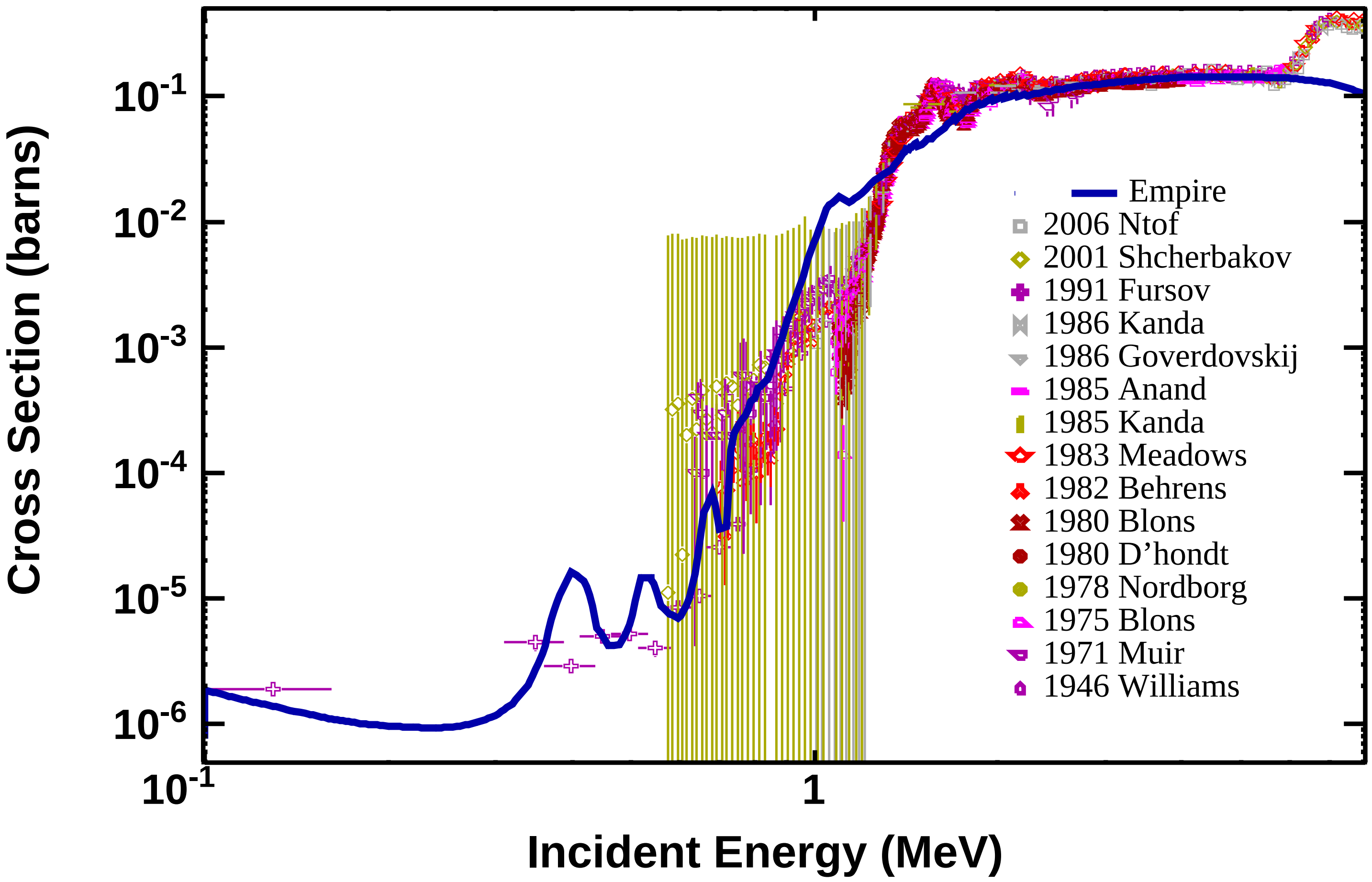
^{239}Pu (n,f)



Impact of class II states

Case of a fertile nucleus

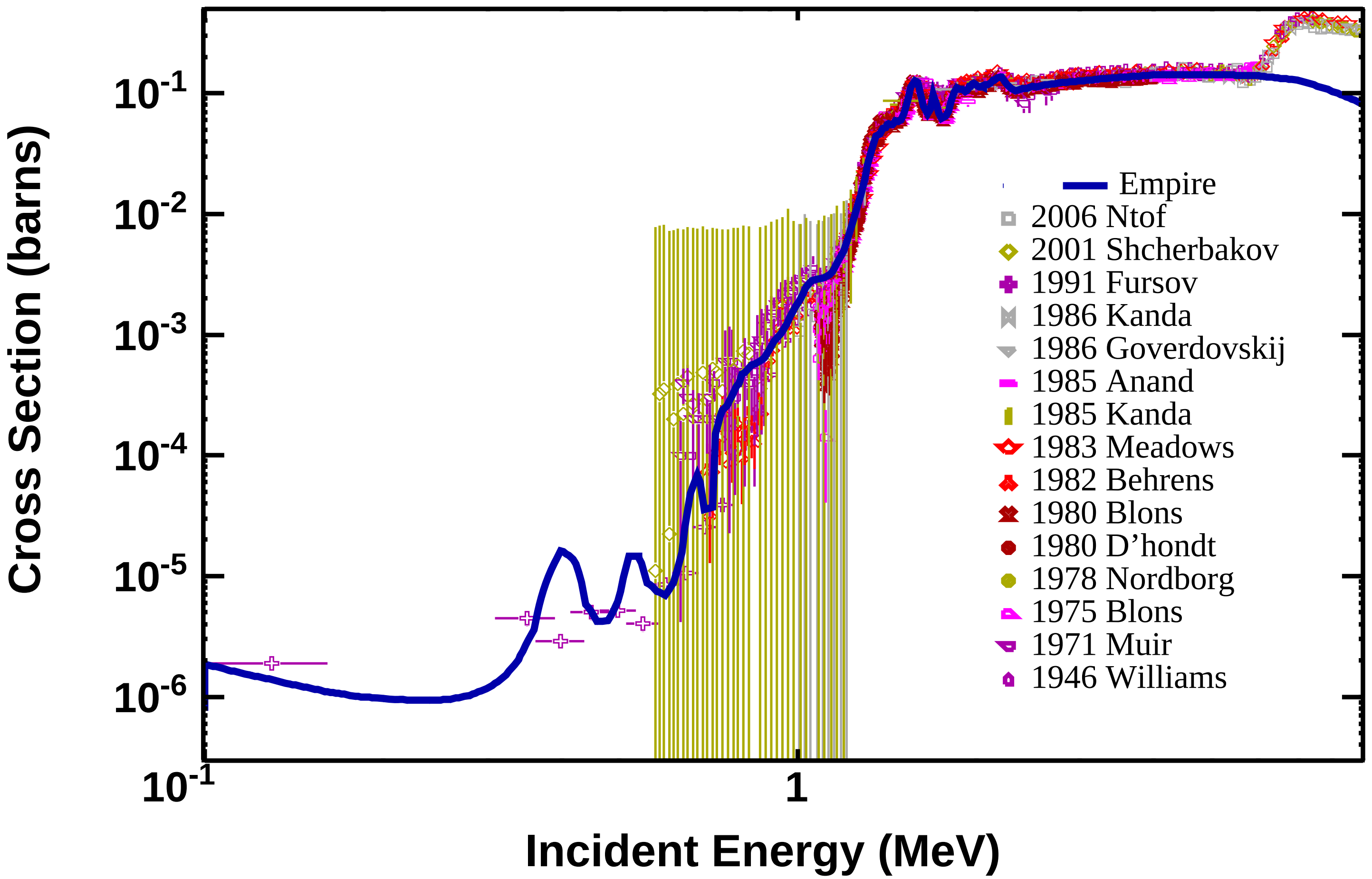
Partially damped class II states. No class III states (fully damped).



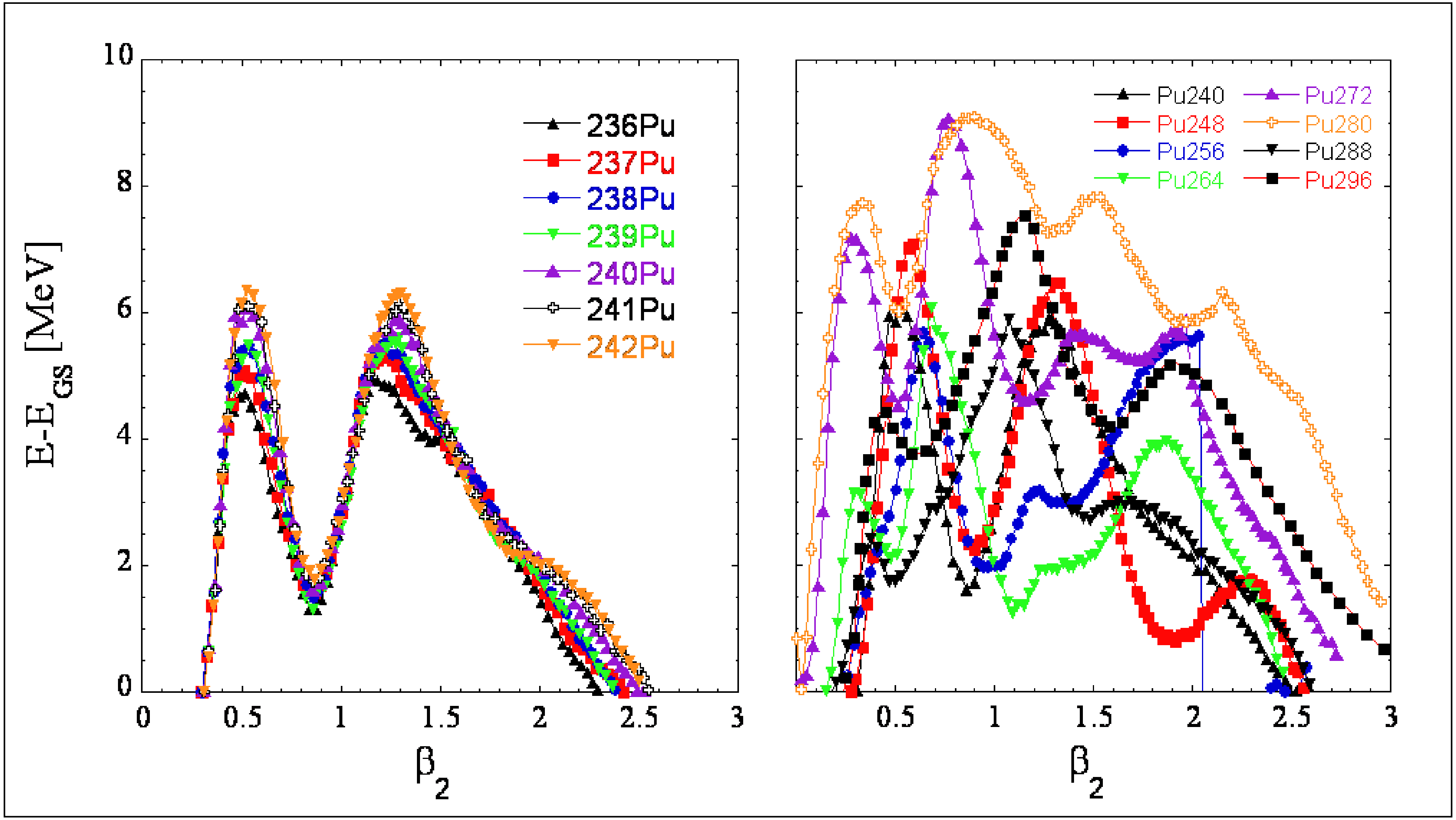
Impact of class II+III states

Case of a fertile nucleus

Class II + III states. Partial damping.

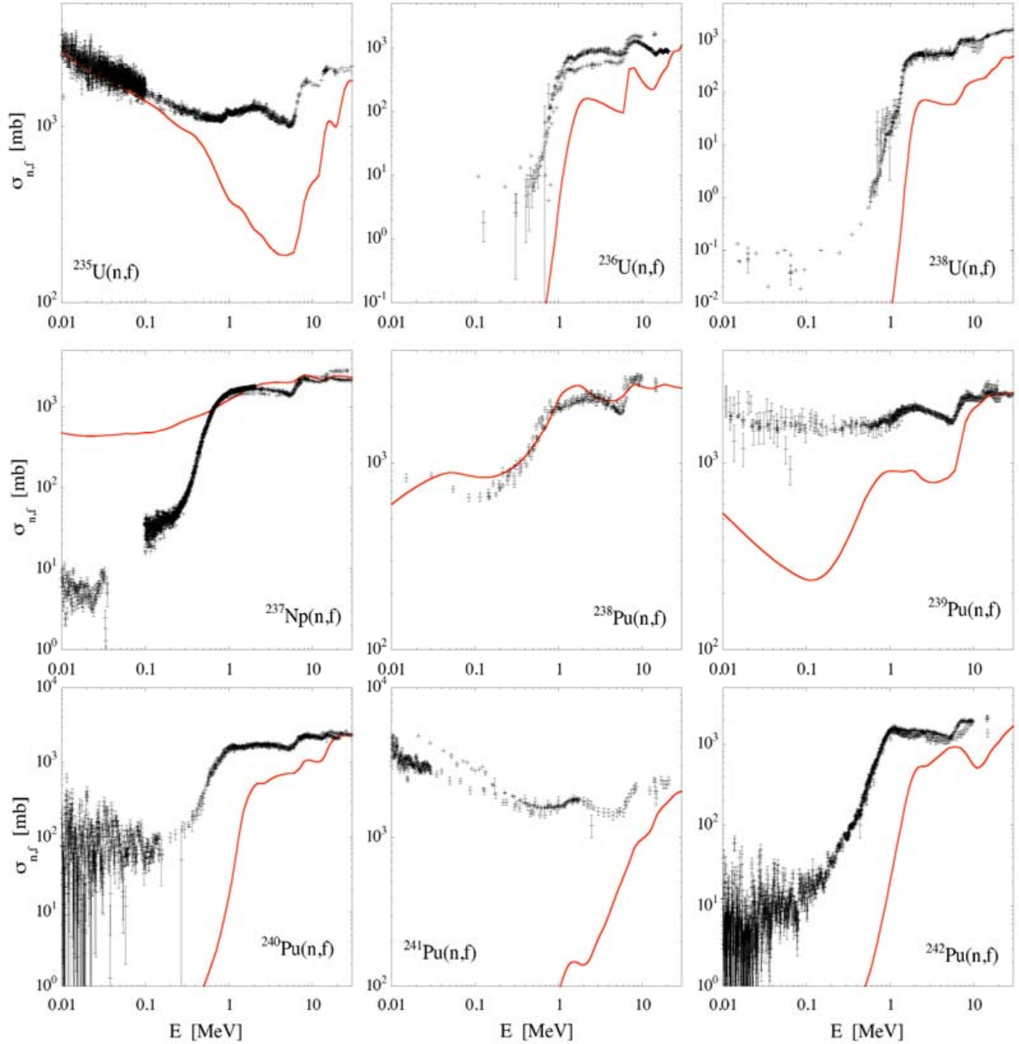


Microscopic fission barrier shapes



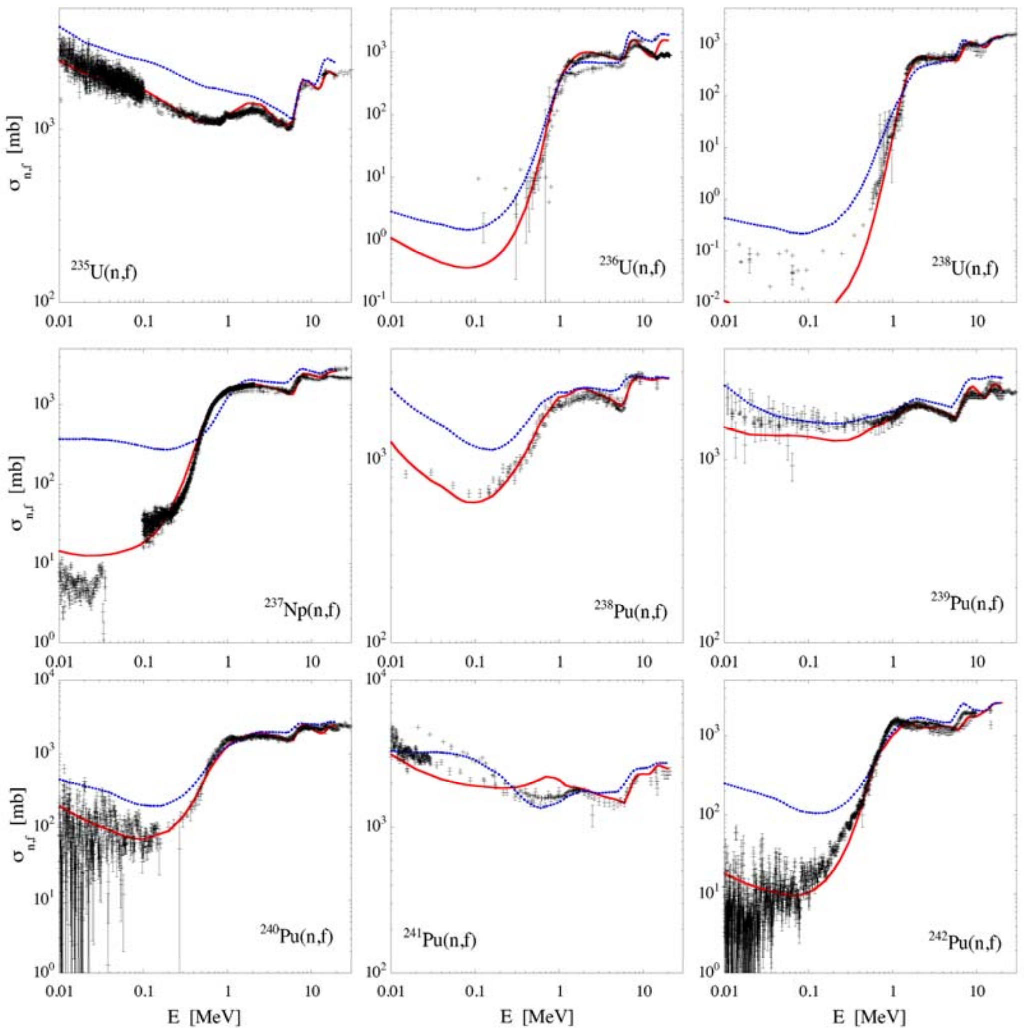
⇒ **For exotic nuclei : strong deviations from Hill-Wheeler.**

Microscopic fission cross sections



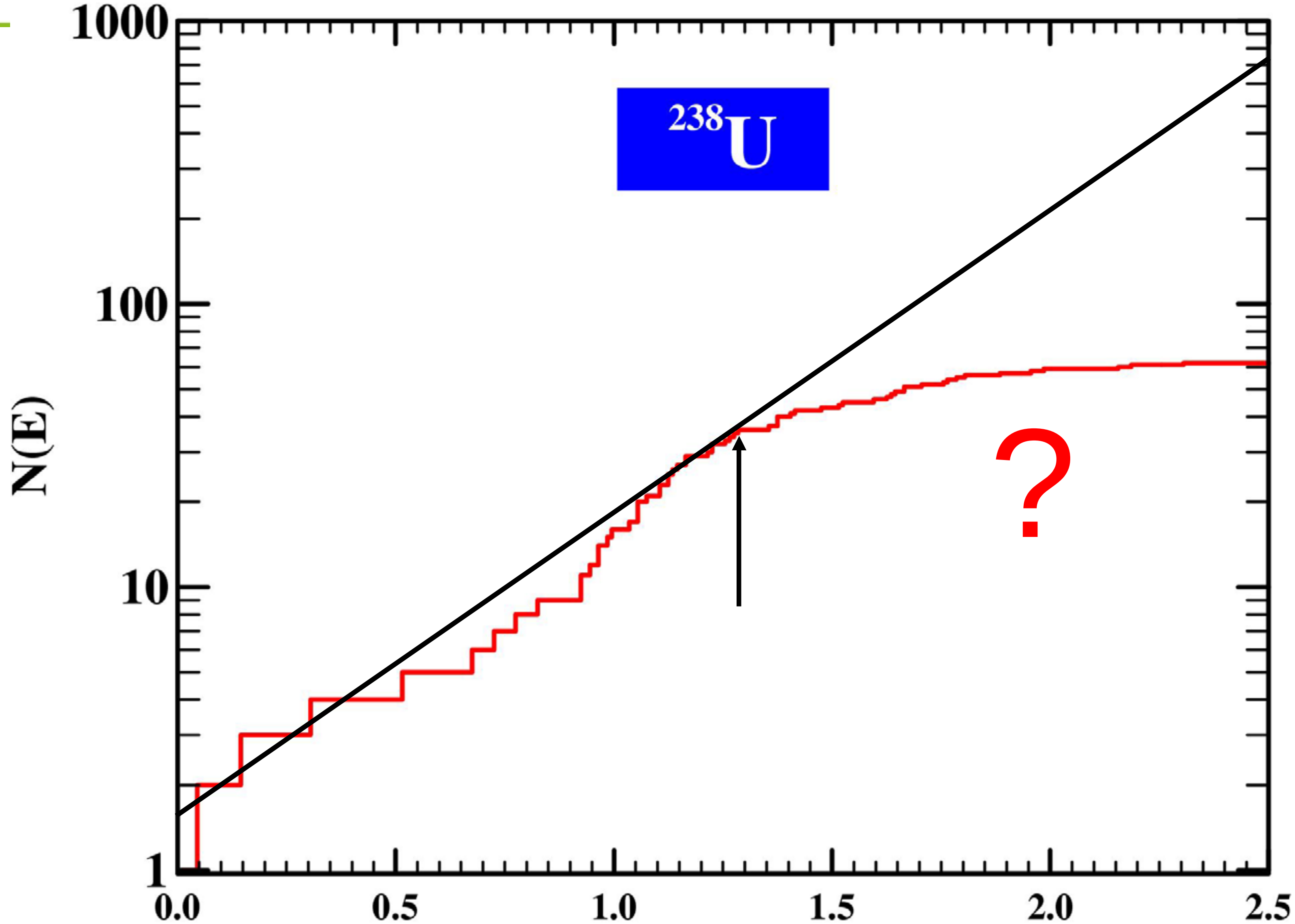
⇒ Default calculations not sufficient for applications.

Microscopic fission cross sections

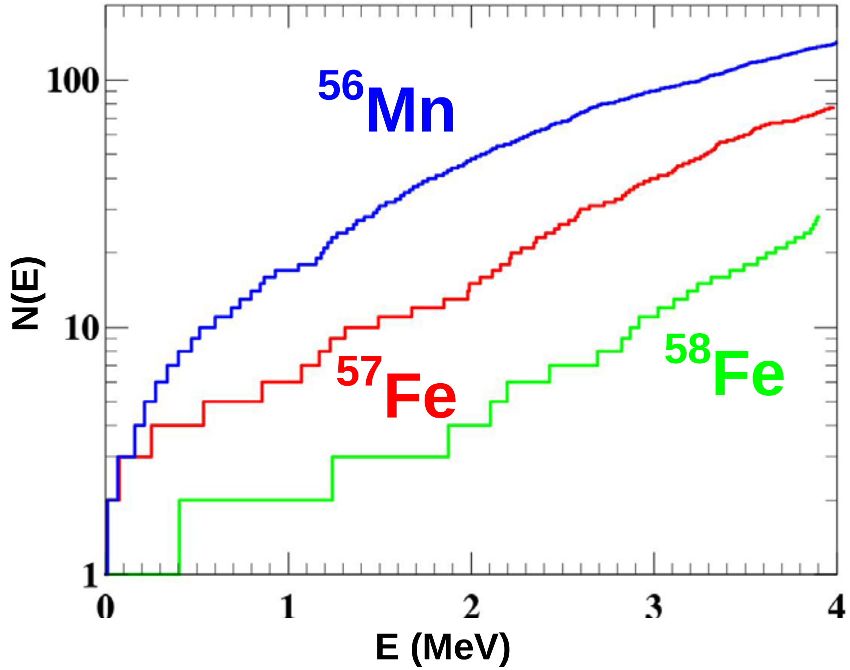


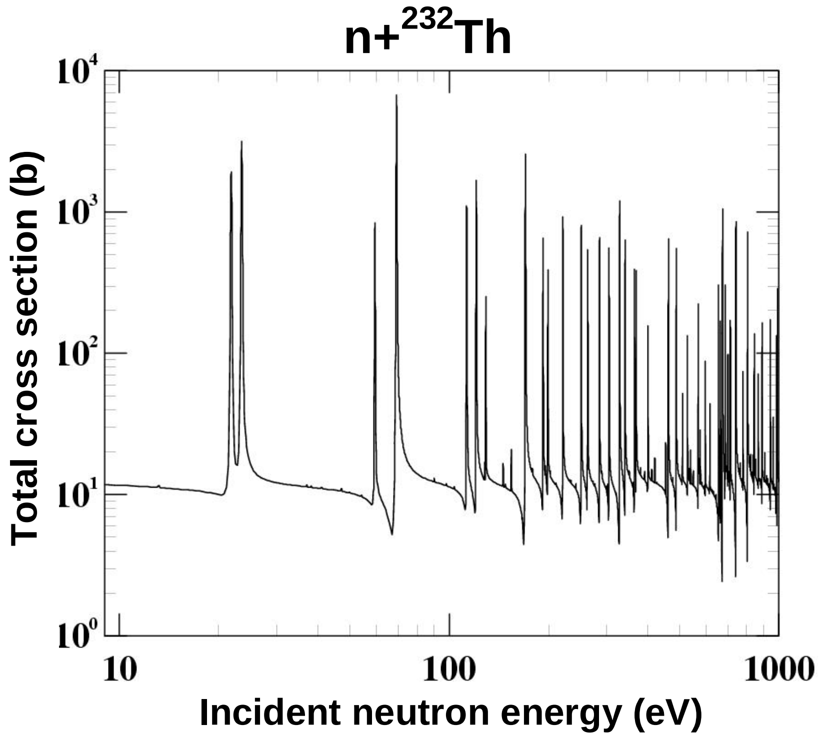
⇒ Not ridiculous after few adjustments.

Level densities : principle



Level densities : qualitative aspects





- **Exponential increase of the cumulated number of discrete levels N(E) with energy**

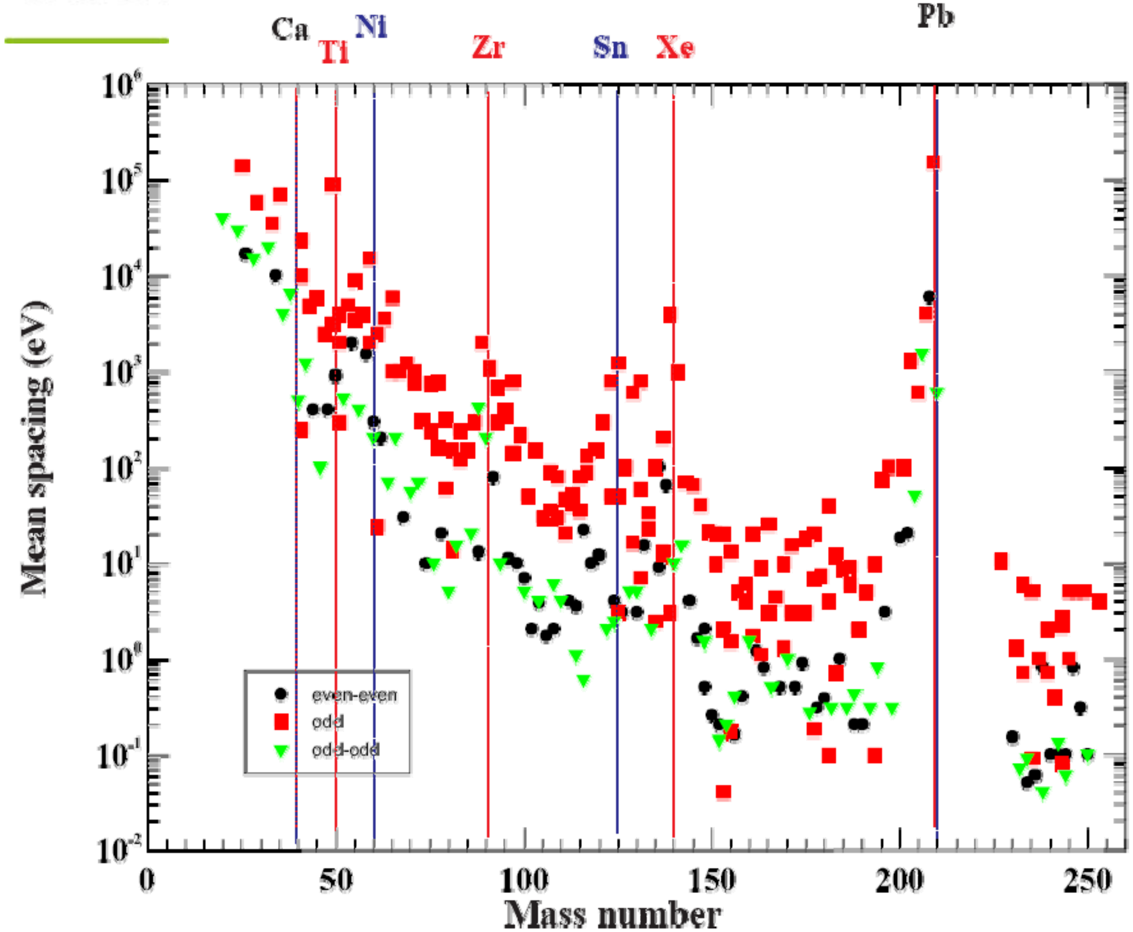
  $\Rightarrow \rho(E) = \frac{dN(E)}{dE}$ **Increases exponentially**

  $\Rightarrow$ **odd-even effects**

- **Mean spacings of s-wave neutron resonances at B_n of the order of few eV**

  $\Rightarrow \rho(B_n)$ **of the order of $10^4 - 10^6$ levels / MeV**

Level densities : qualitative aspects



Iljinov et al., NPA 543 (1992) 517.

$\Rightarrow$ **Mass dependency**
Odd-even effects
Shell effects

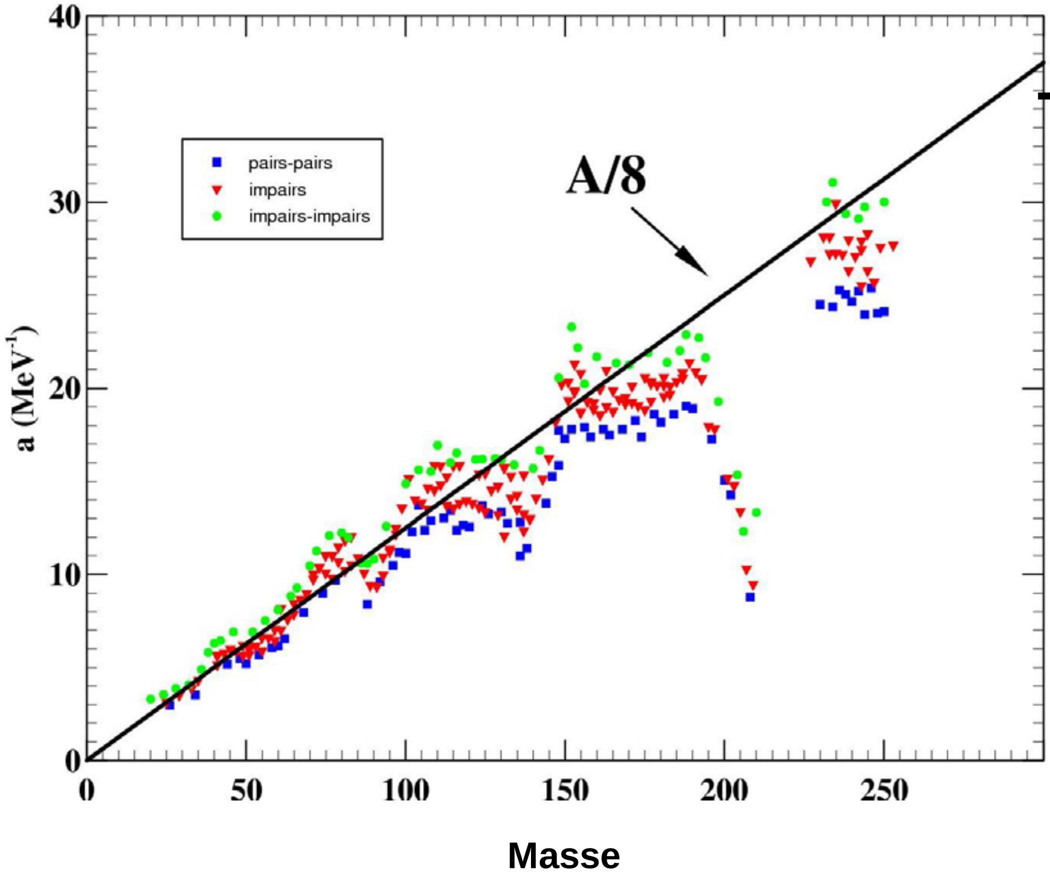
$$\frac{1}{D_0} = \rho\,(B_n, 1/2, \pi_t) \text{ for an even-even target}$$

$$= \rho\,(B_n, I_t+1/2, \pi_t) + \rho\,(B_n, I_t-1/2, \pi_t) \text{ otherwise}$$

Level densities : quantitative analysis

$$\rho(U, J, \pi) = \frac{1}{2}\,\frac{\sqrt{\pi}}{12}\,\frac{\exp\left(2\sqrt{aU}\right)}{a^{1/4}U^{5/4}}\,\frac{2J+1}{2\sqrt{2\pi}\,\sigma^3}\,\exp-\left[\frac{(J+\frac{1}{2})^2}{2\sigma^2}\right]$$

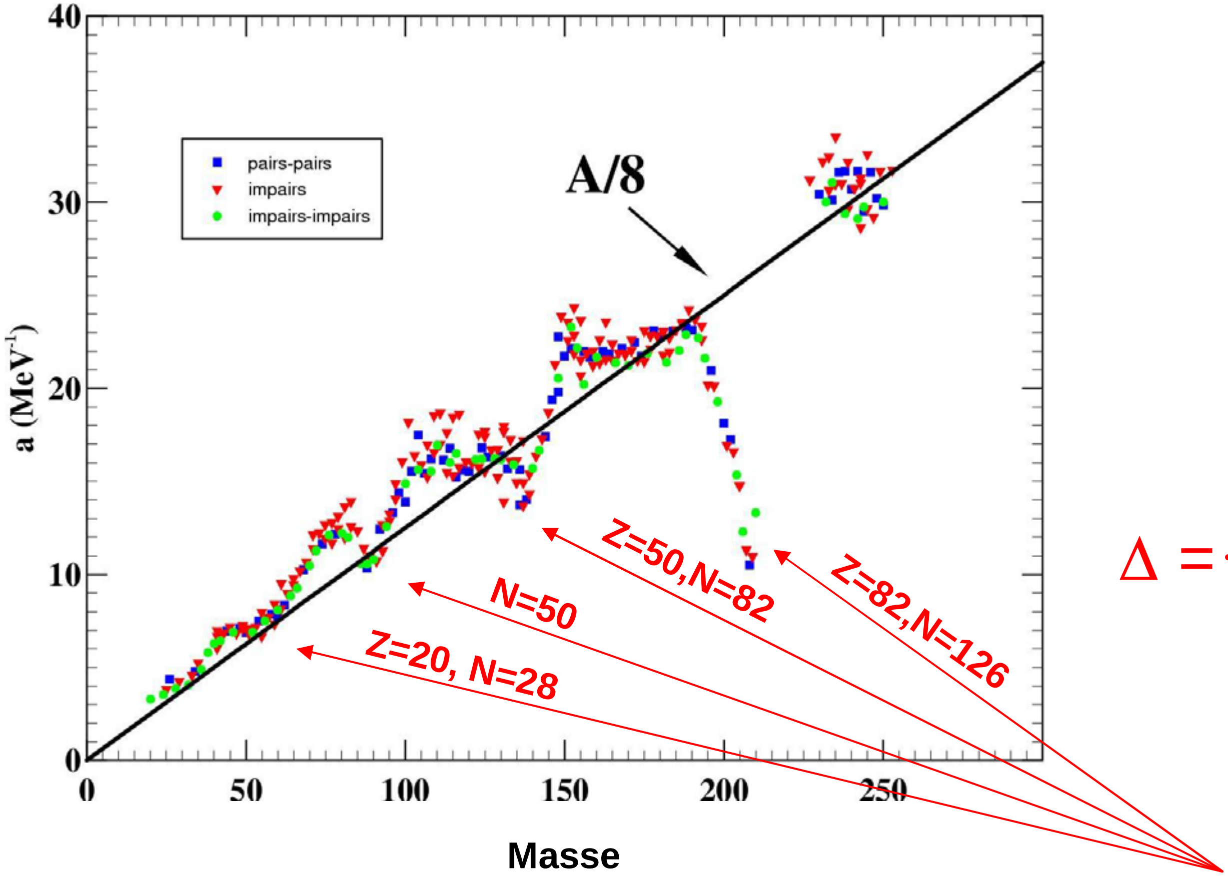
$$+\quad \sigma^2 = I_{rig}\sqrt{\frac{U}{a}}$$



$\Rightarrow$ **odd-even effects**

Level densities : quantitative analysis

$$\rho(U, J, \pi) = \frac{1}{2}\,\frac{\sqrt{\pi}}{12}\,\frac{\exp\left(2\sqrt{aU}\right)}{a^{1/4}U^{5/4}}\,\frac{2J+1}{2\sqrt{2\pi}\,\sigma^3}\,\exp - \left[\frac{\left(J+\frac{1}{2}\right)^2}{2\sigma^2}\right]$$



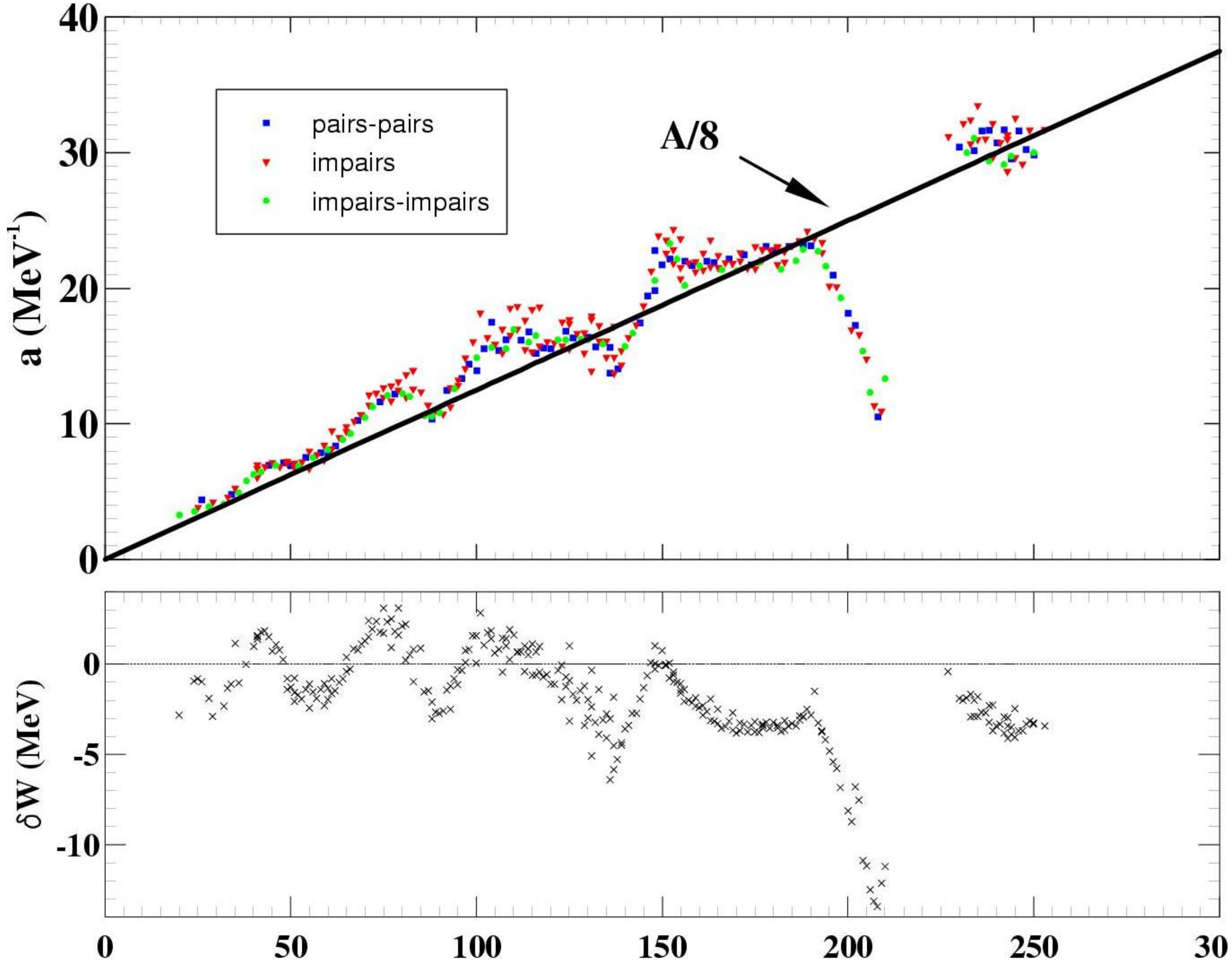
Odd-even effects accounted for

$$U \rightarrow U^* = U - \Delta$$

$$\Delta = \begin{cases} 0 & \text{odd-odd} \\ 12/\sqrt{A} & \text{odd-even} \\ 24/\sqrt{A} & \text{even-even} \end{cases}$$

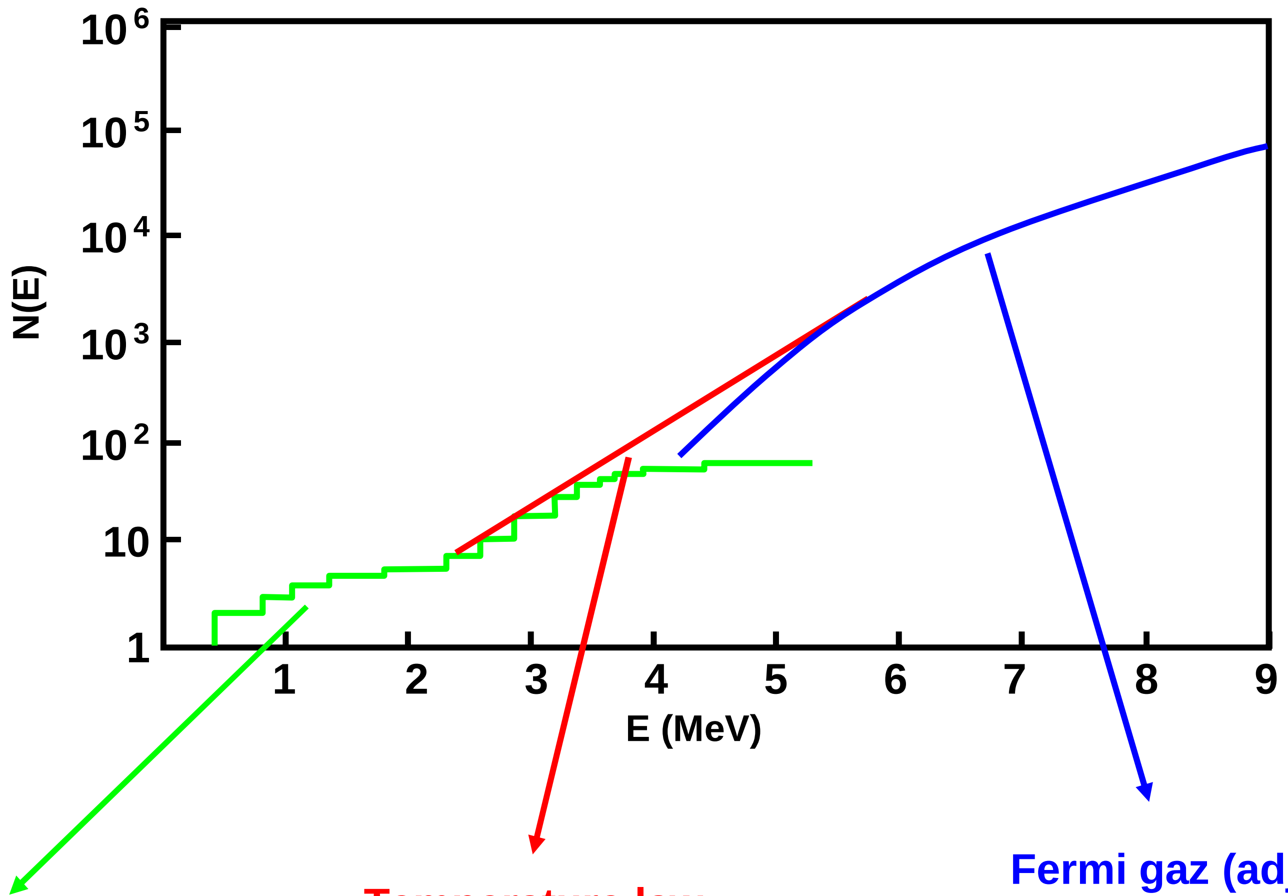
Shell effects

Level densities : Ignatyuk formula



$$a\,(N, Z, U^*) = \tilde{a}\,(A) \left[1 + \delta W(N,Z) \; \frac{1 - \exp(-\gamma\, U^*)}{U^*} \right]$$

Full description of level densities



Fermi gaz (adjusted at B_n)

Temperature law

Discrete levels
(spectroscopy)

$$N(E)=\exp\left(\frac{E-E_0}{T}\right)$$

$$\rho(E)=\alpha\,\frac{\exp\left(2\sqrt{aU^*}\right)}{a^{1/4}U^{*5/4}}$$

The combinatorial method

See PRC 78 (2008) 064307 for details

- **HFB + effective nucleon-nucleon interaction ⇒ single particle level schemes**

- **Combinatorial calculation ⇒ intrinsic p-h and total state densities ω_i (U, K, π)**

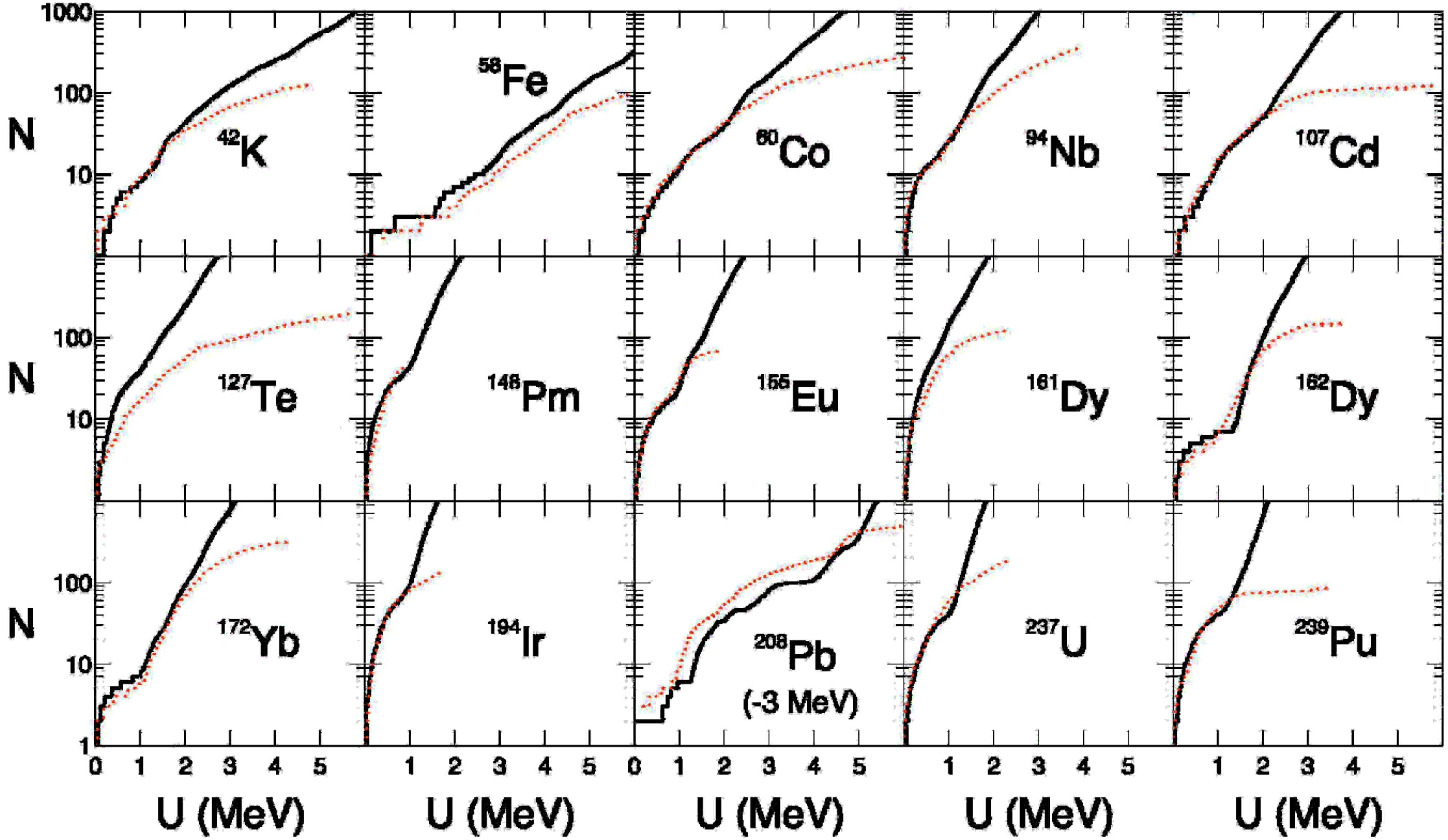
- **Collective effects ⇒ from state to level densities ρ(U, J, π)**

2006 Approximation : ~~1) construction of rotational bands~~
~~2) multiplication by vibrational enhancement~~

Current treatment : 1) folding of intrinsic and vibrational state densities
2) construction of rotational bands

- **Phenomenological transition for deformed/spherical nucleus**

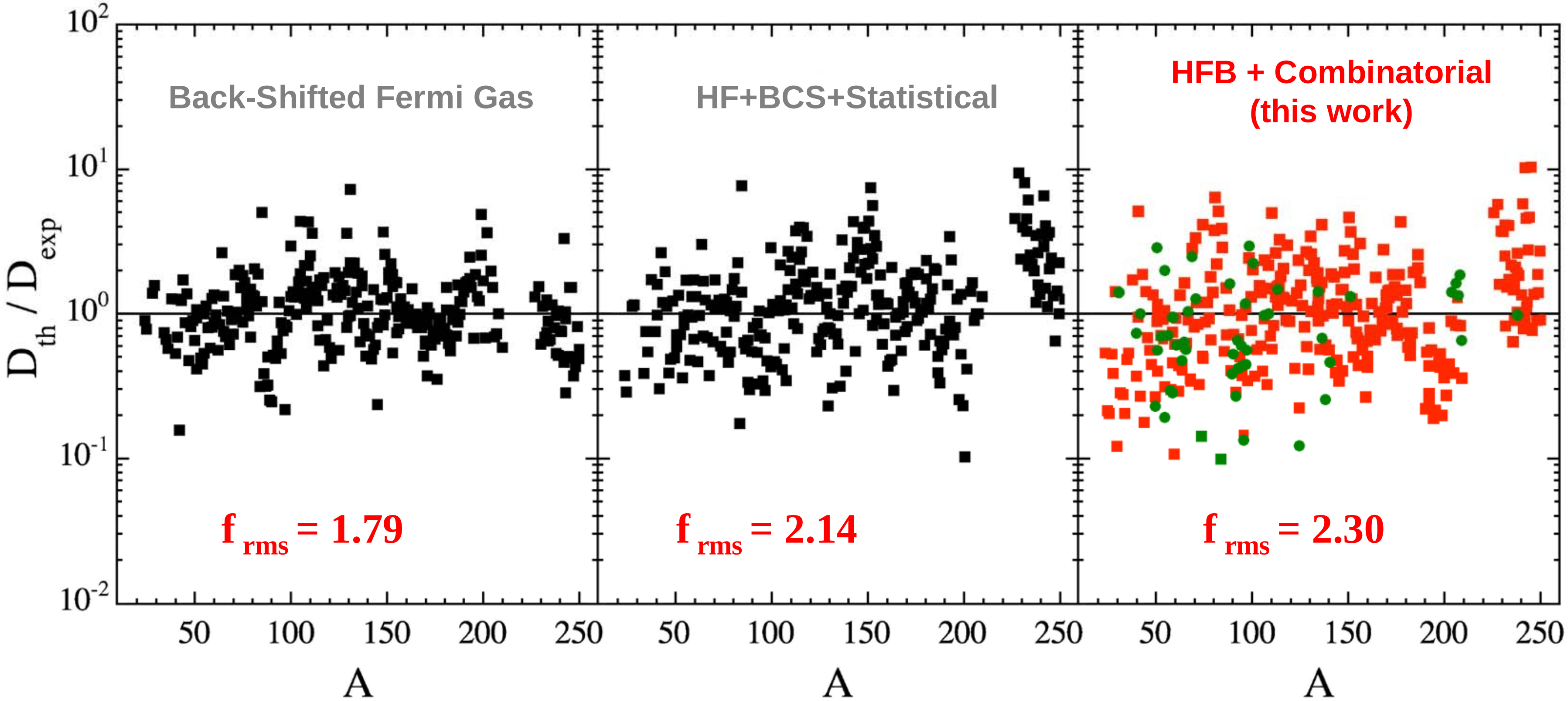
Results for cumulated histograms



➡ **Structures typical of non-statistical feature**

Results at B_n

D values (s-waves & p-waves)

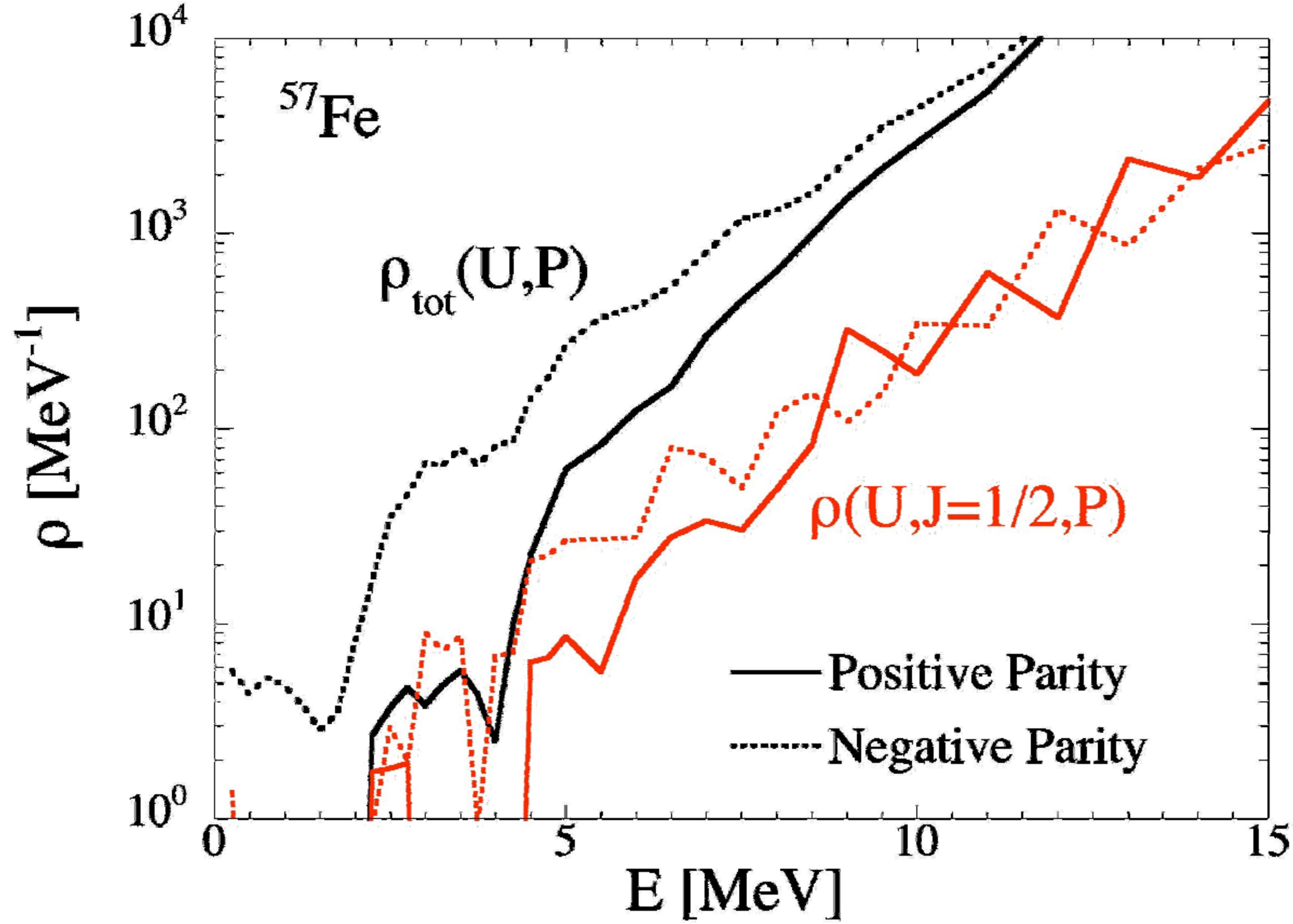


➡ **Description similar to that obtained with other global approaches**

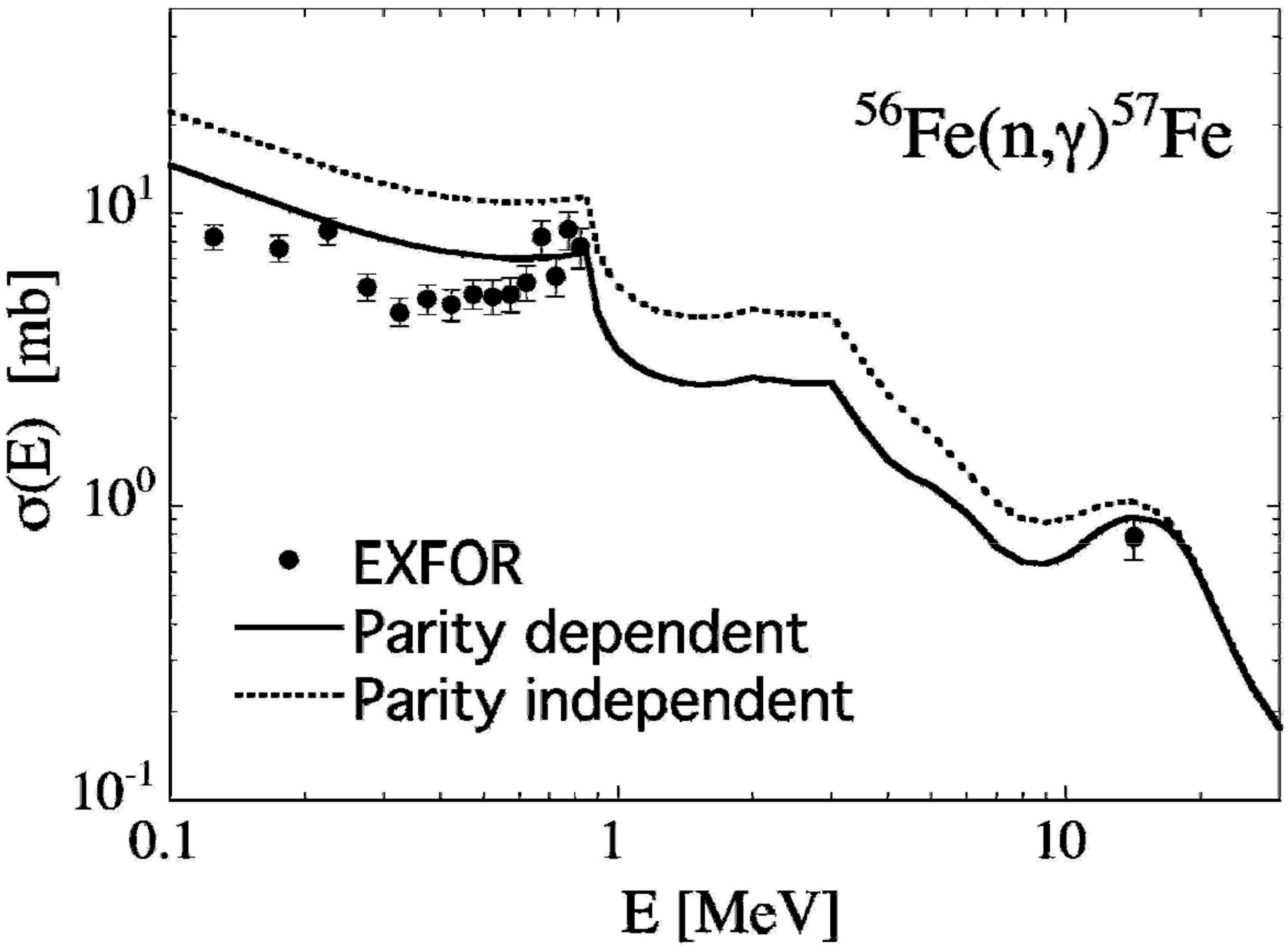
Combinatorial level densities

Talys deals with realistic (non statistical) parity and spin distributions

Combinatorial level densities

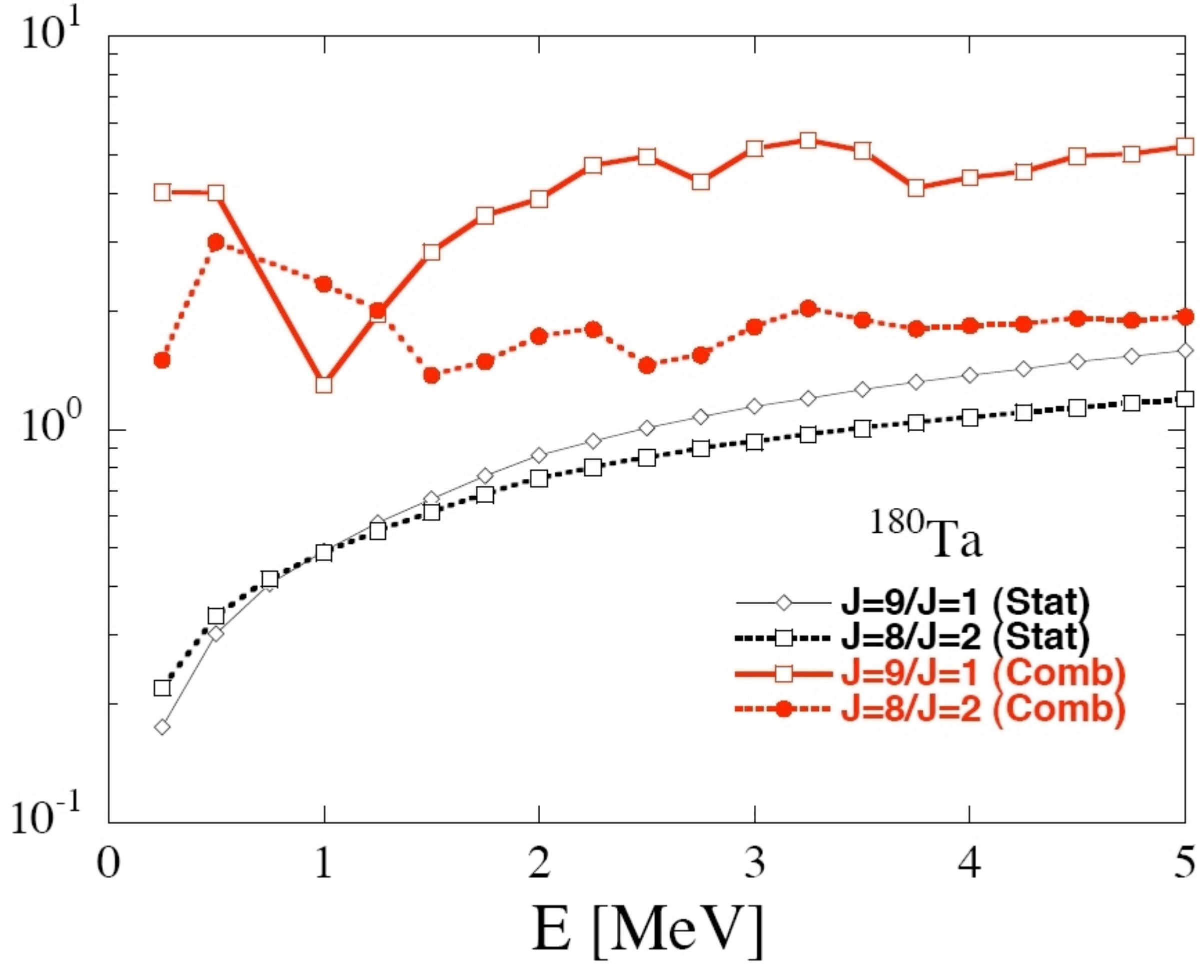


Combinatorial level densities



Combinatorial level densities

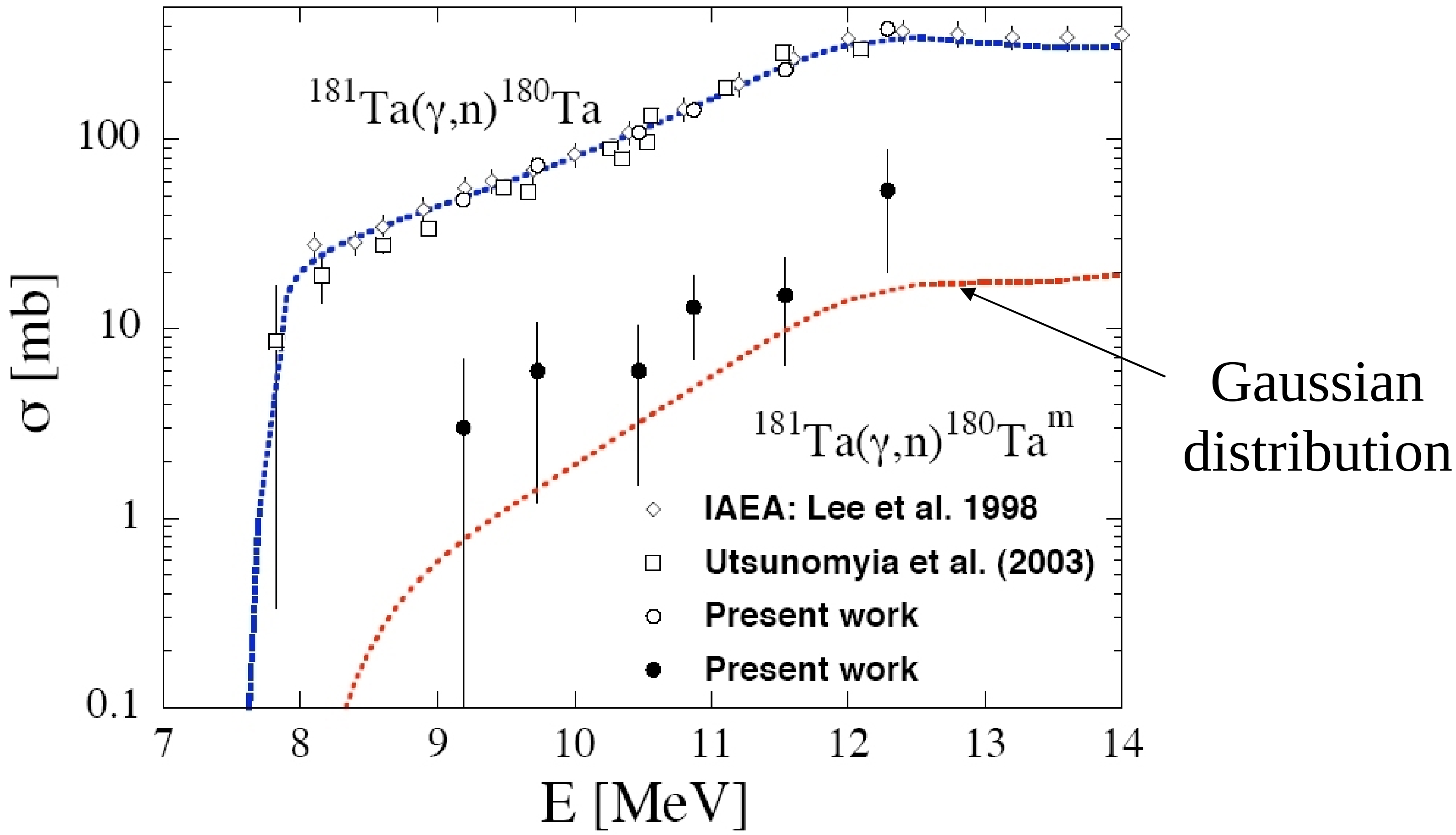
Talys deals with realistic (non statistical) parity and spin distributions



➡ **Non-statistical feature imply significant deviations from the usual gaussian spin dependence**

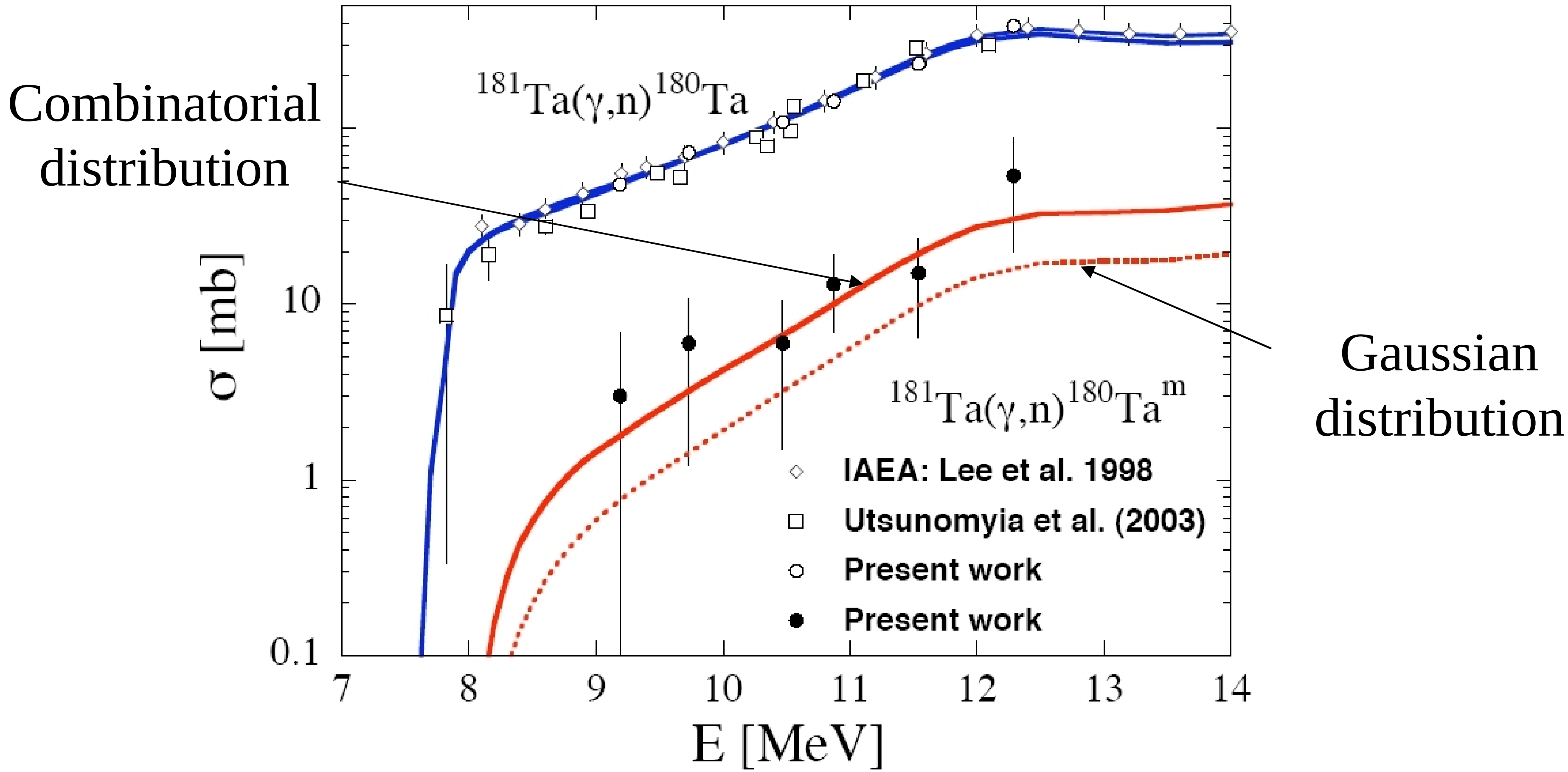
Combinatorial level densities

See PRL 96 (2006) 192501 for details



Combinatorial level densities

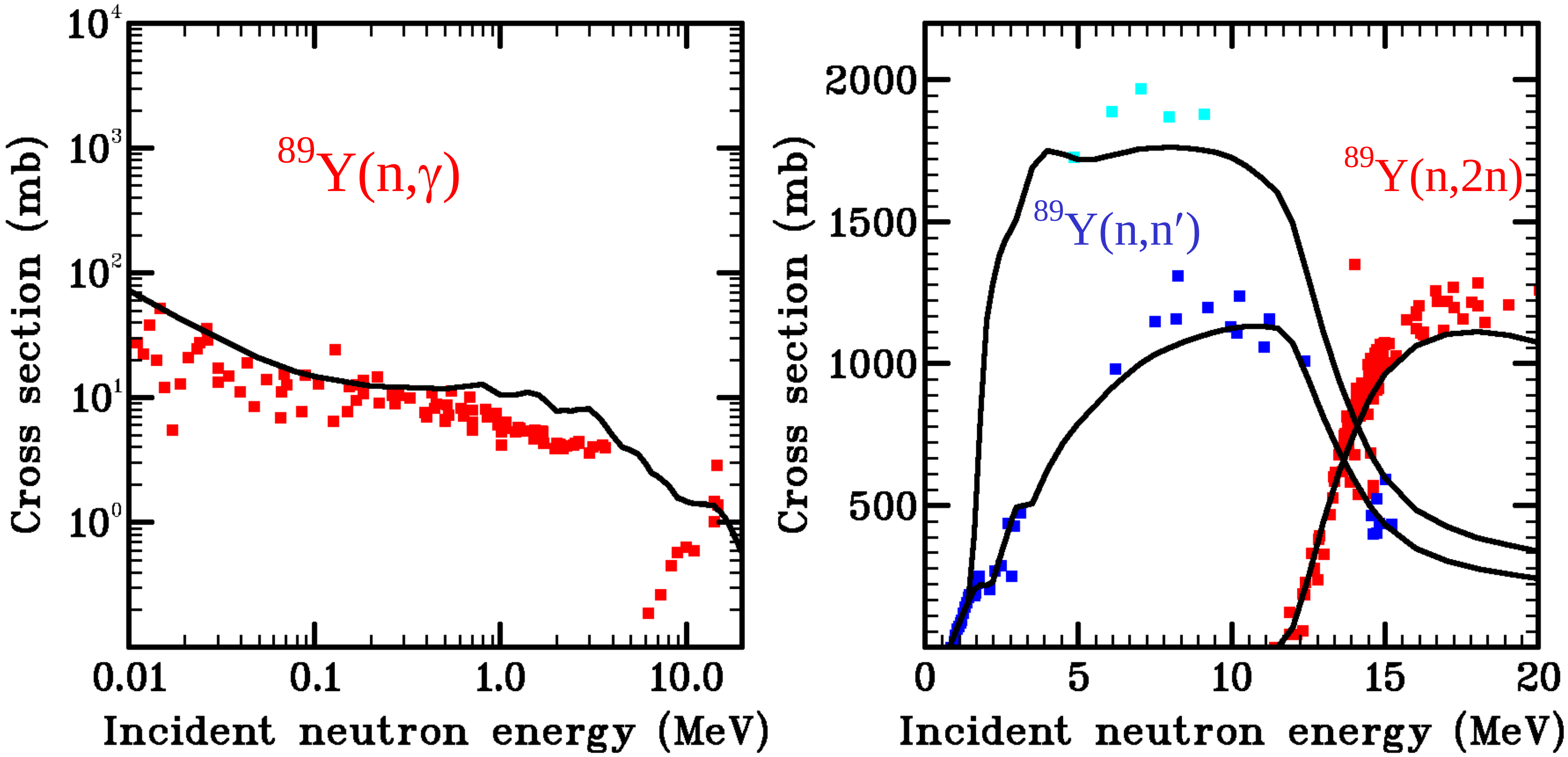
See PRL 96 (2006) 192501 for details



➡ **Deviations from the usual gaussian spin dependence can have large impact on isomeric level production cross sections**

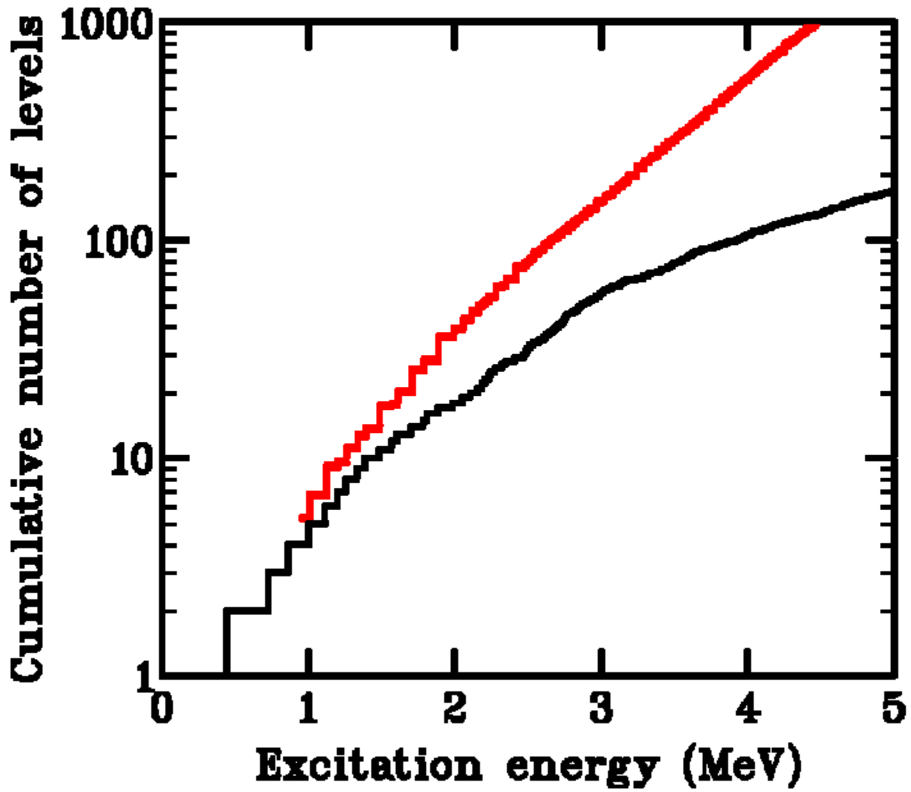
Adjustable level densities : recipe & impact

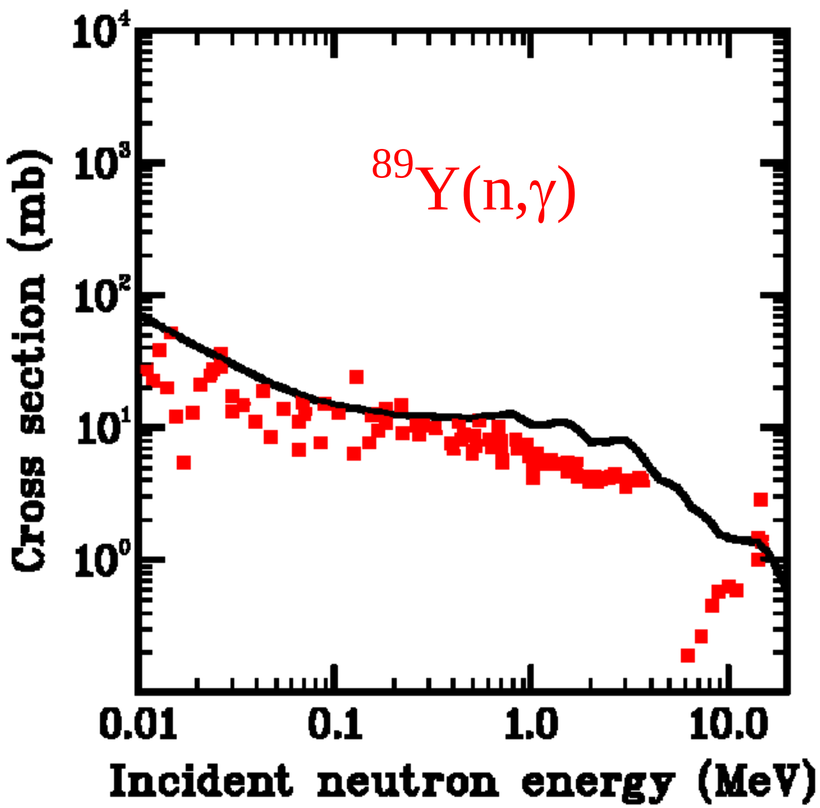
$$\rho_{renorm}(U) = e^{\alpha\sqrt{(U-\delta)}}\,\rho_{global}(U-\delta)$$



Adjustable level densities : recipe & impact

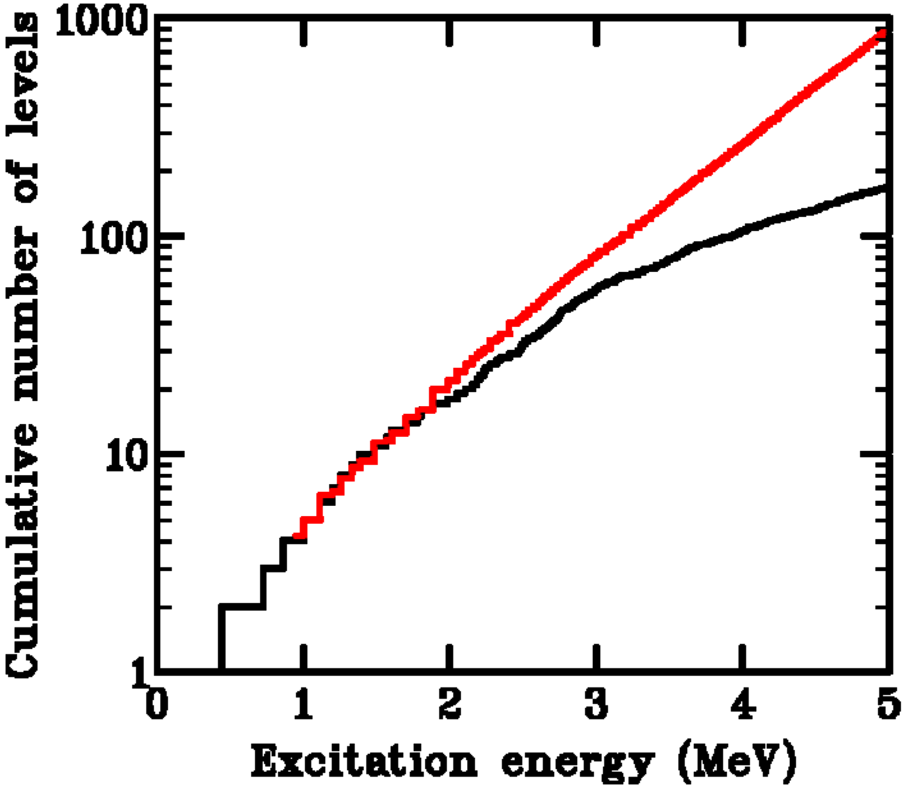
$$\rho_{renorm}(U) = e^{\alpha\sqrt{(U-\delta)}}\,\rho_{global}(U-\delta)$$

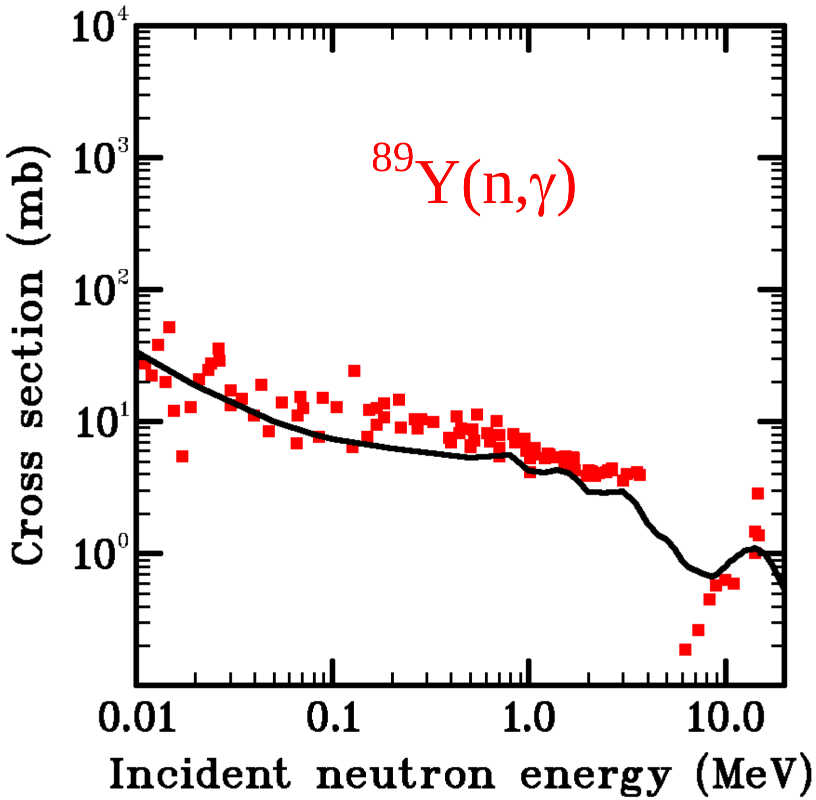




Adjustable level densities : recipe & impact

$$\rho_{renorm}(U) = e^{\alpha\sqrt{(U-\delta)}}\,\rho_{global}(U-\delta)$$

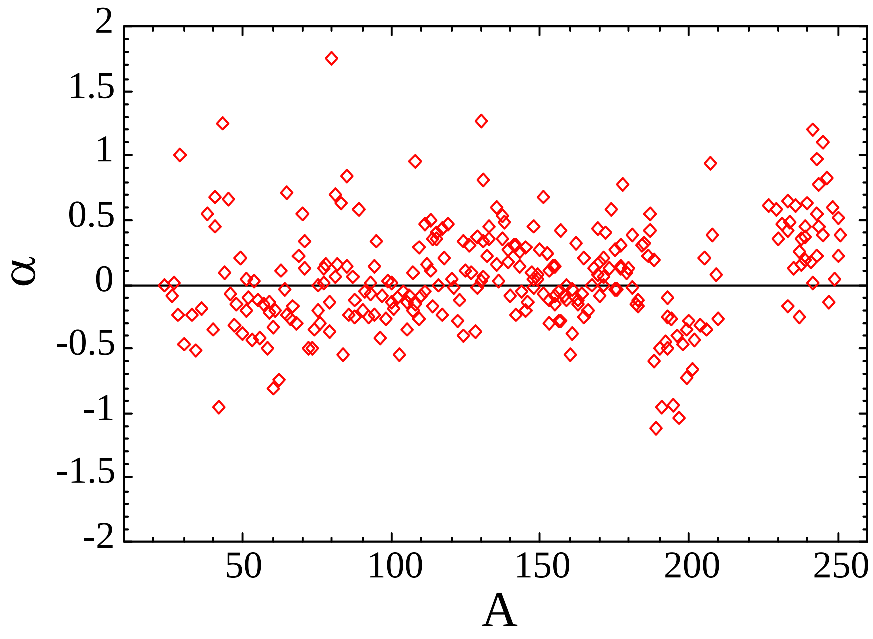


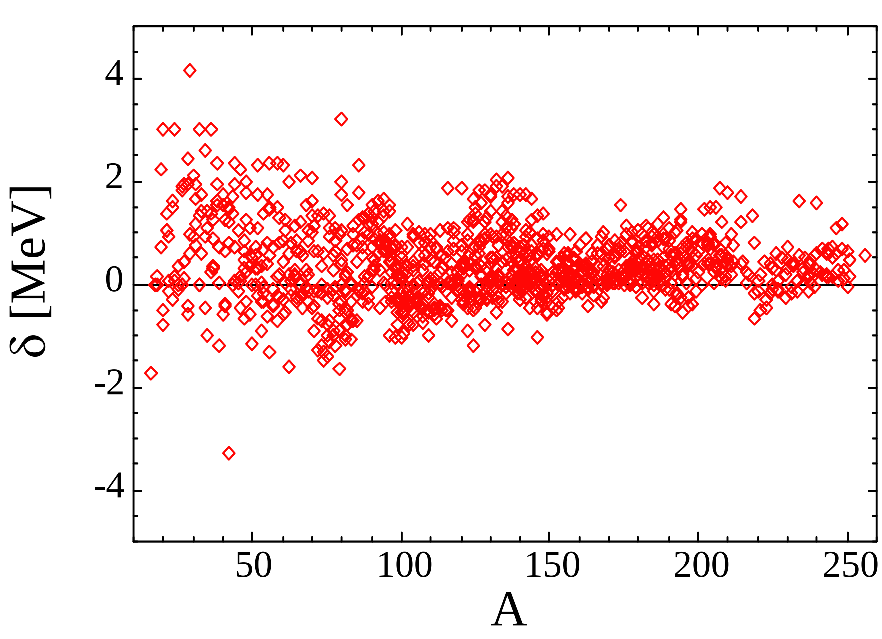


Global adjustment

See NPA 810 (2008) 13 for details

α and δ adjusted to fit discrete levels (≈ 1200 nuclei) and D_0's (≈ 300 nuclei) using the TALYS code





Levels density models implemented in TALYS

- **Gilbert-Cameron model + Ignatyuk**

  $\Rightarrow$ **Default**

- **Back-Shifted Fermi Gas model + Ignatyuk**

  $\Rightarrow$ **Default**

- **(Generalized) Superfluid model**

  $\Rightarrow$ **More rigourous treatment of pairing correlation at low energy**
  $\Rightarrow$ **Fermi gaz + Ignatyuk law above some critical energy**
  $\Rightarrow$ **Explicit treatment of collective effects**

- **Combinatorial approach**

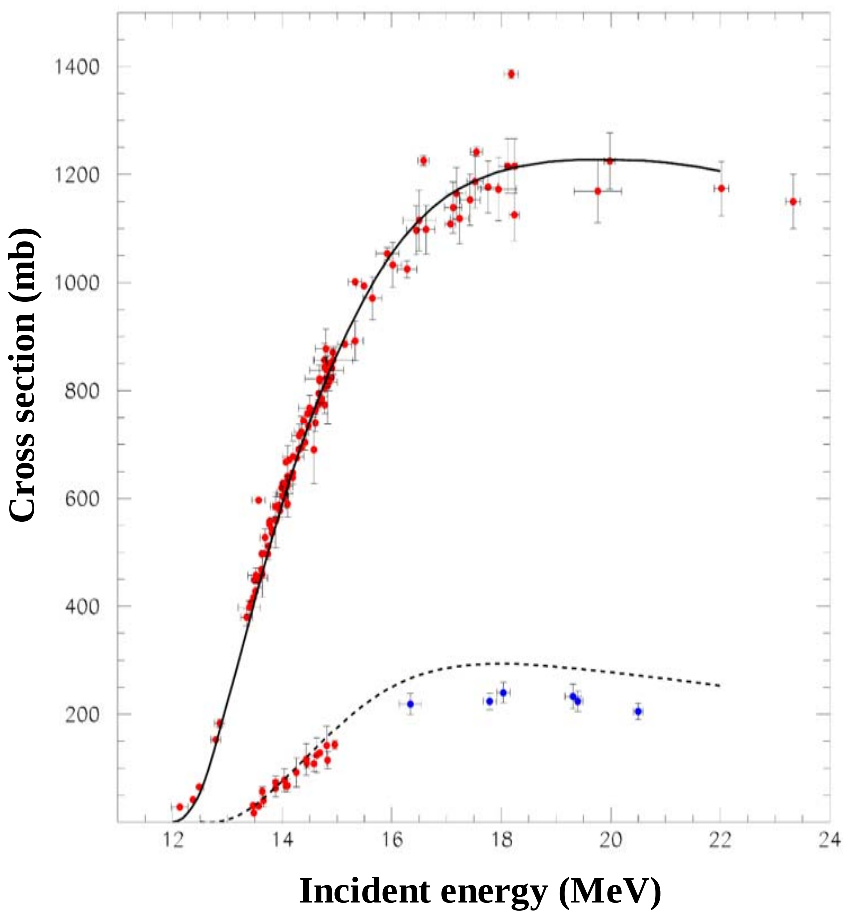
  $\Rightarrow$ **Direct counting method of both partial and total level densities**
  $\Rightarrow$ **Access to non statistical effects**

Phenomenological ⇒ microscopic predictions ?

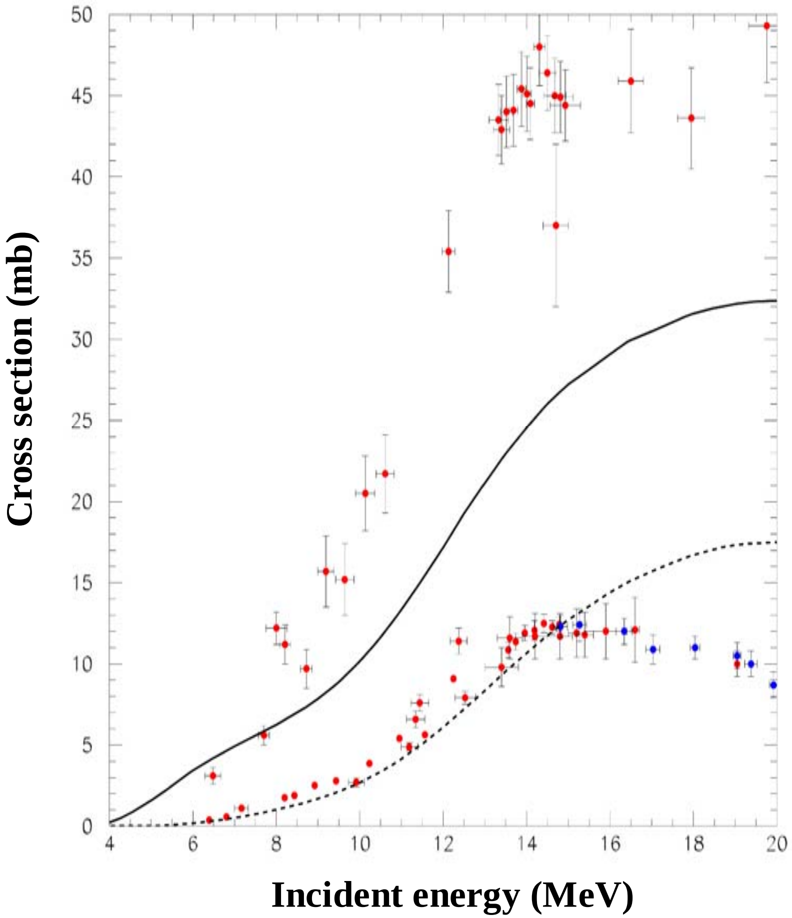
Experimentally known (deduced)		Theoretically predicted
Nuclear properties - Level properties (E, J^π, branching ratios) - deformations	⇒	**HFB + ν-ν interaction**
Level densities - Gilbert & Cameron - Back Shifted Fermi Gas - Generalized Superfluid Model - Williams + several corrections (p-h)	⇒	**Combinatorial method** - Total level densities - p-h level densities
Optical model - Koning & Delaroche - Soukhovistkii (actinides) - Tabulated	⇒	**Semi-microscopic JLM**
γ-strength functions - Kopecky-Uhl, Brink-Axel	⇒	**HFBCS or HFB Tables**
Fission paths - Hill-Wheeler	⇒	**HFB shapes with WKB penetrabilities**

Some TALYS results

^{90}Zr (n,2n) ^{89}Zr



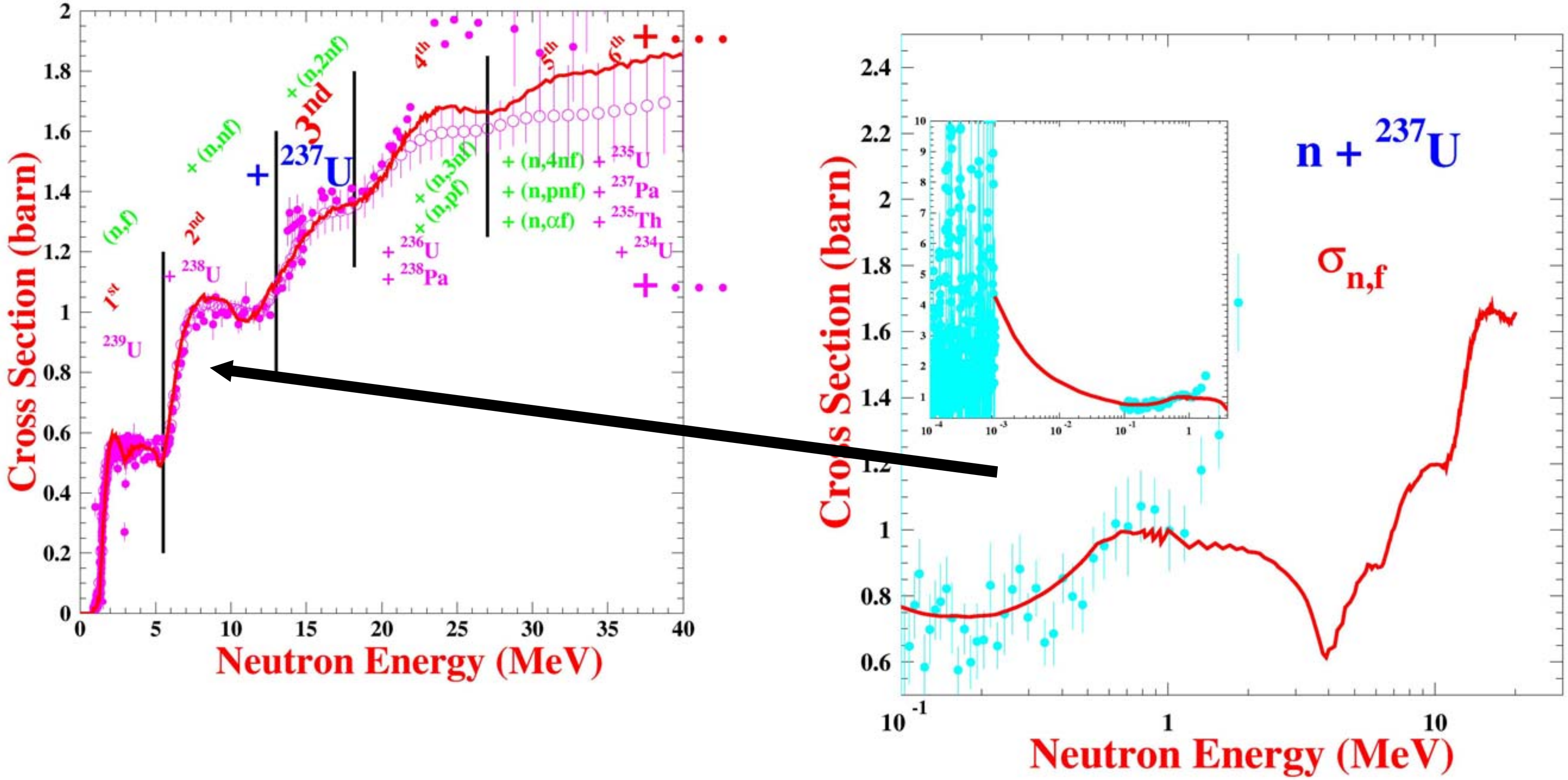
^{90}Zr (n,p) ^{90}Y



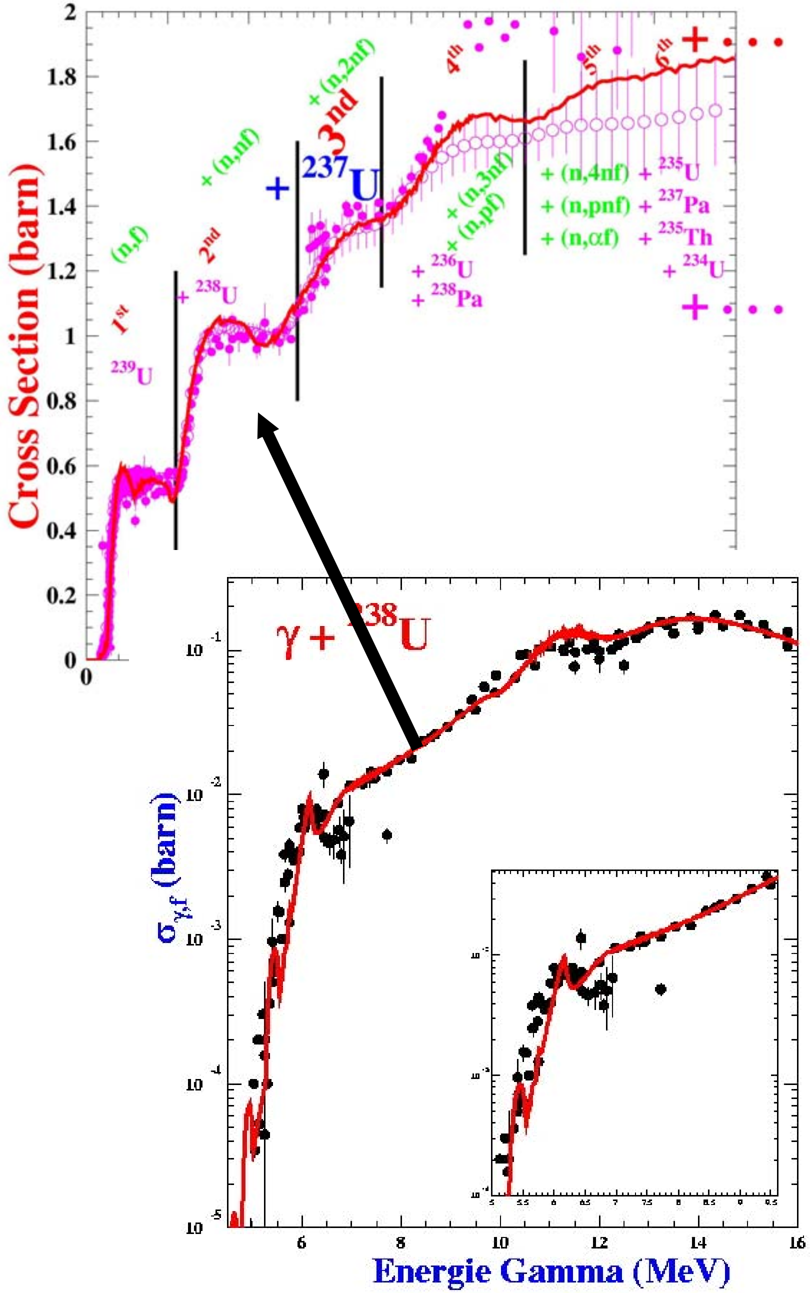
Coherent fission cross sections with phenomenological approach

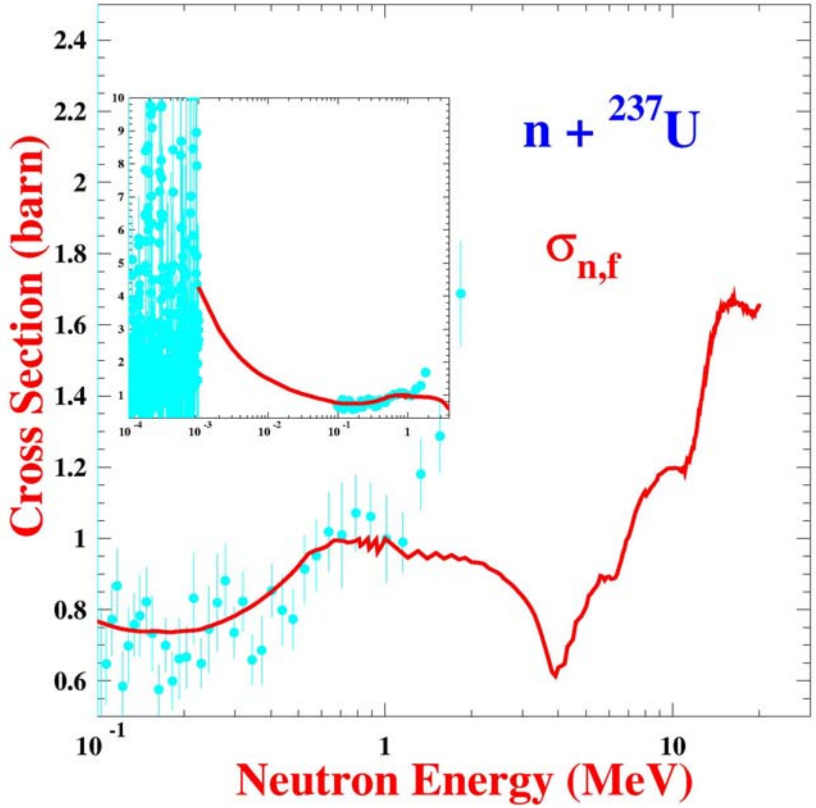
Neutron induced fission on ^{238}U

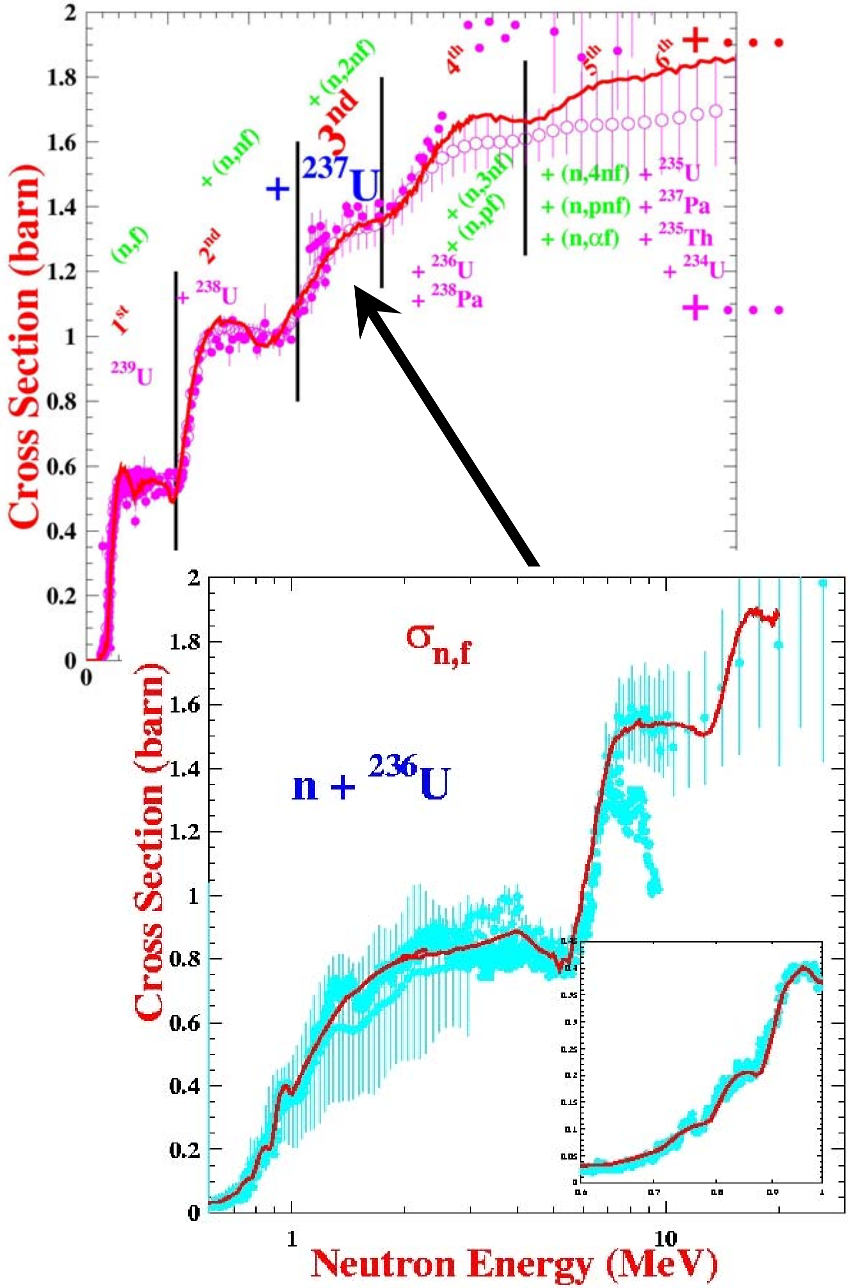
- several hundreds of parameters
- unique set for all fission chances or U targets

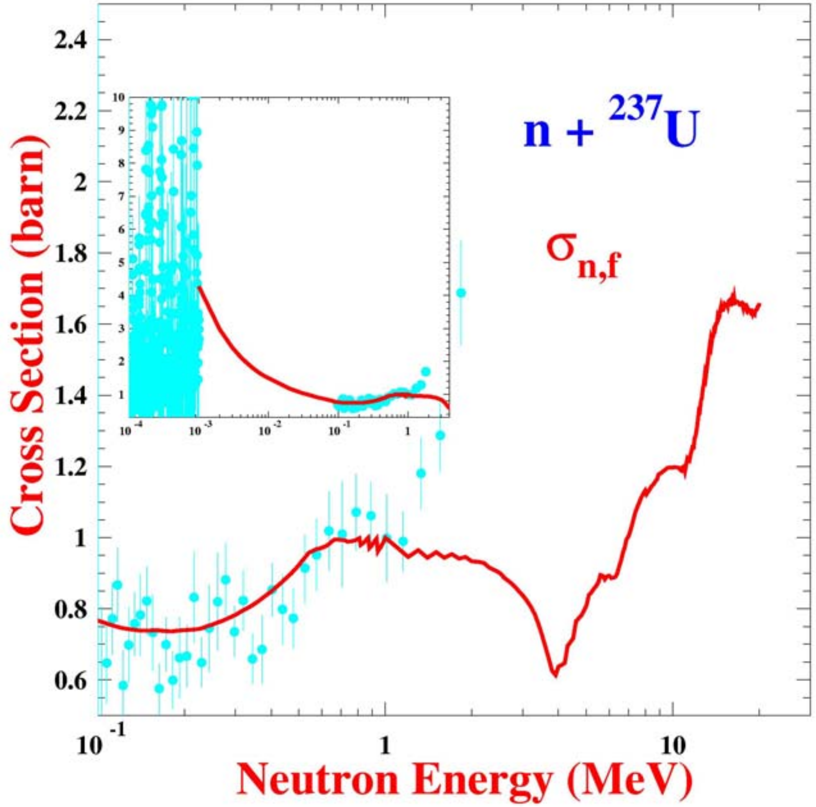


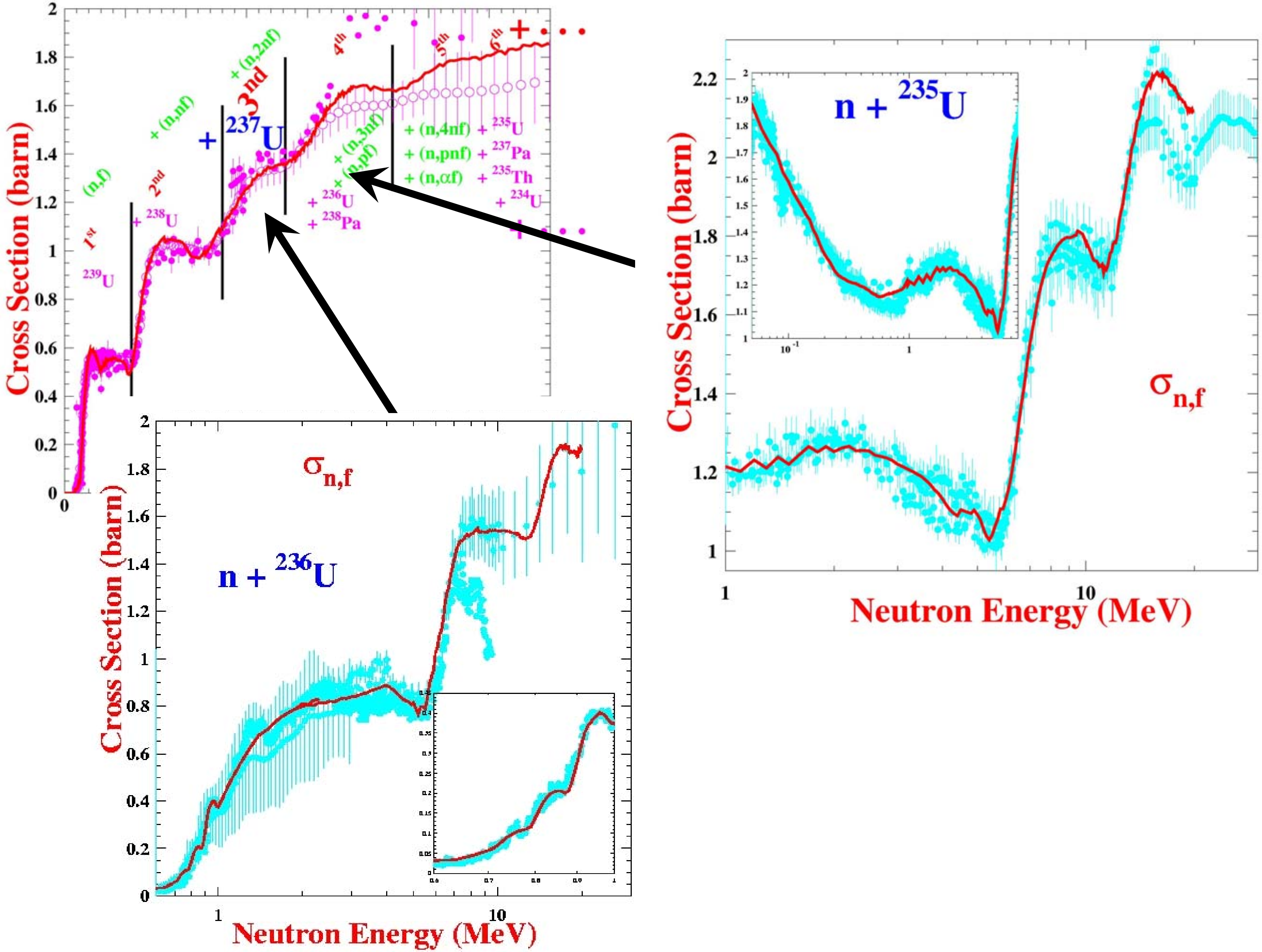
Cross Section (barn)
Neutron Energy (MeV)
(n,f)
+ (n,nf)
+ (n,2nf)
1st
2nd
3nd
4th
5th
6th
239U
+ 238U
+ 237U
+ 236U
+ 238Pa
+ (n,3nf)
+ (n,pf)
+ (n,4nf) + 235U
+ (n,pnf) + 237Pa
+ (n,αf) + 235Th
+ 234U
n + 237U
σn,f

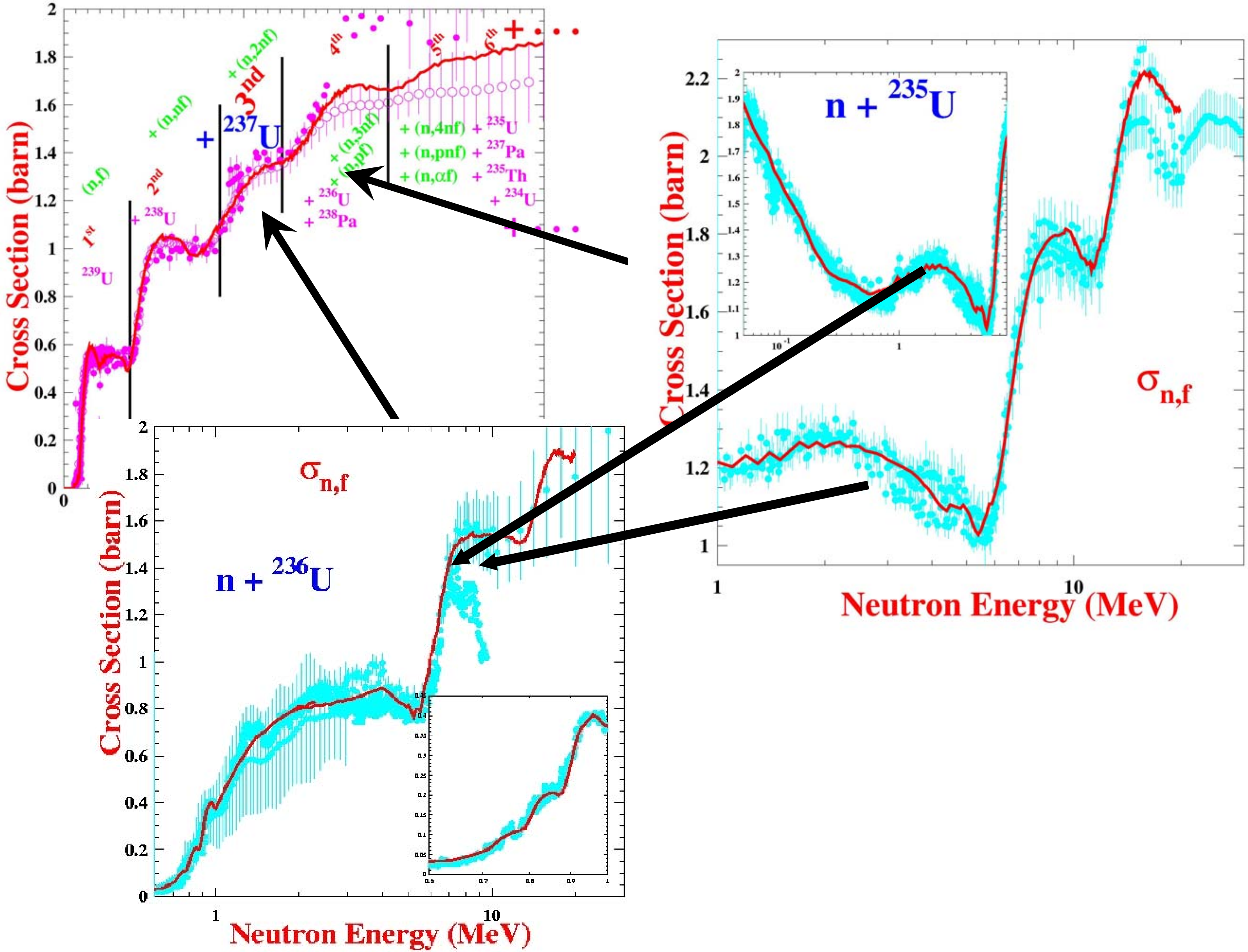

Cross Section (barn)
(n,f)
1st
239U
2nd
+ 238U
+ (n,nf)
+ 237U
3nd
+ (n,2nf)
4th
5th
6th
+ (n,3nf)
+ (n,pf)
+ 236U
+ 238Pa
+ (n,4nf) + 235U
+ (n,pnf) + 237Pa
+ (n,αf) + 235Th
+ 234U
γ + 238U
σγ,f (barn)
Energie Gamma (MeV)

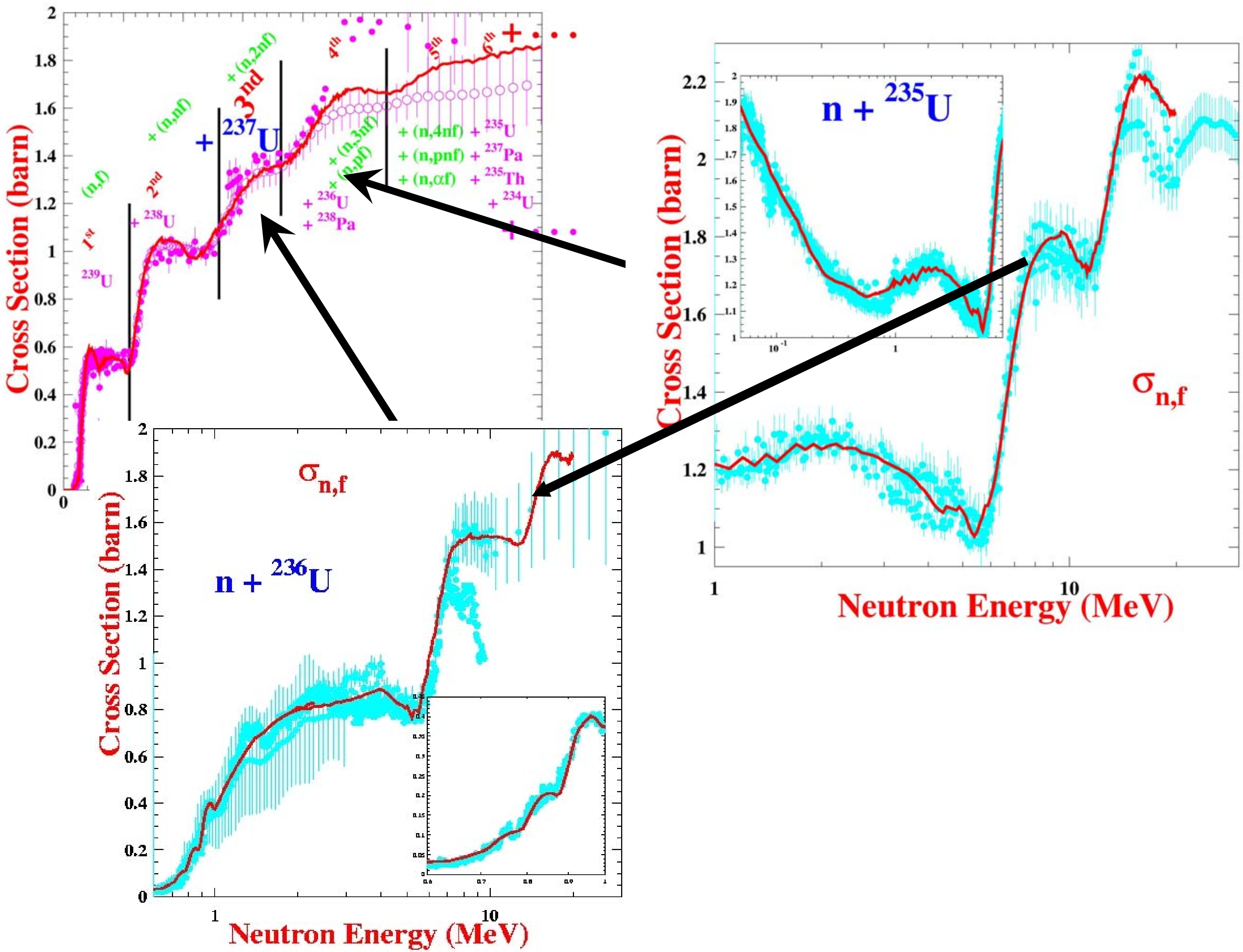

n + 237U
σn,f
Cross Section (barn)
Neutron Energy (MeV)

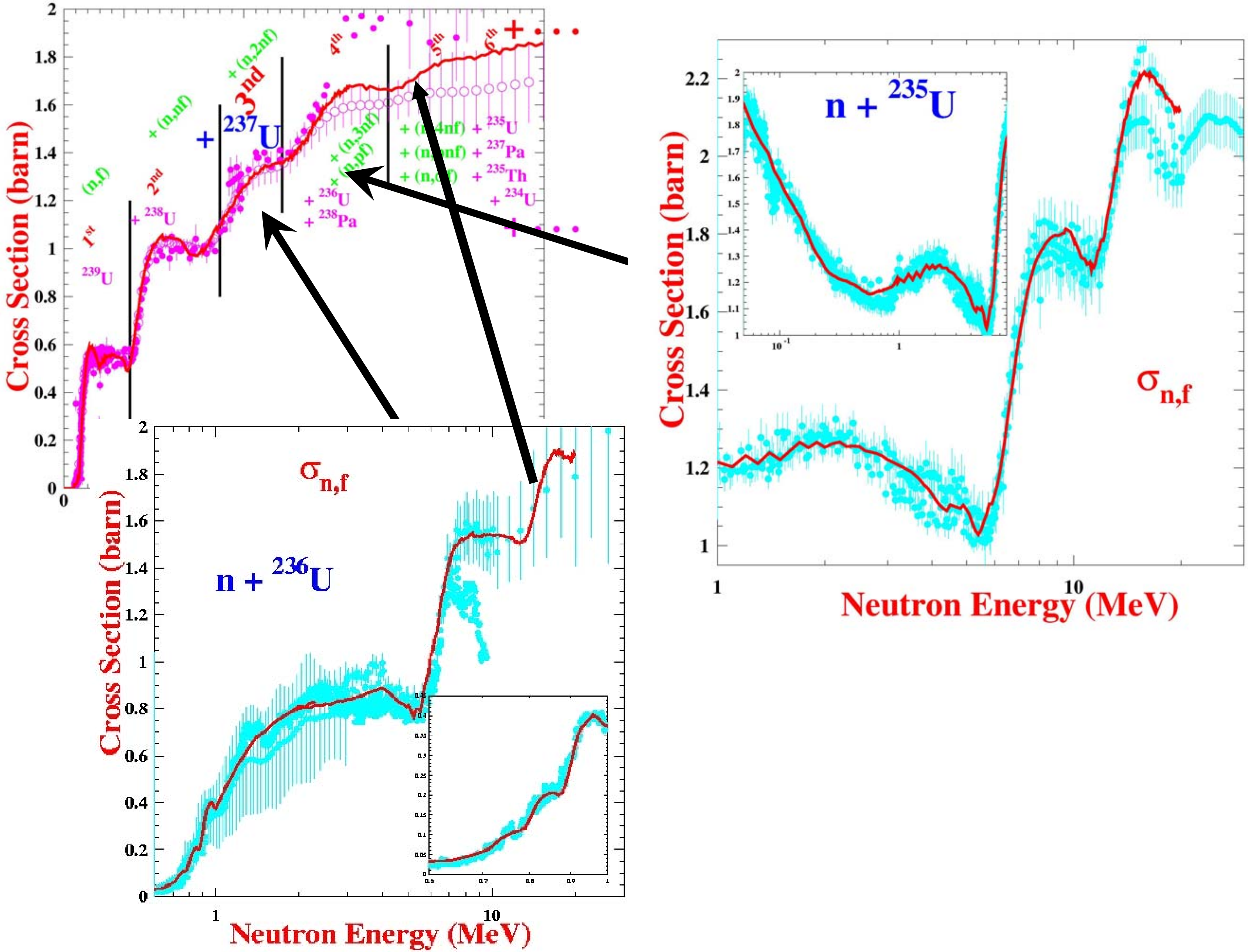

Cross Section (barn)
(n,f)
1st
239U
2nd
+ 238U
+ (n,nf)
3rd
+ 237U
+ (n,2nf)
4th
5th
6th
+ (n,3nf)
+ (n,pf)
+ 236U
+ 238Pa
+ (n,4nf) + 235U
+ (n,pnf) + 237Pa
+ (n,αf) + 235Th
+ 234U
σn,f
n + 236U
Cross Section (barn)
Neutron Energy (MeV)


n + 237U
σn,f
Cross Section (barn)
Neutron Energy (MeV)

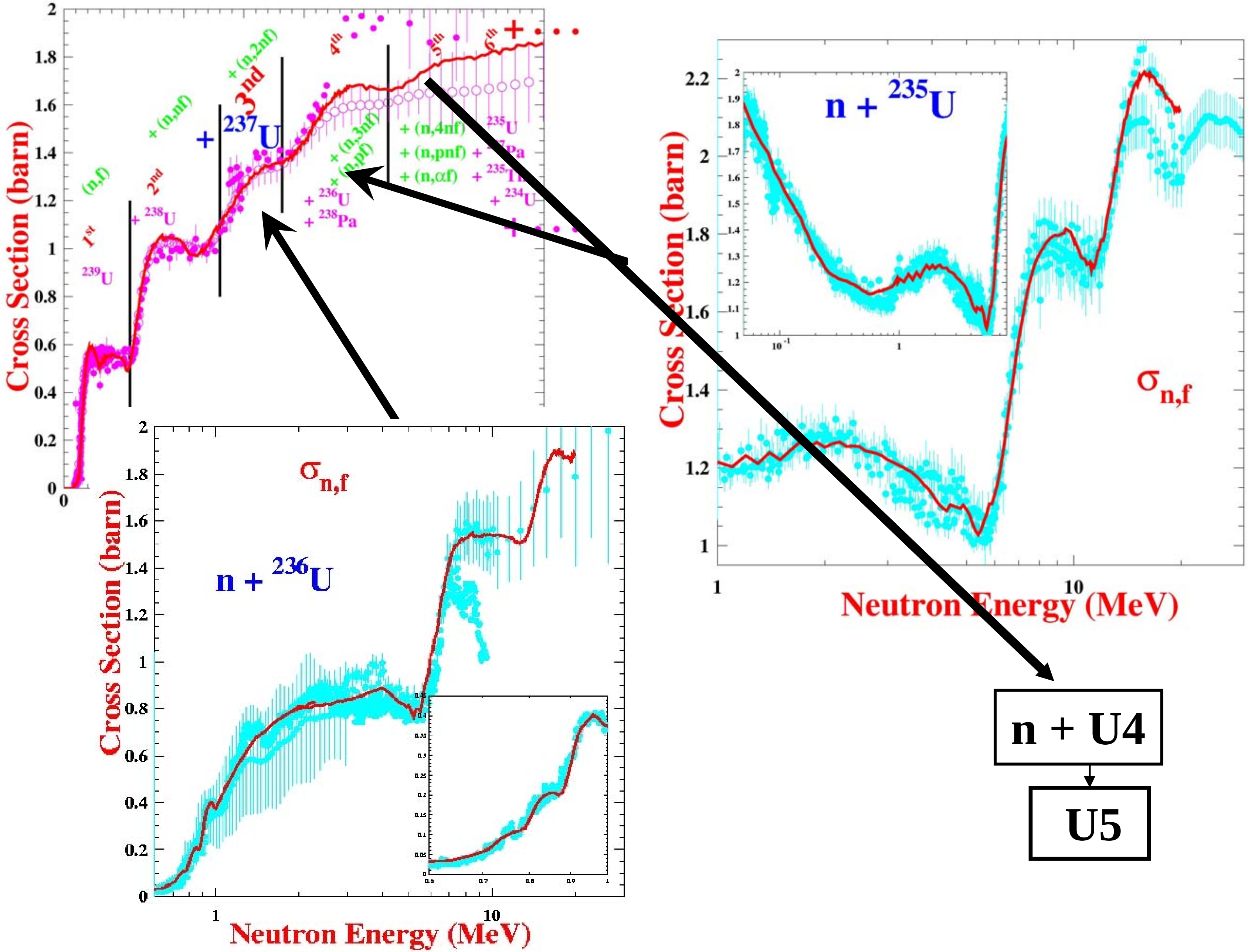

Cross Section (barn)
(n,f)
+ (n,nf)
+ (n,2nf)
+ (n,3nf)
+ (n,pf)
+ (n,4nf) + 235U
+ (n,pnf) + 237Pa
+ (n,αf) + 235Th
+ 234U
1st
2nd
3nd
4th
5th
6th
239U
+ 238U
+ 237U
+ 236U
+ 238Pa
n + 236U
σn,f
Neutron Energy (MeV)
n + 235U
σn,f
Cross Section (barn)
Neutron Energy (MeV)


Cross Section (barn)
(n,f)
(n,nf)
(n,2nf)
1st
2nd
3nd
4th
5th
6th
239U
+ 238U
+ 237U
+ (n,3nf)
+ (n,pf)
+ 236U
+ 238Pa
+ (n,4nf) + 235U
+ (n,pnf) + 237Pa
+ (n,αf) + 235Th
+ 234U
n + 235U
σn,f
Cross Section (barn)
Neutron Energy (MeV)
n + 236U
σn,f
Cross Section (barn)
Neutron Energy (MeV)


Cross Section (barn)
1st
2nd
3nd
4th
5th
6th
(n,f)
+ (n,nf)
+ (n,2nf)
+ (n,3nf)
+ (n,pf)
+ (n,4nf)
+ (n,pnf)
+ (n,αf)
+ 237U
239U
+ 238U
+ 236U
+ 238Pa
+ 235U
+ 237Pa
+ 235Th
+ 234U
n + 236U
σn,f
Neutron Energy (MeV)
n + 235U
σn,f
Cross Section (barn)
Neutron Energy (MeV)



Cross Section (barn)
(n,f)
(n,nf)
+ (n,2nf)
1st
2nd
3nd
4th
5th
6th
^{239}U
+ ^{238}U
+ ^{237}U
+ (n,3nf)
+ (n,pf)
+ ^{236}U
+ ^{238}Pa
+ (n,4nf) + ^{235}U
+ (n,pnf) + ^{237}Pa
+ (n,αf) + ^{235}Th
+ ^{234}U
$\sigma_{n,f}$
n + ^{236}U
Neutron Energy (MeV)
n + ^{235}U
$\sigma_{n,f}$
Cross Section (barn)
Neutron Energy (MeV)


Cross Section (barn)
1st
2nd
3nd
4th
5th
6th
(n,f)
+ (n,nf)
+ (n,2nf)
+ (n,3nf)
+ (n,pf)
+ (n,4nf)
+ (n,pnf)
+ (n,αf)
239U
+ 238U
+ 237U
+ 236U
+ 238Pa
235U
235Th
234U
n + 236U
σn,f
Neutron Energy (MeV)
n + 235U
σn,f
Cross Section (barn)
Neutron Energy (MeV)
n + U4
U5

Coherent fission cross sections With microscopic ingredients

HFB-14 predictions of fission barriers and NLD at saddle points, including renormalization (max 5 parameters) of

- fission path height: $B_f'(\beta_2) = B_f(\beta_2) \times v_{corr}$
- NLD at 1st and 2d saddle points:

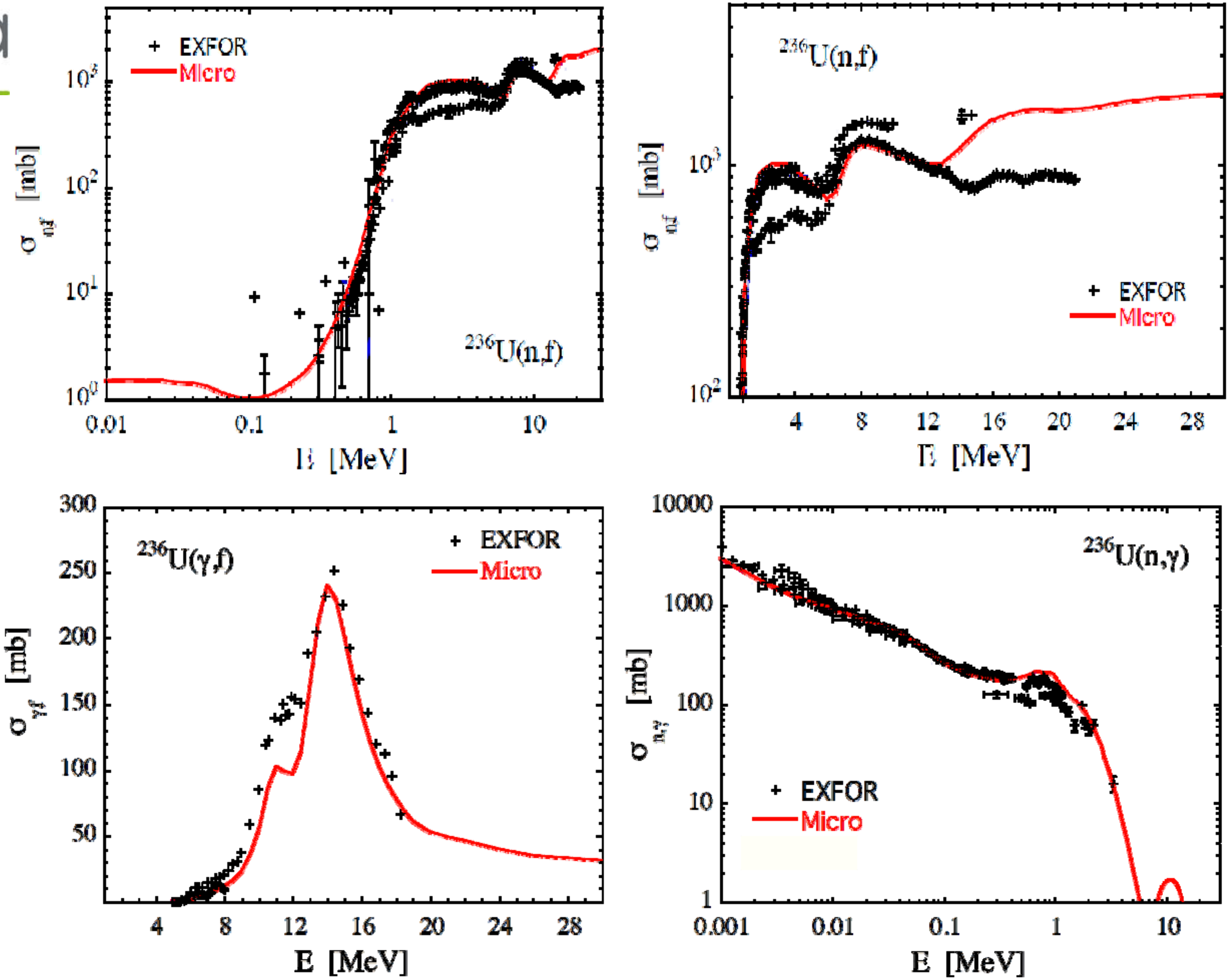
$$\rho'(U,J,P) = \rho(U-\delta,J,P)e^{\alpha\sqrt{U-\delta}}$$

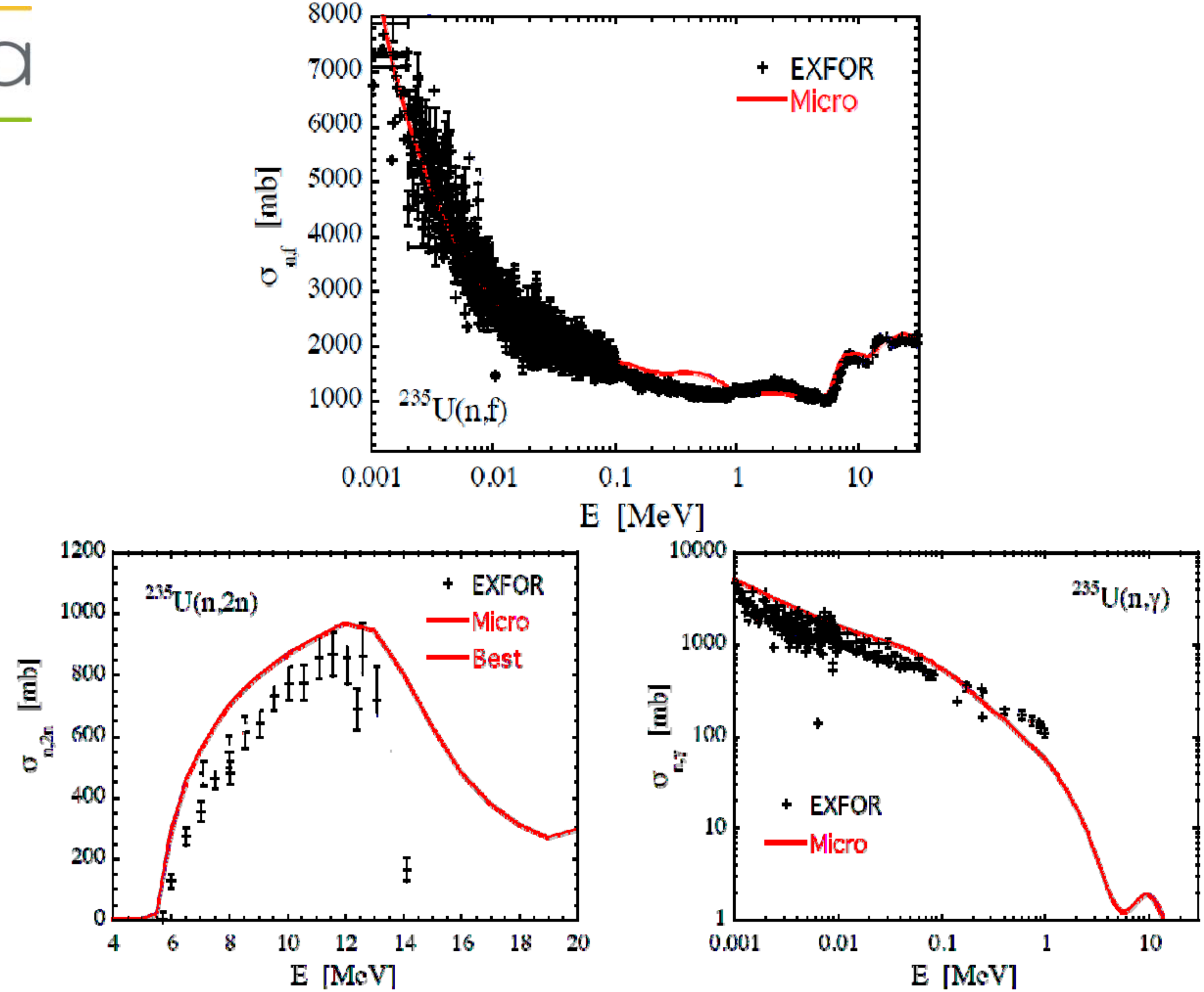
Additional nuclear inputs:

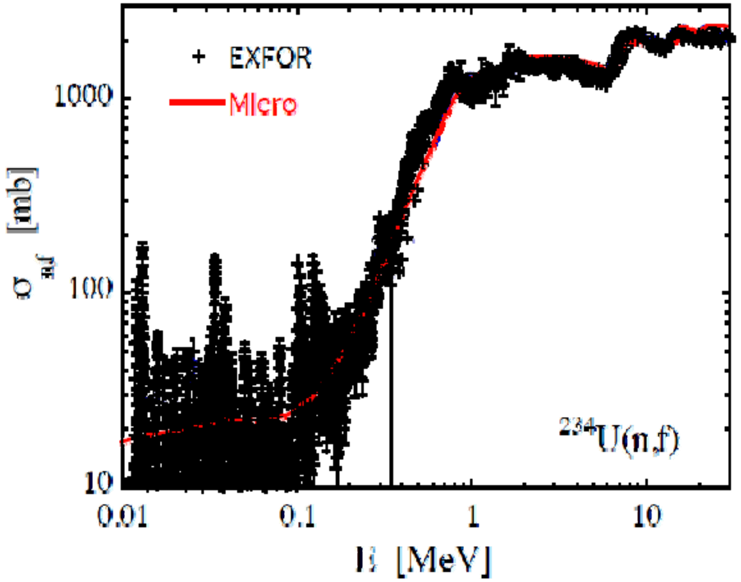
- Nuclear structure properties: HFB-14 (Goriely et al. 2007)
- Optical potential: Soukhovitskii et al. (2004)
- γ-ray strength: Hybrid model (Goriely, 1998)
- NLD: HFB-14 plus combinatorial model (Goriely et al., 2008) normalized on s-wave spacings and discrete excited levels

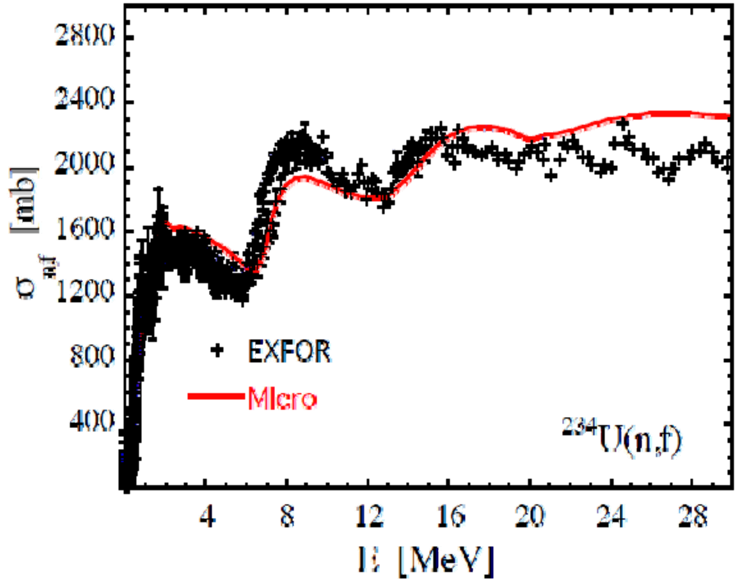
Note:

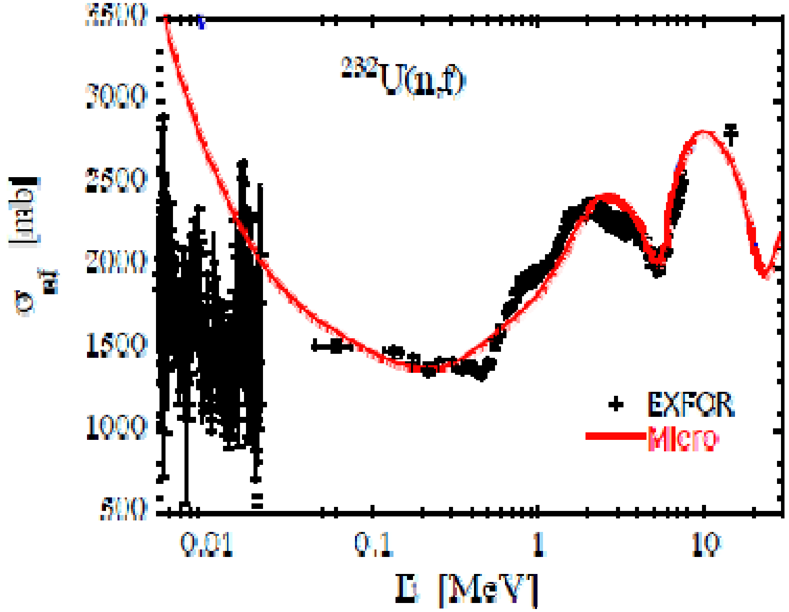
- 1 UNIQUE set of nuclear ingredients for all U isotopes
- no class 2 states included
- no discrete transition states included


EXFOR
Micro
236U(n,f)
σ n,f [mb]
E [MeV]
236U(n,f)
EXFOR
Micro
σ n,f [mb]
E [MeV]
236U(γ,f)
EXFOR
Micro
σ γf [mb]
E [MeV]
236U(n,γ)
EXFOR
Micro
σ n,γ [mb]
E [MeV]


EXFOR
Micro
235U(n,f)
σn,f [mb]
E [MeV]
235U(n,2n)
EXFOR
Micro
Best
σn,2n [mb]
E [MeV]
235U(n,γ)
EXFOR
Micro
σn,γ [mb]
E [MeV]


EXFOR
Micro
1000
100
10
0.01
0.1
1
10
E [MeV]
σ n,f [mb]
234U(n,f)


2800
2400
2000
1600
1200
800
400
EXFOR
Micro
4
8
12
16
20
24
28
E [MeV]
σ n,f [mb]
234U(n,f)


232U(n,f)
3000
2500
2000
1500
1000
500
EXFOR
Micro
0.01
0.1
1
10
E [MeV]
σ n,f [mb]

Conclusions and prospects

- ***Cross section modeling quite easy for non fissile nuclei***

  Microscopic or Phenomenological OMP, Γ_γ, LDs

  ⇒ full microscopic calculation for non fissile nuclei almost possible

- ***Difficult cross section modeling for fissile nuclei***

- ***Web site opened in October 2006 : www.talys.eu***

  ⇒ All microscopic ingredients mentionned included in the distribution

Conclusions and prospects

- ***New level densities for pre-equilibrium (done but not tested)***
- ***JLM OMP : spherical (OK) – deformed (soon)***
- ***Neutron multiplicities from FF decay (under dev.)***
- ***Microscopic ingredients with Gogny instead of Skyrme (under dev.)***