The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

1944-6

Joint ICTP-IAEA Workshop on Nuclear Reaction Data for Advanced Reactor Technologies

19 - 30 May 2008

Statistical Nuclear Reaction Modeling. DIF/DPTA/SPN/LMED

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Statistical Nuclear Reaction Modeling

DIF/DPTA/SPN/LMED

S.Hilaire

Nuclear data needs

Nuclear data needed for

- Understanding basic reaction mechanism between particles and nuclei
- Astrophysical applications (Age of the Galaxy, element abundancies …)
- Existing or future nuclear reactors simulations
- Medical applications, oil well lodging, wastes transmutation …

But

- Finite number of experimental data (price, safety or counting rates)
- Complete measurements restricted to low energies (< 1 MeV)

Predictive Nuclear models (codes) essential

Content

- Why and for whom ?
- How ?
- Modern methods
- Few realistic examples
- Future developments

1st PART

Why and for whom ?

Why and for whom ?

- What does the final product look like ?
- What does it contain ?
- What is it used for ?
- Why do we need to perform evaluations ?

Portion of a evaluated file
(FORMAT ENDF)

Target identification (^{151}Sm)

Target mass

Content nature (σ)

```
 6.215100+4 1.496234+2          0          0          0          06210 3 16  350
-5.596445+6-5.596445+6          0          0          1       1336210 3 16  351
        133          2                                           6210 3 16  352
 5.633849+6 0.000000+0 5.700000+6 1.580180-3 5.800000+6 6.073681-36210 3 16  353
 5.900000+6 1.347960-2 6.000000+6 2.690410-2 6.100000+6 4.687551-26210 3 16  354
 6.200000+6 7.598900-2 6.300000+6 1.119810-1 6.400000+6 1.518520-16210 3 16  355
 6.500000+6 2.016680-1 6.600000+6 2.528690-1 6.700000+6 3.144490-16210 3 16  356
 6.800000+6 3.780410-1 6.900000+6 4.433380-1 7.000000+6 5.136740-16210 3 16  357
 7.100000+6 5.833550-1 7.200000+6 6.576591-1 7.300000+6 7.306390-16210 3 16  358
 7.400000+6 8.033710-1 7.500000+6 8.746620-1 7.600000+6 9.434911-16210 3 16  359
 7.700000+6 1.010920+0 7.800000+6 1.078550+0 7.900000+6 1.140340+06210 3 16  360
 8.000000+6 1.202710+0 8.100000+6 1.257750+0 8.200000+6 1.313880+06210 3 16  361
 8.300000+6 1.367080+0 8.400000+6 1.416210+0 8.500000+6 1.463580+06210 3 16  362
 8.600000+6 1.506400+0 8.700000+6 1.546900+0 8.800000+6 1.586770+06210 3 16  363
 8.900000+6 1.623670+0 9.000000+6 1.656720+0 9.100000+6 1.687830+06210 3 16  364
 9.200000+6 1.717430+0 9.300000+6 1.745200+0 9.400000+6 1.771480+06210 3 16  365
 9.500000+6 1.796050+0 9.600000+6 1.817200+0 9.700000+6 1.837390+06210 3 16  366
 9.800000+6 1.858090+0 9.900000+6 1.876590+0 1.000000+7 1.893530+06210 3 16  367
```

Values

Number of values

Material number

Content type (n,2n)

Content of an evaluated file

- General Informations (authors, method used, date, version, etc …)
- Resonances parameters
- Cross sections
  - Integrated, spectra and angular distribution, doubly differential
  - (n,f), (n,γ), (n,n'), (n,p), (n,d), …, (n,2n), …,(n,2nα), (n,pα), ……….
- Decay schemes
- Multiplicities
- Uncertainties, Covariance data

What is it used for ?

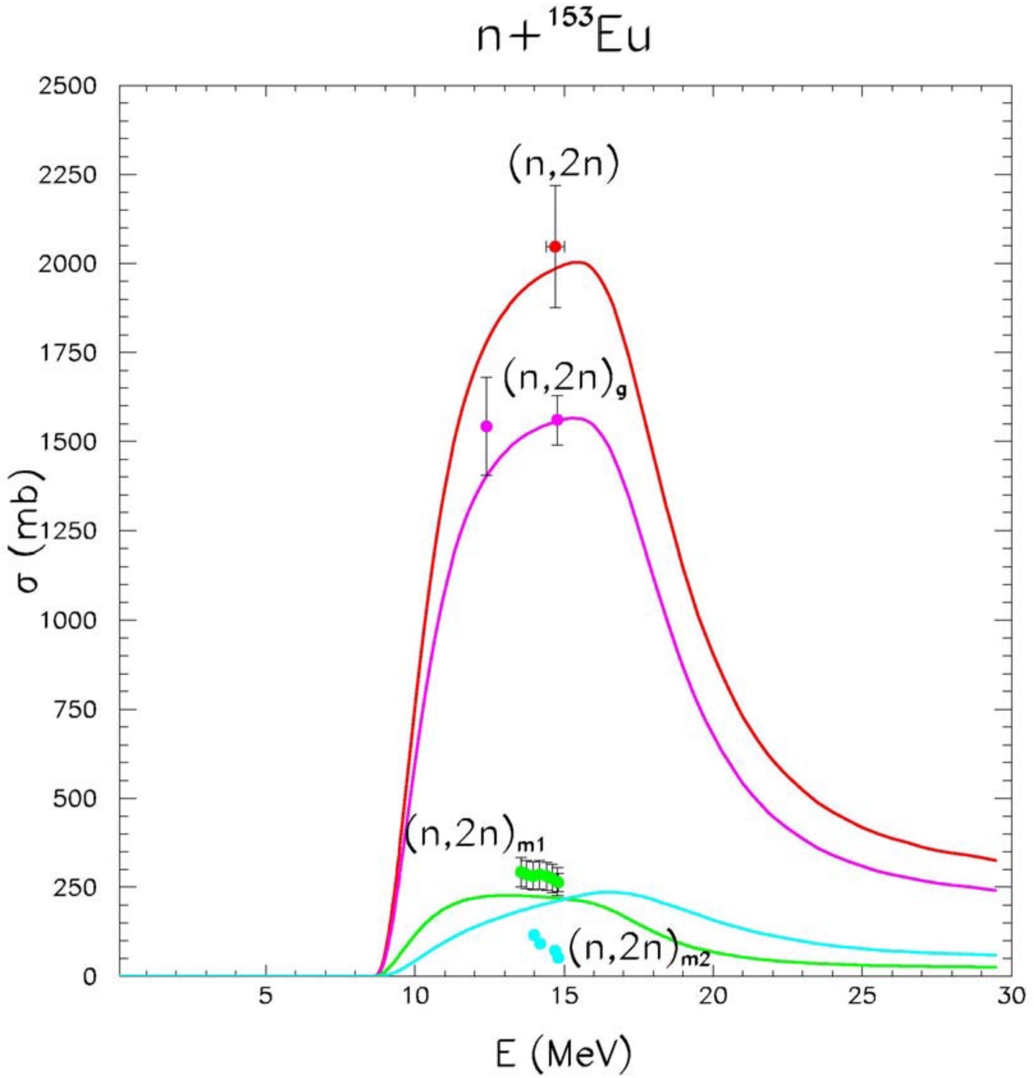
- Produce nuclear data libraries
  - (ENDF, CENDL, BROND, JENDL, JEFF)
- Feed codes with evaluated nuclear «constants»
  - Non-proliferation and lugage scan
  - Nuclear power plants (classical or new generation)
  - Electronic damage (space)
  - Radiotherapy
  - Geology (oil well logging, …)
  - Non-destructive control
  - Fuel cycle, waste management …

Why do we need data evaluations ?

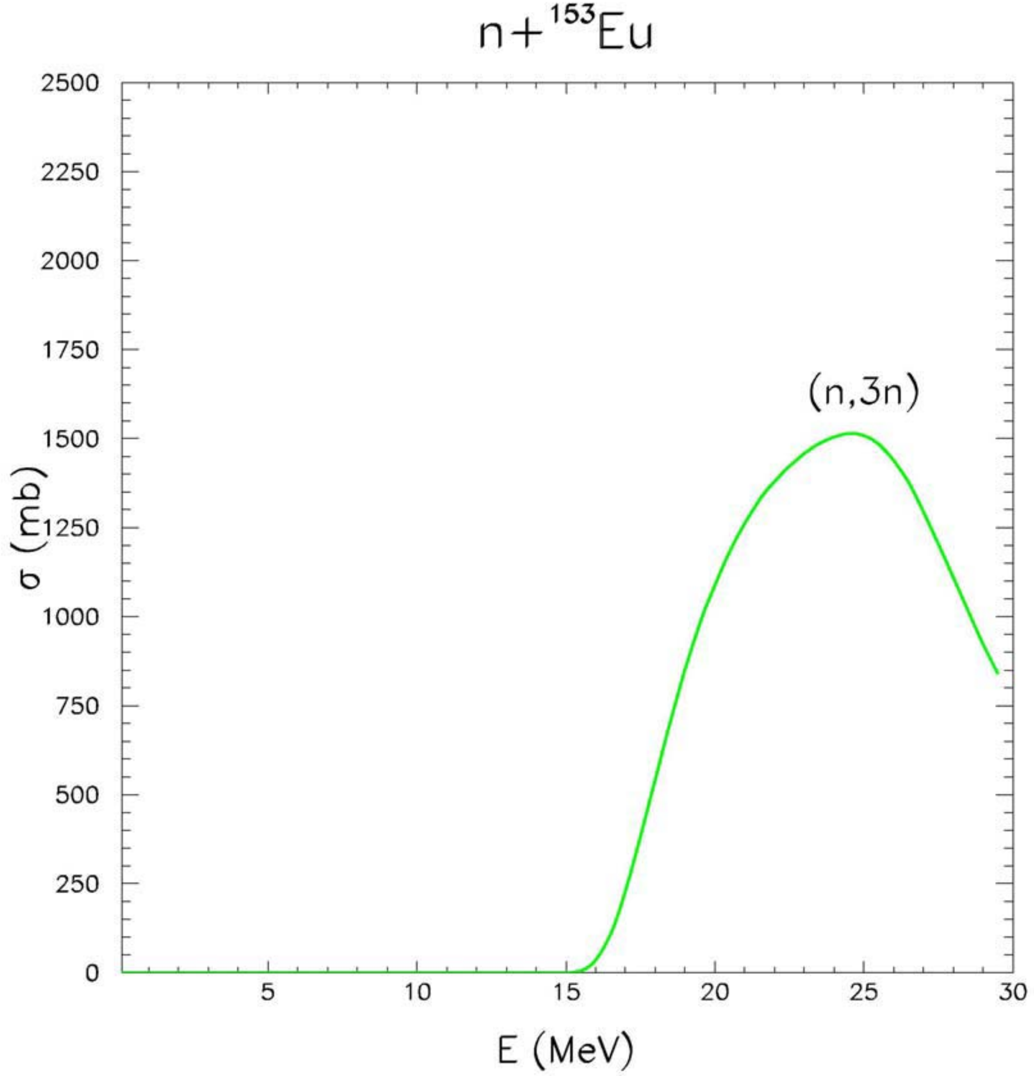
Problems due to microscopic data

- Too few or no experimental data

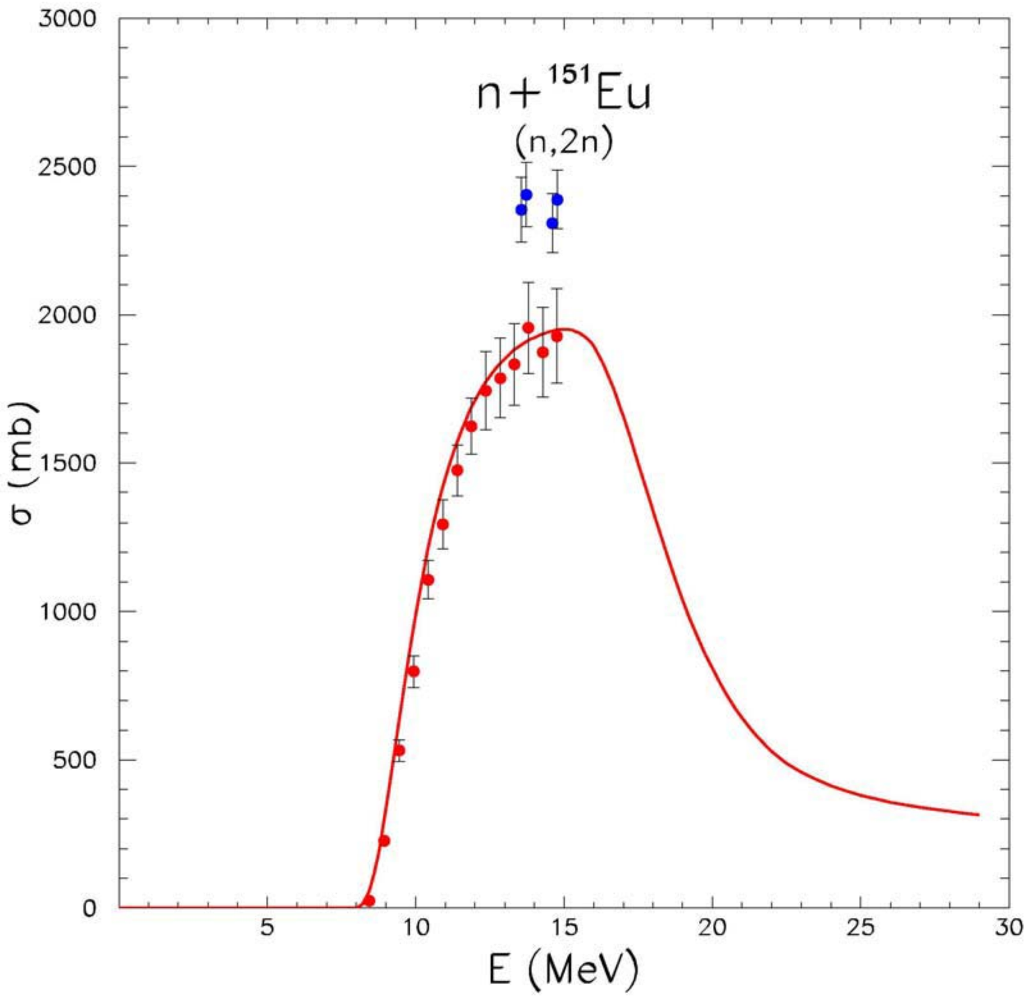
Too few experimental data



No experimental data



Incoherent experimental data



Bad description of integral experiment

Benchmark JEZEBEL ^{240}Pu

CRITICAL SPHERE

Atomic composition

^{239}Pu	73.8 %
^{240}Pu	19.4 %
^{241}Pu	3.00 %
^{242}Pu	0.40 %
Ga	3.40 %

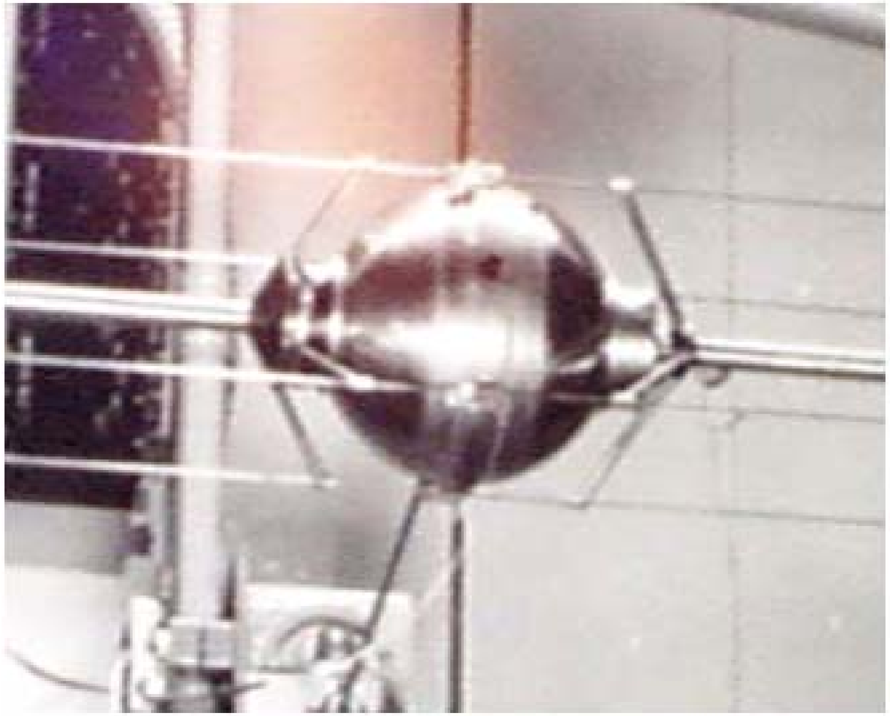
Geometry

M = 19.46 ± 0.156 Kg
ρ = 15.73 g/cm^3
R = 6.66 cm

K effectif

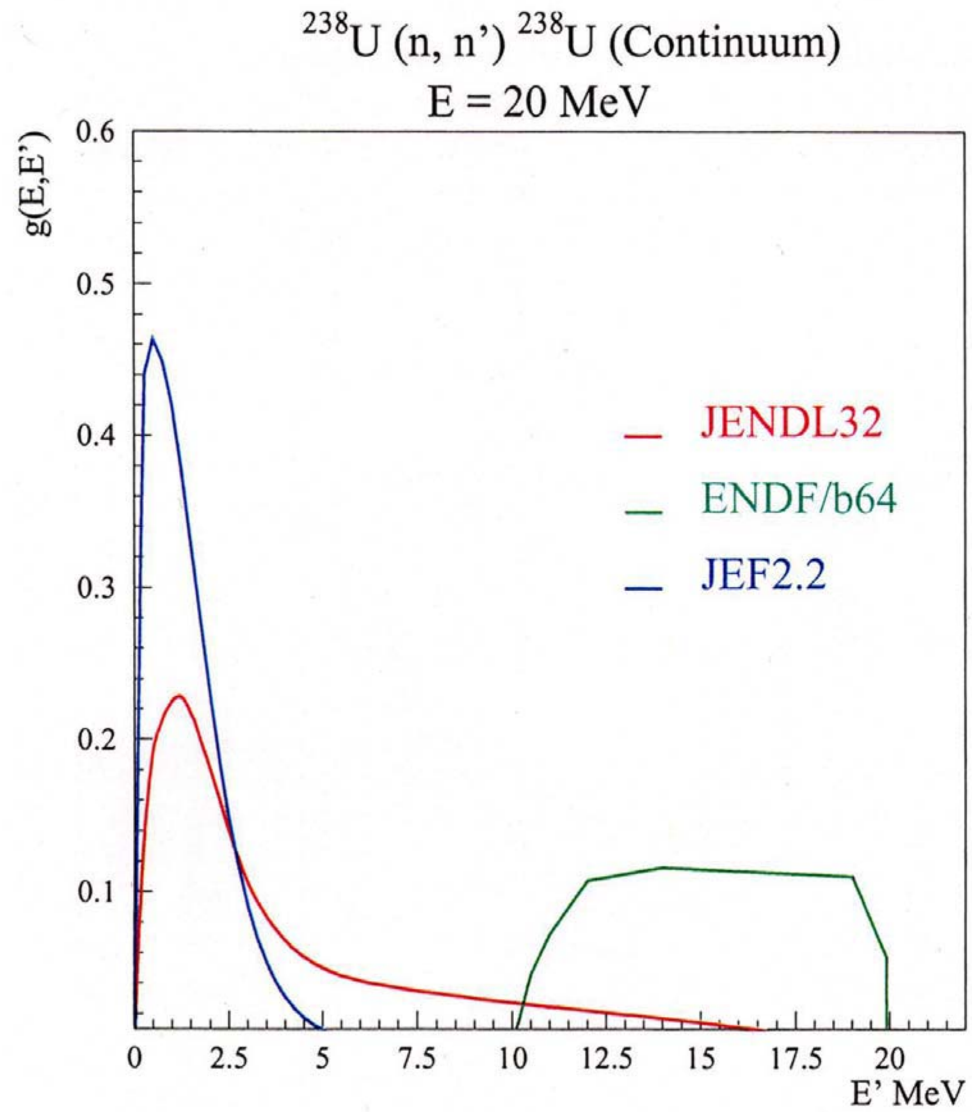
1.00000 ± 0.002

SIMULATION

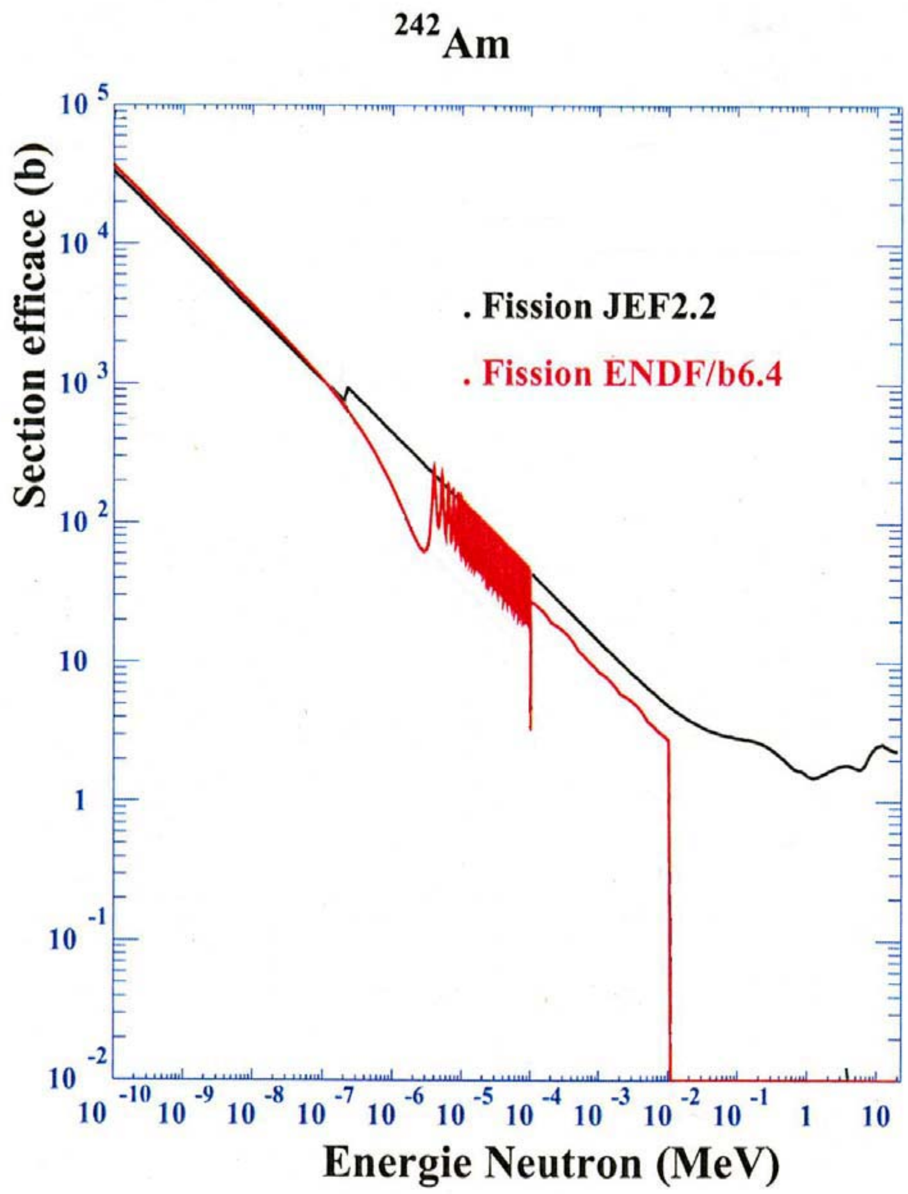


JENDL3.3	1.00341 ± 0.00110

Bad evaluations



Partial evaluations



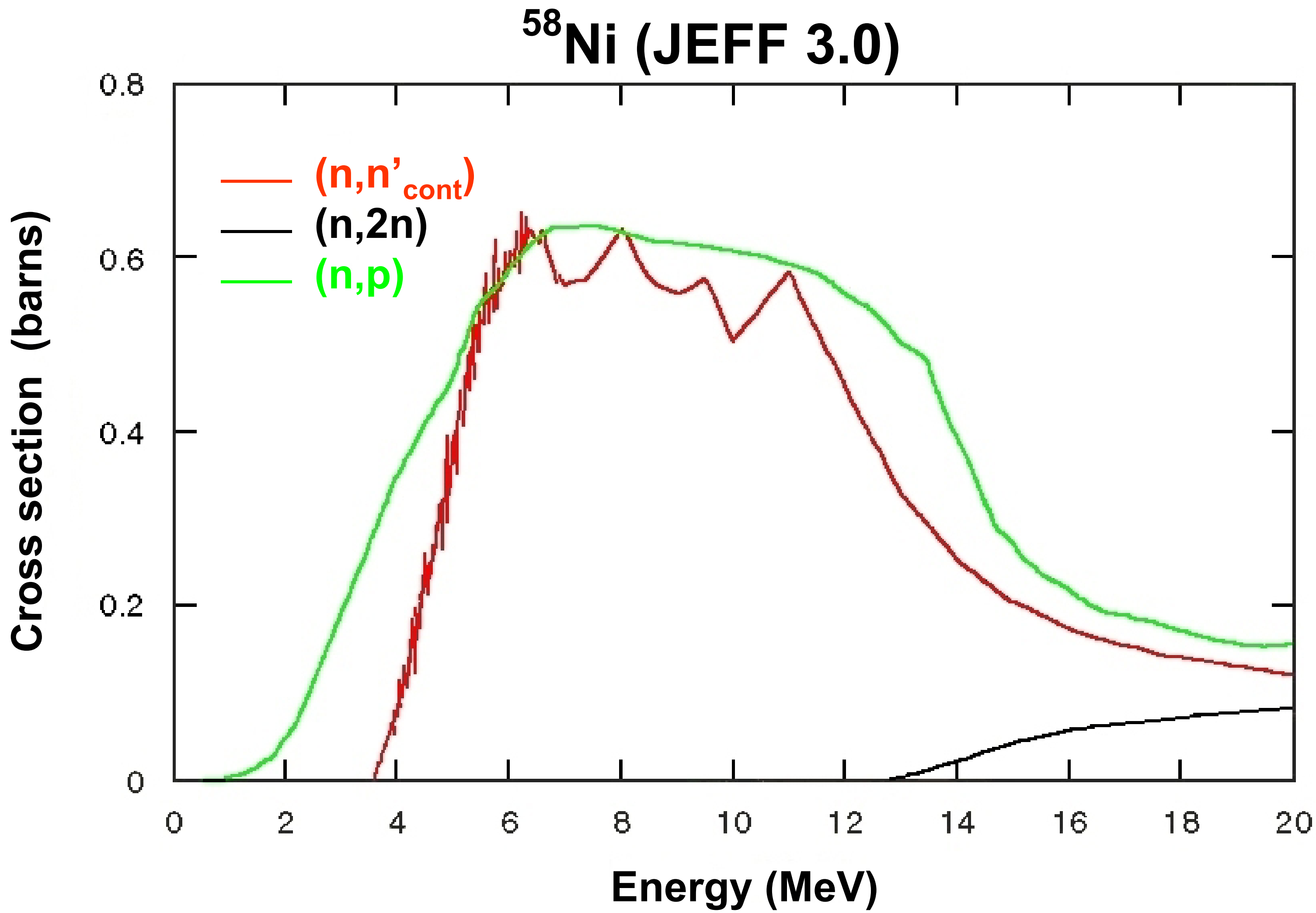
2nd PART

How ?

How ?

- Experimental data interpolation
- Bayesian methods
- Renormalisations of existing evaluations
- Copy/Paste of other evaluations
- Nuclear reaction modeling

Experimental data interpolation



Bayesian methods

- **Method :**

  Account for new experimental data to improve an existing evaluation without re-doing everything.

  Suppress crazy data points.

- **Advantages :**

  Provides variances & covariances simultaneously with the new evaluation.

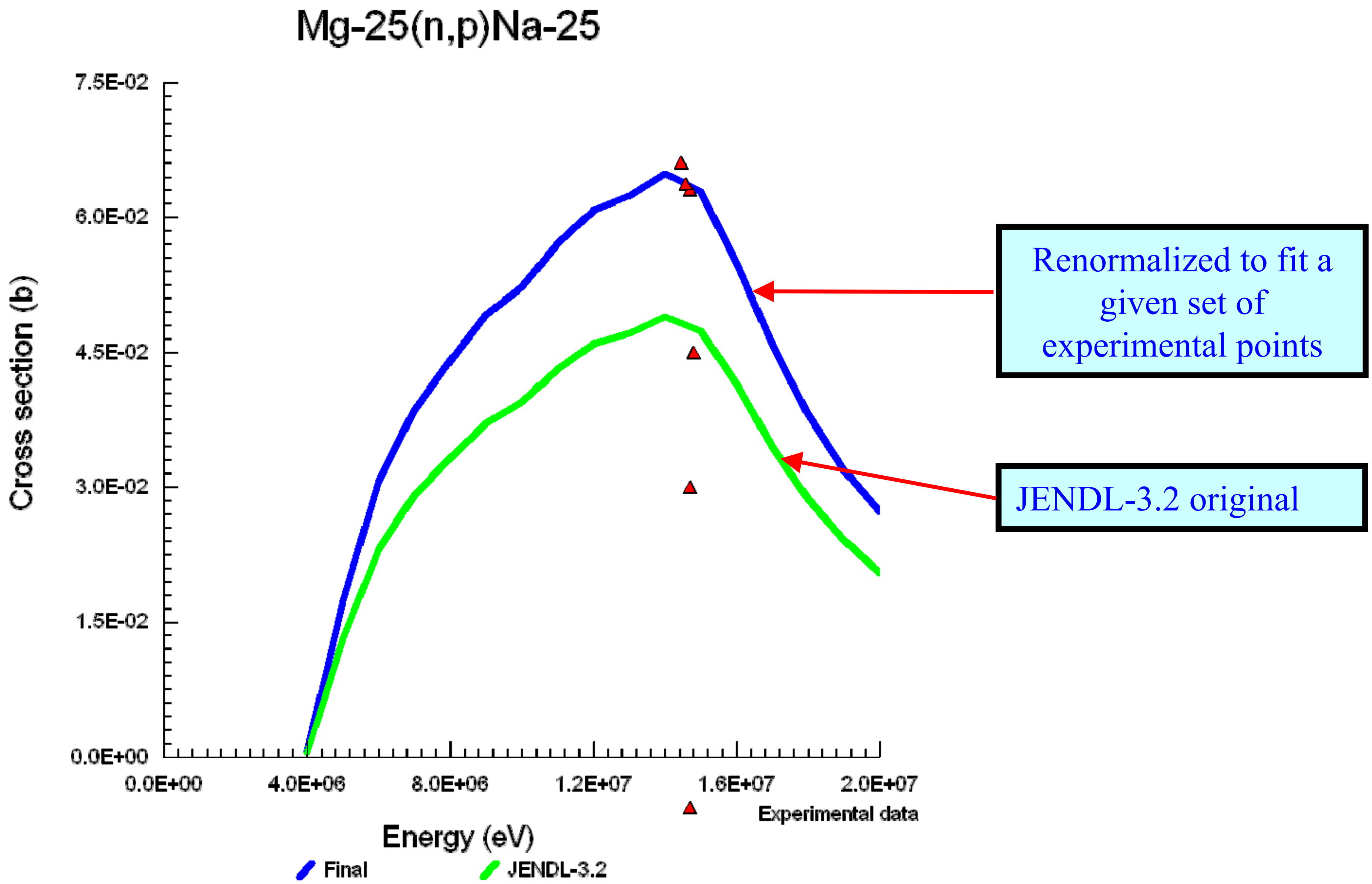
  Perfect agreement with the available experimental points.

- **Drawbacks :**

  A large quantity of experimental points are required.

  Depends on the choice of the « prior »

Renormalisations



Cut and Paste

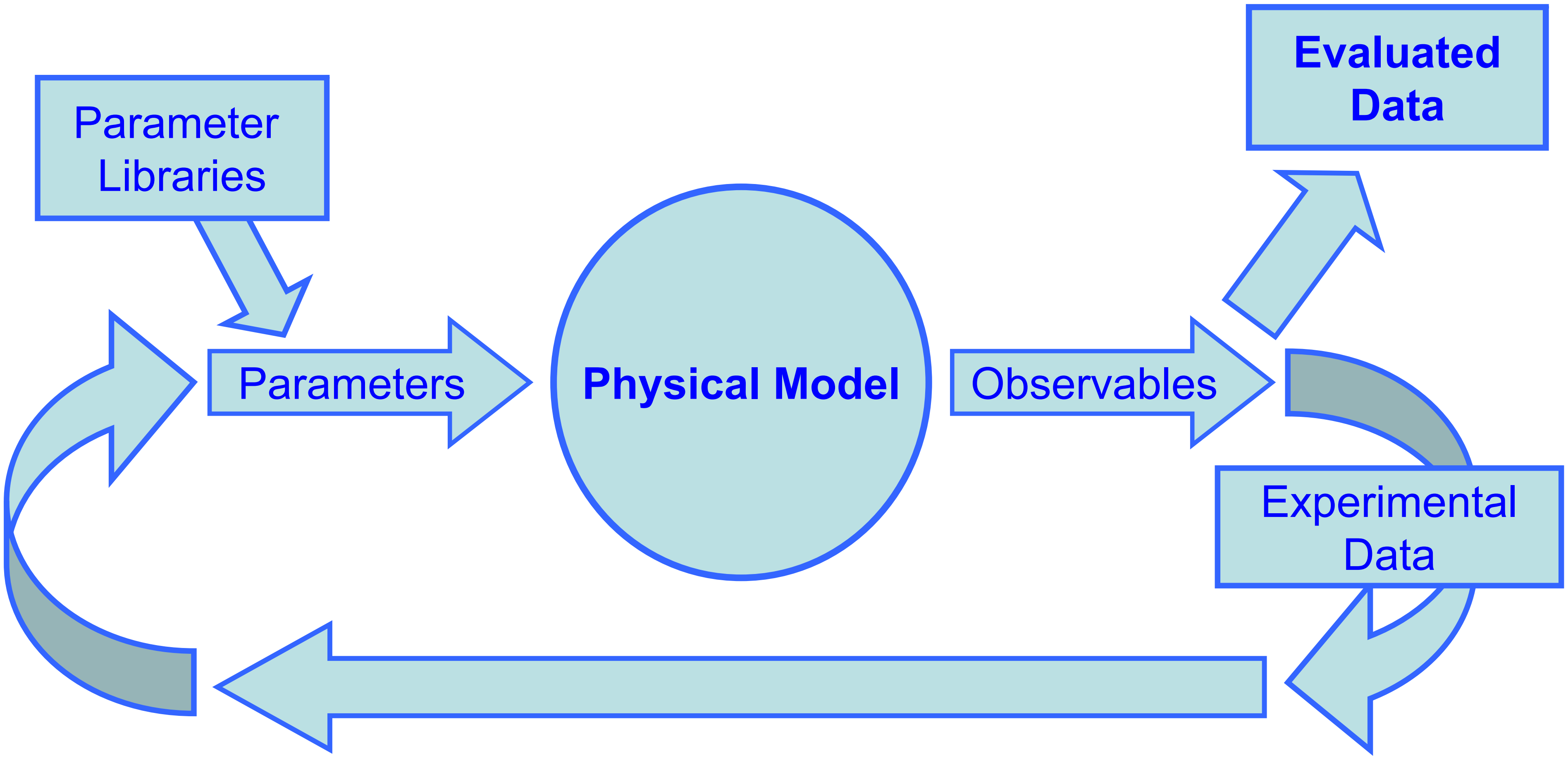
Á new evaluation can be restricted (only specific cross section are given) or only a given energy range is covered (ex: E > 1keV).

A complete evaluation is obtained by copiing selected parts from other evaluations correctly chosen

Expertise.

Nuclear Reaction Modeling

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

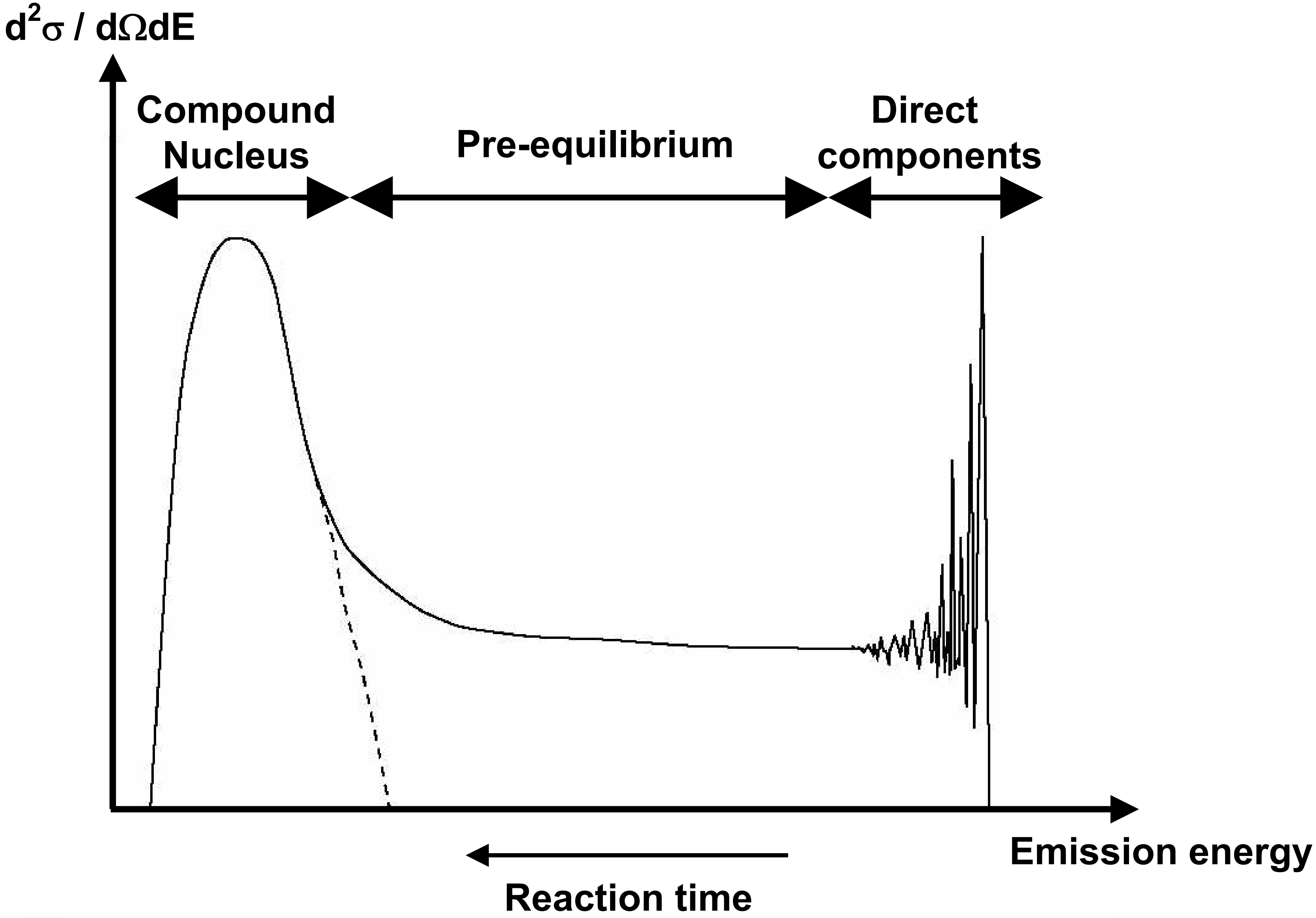


3rd PART

Nuclear Reaction Modeling

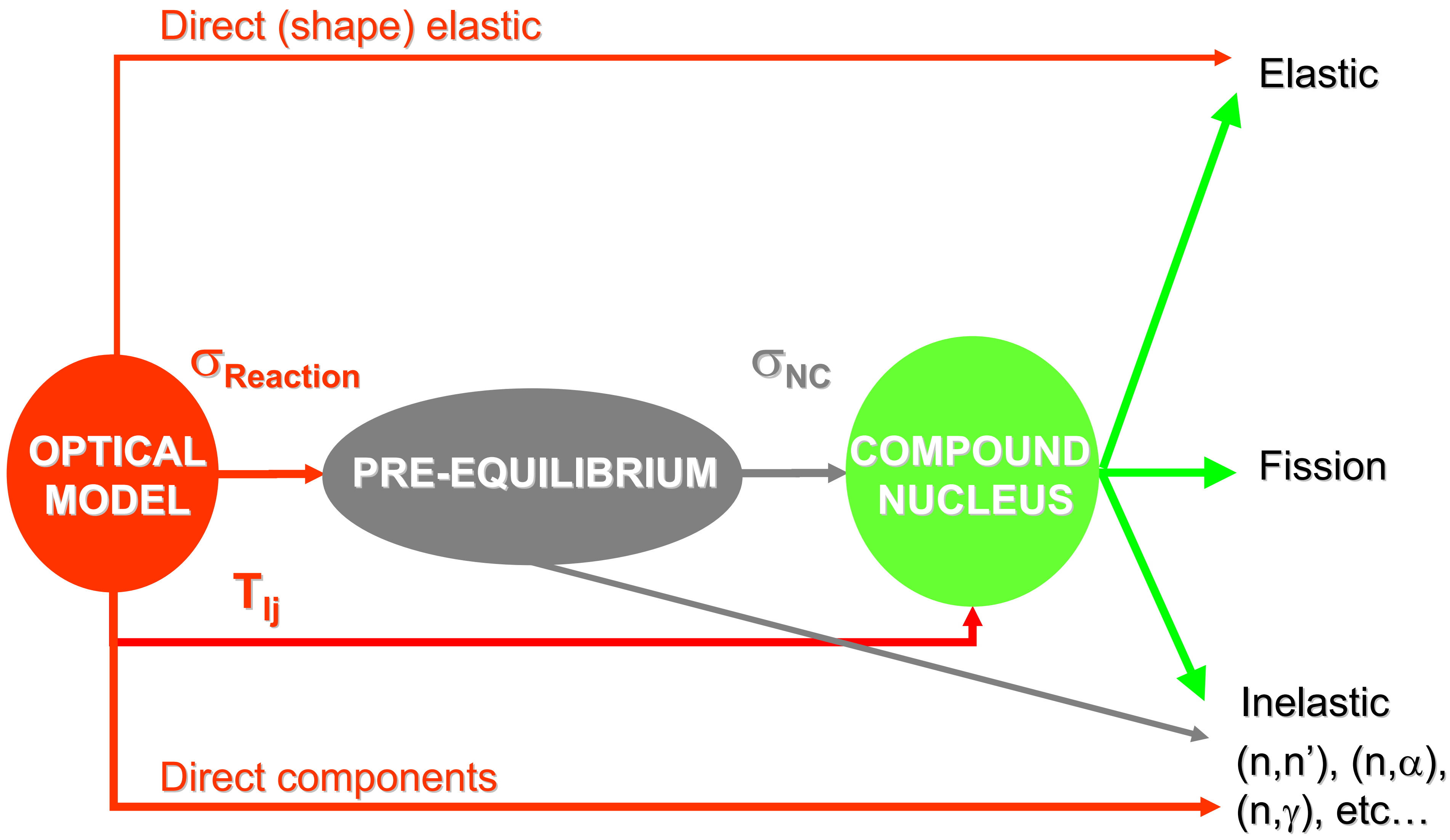
Nuclear Reaction Modeling

- **Models sequence**
- **Optical model and direct reactions**
- **Pre-equilibrium model**
- **Compound Nucleus model**
- **Fission**
- **Level densities**
- **Neutron multiplicities**
- **Uncertainties**



$d^2\sigma / d\Omega dE$
Compound Nucleus
Pre-equilibrium
Direct components
Emission energy
Reaction time

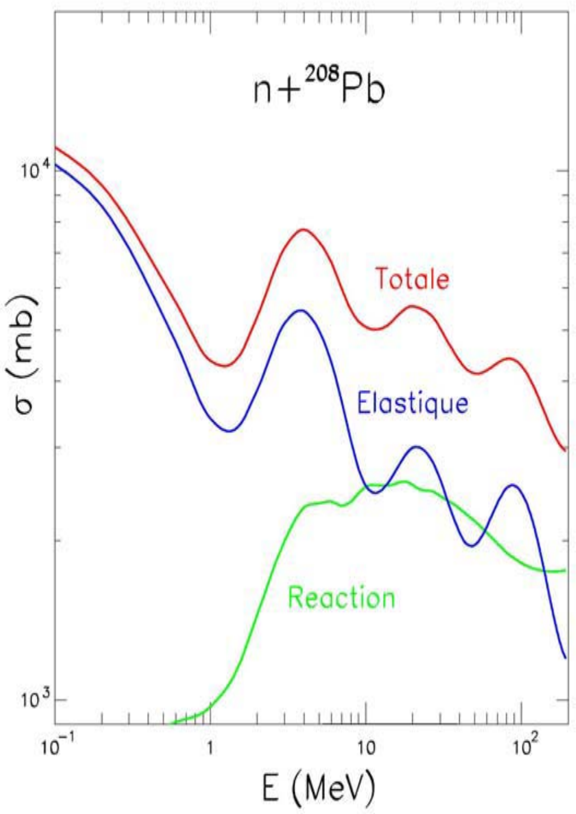
Models sequence



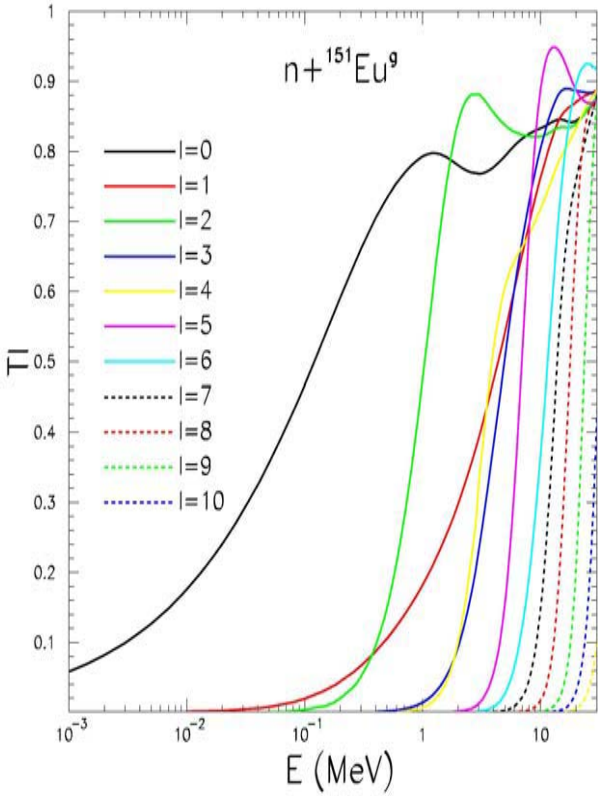
Optical model

This model yields :

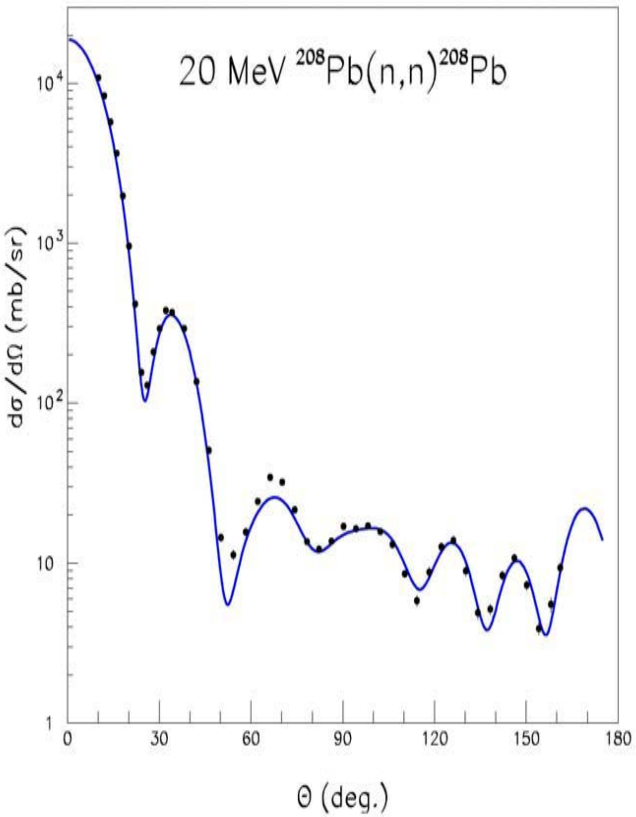
Integrated cross sections



Transmission coefficients



Angular distributions



Optical Model

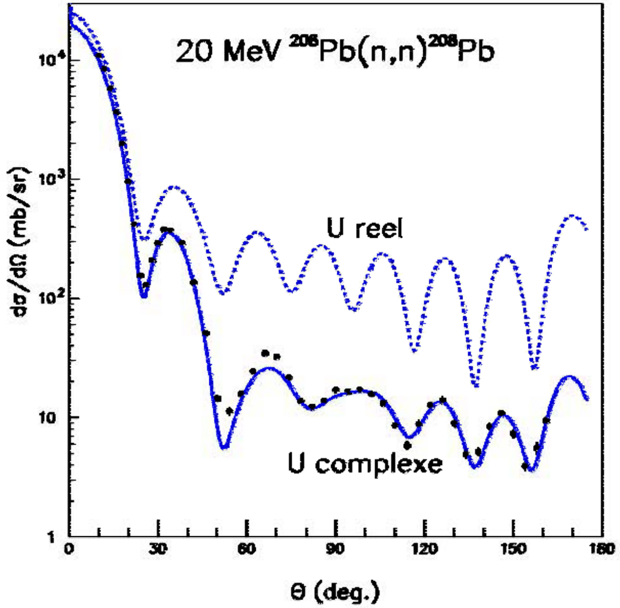
Direct interaction of a projectile with a target nucleus considered as a whole
Quantum model $\rightarrow$ Schrödinger equation

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

Complex potential:

$$U = V + iW$$

Refraction (V) — Absorption (iW)



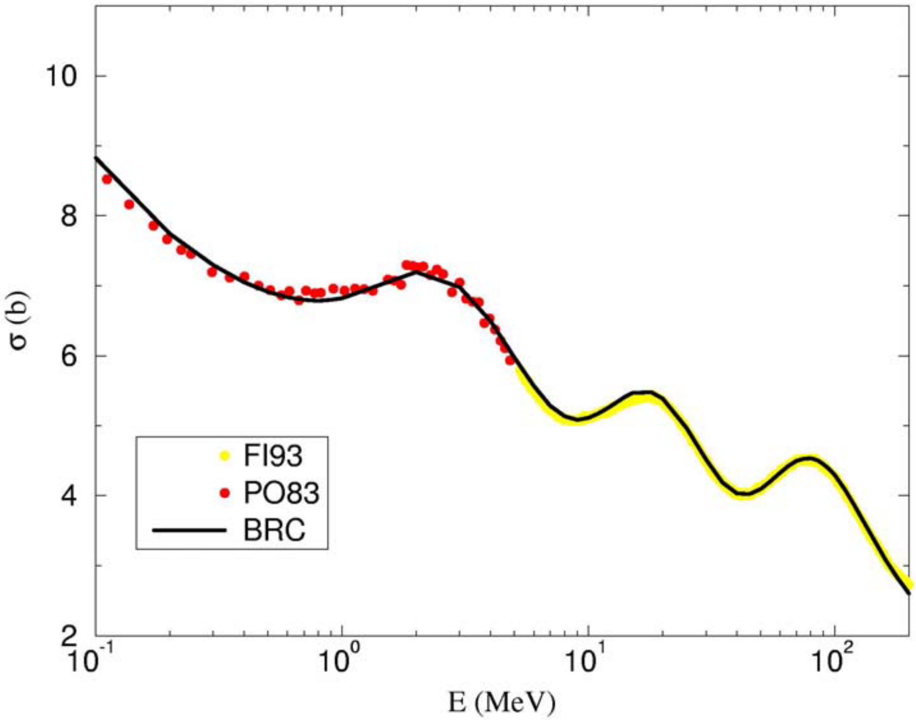
Two types of approaches

Phenomenologic

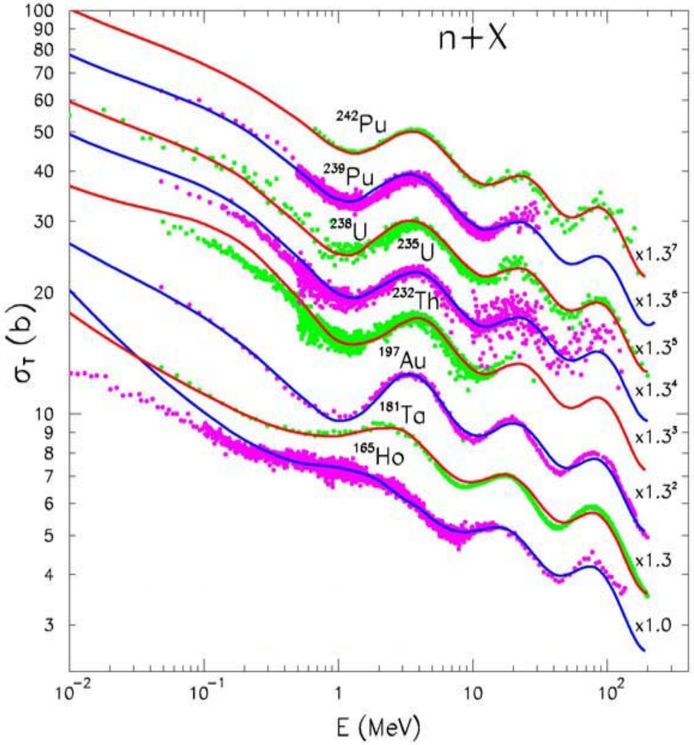
Adjusted parameters
Weak predictive power
Very precise (≈ 1%)
Important work

Microscopic

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

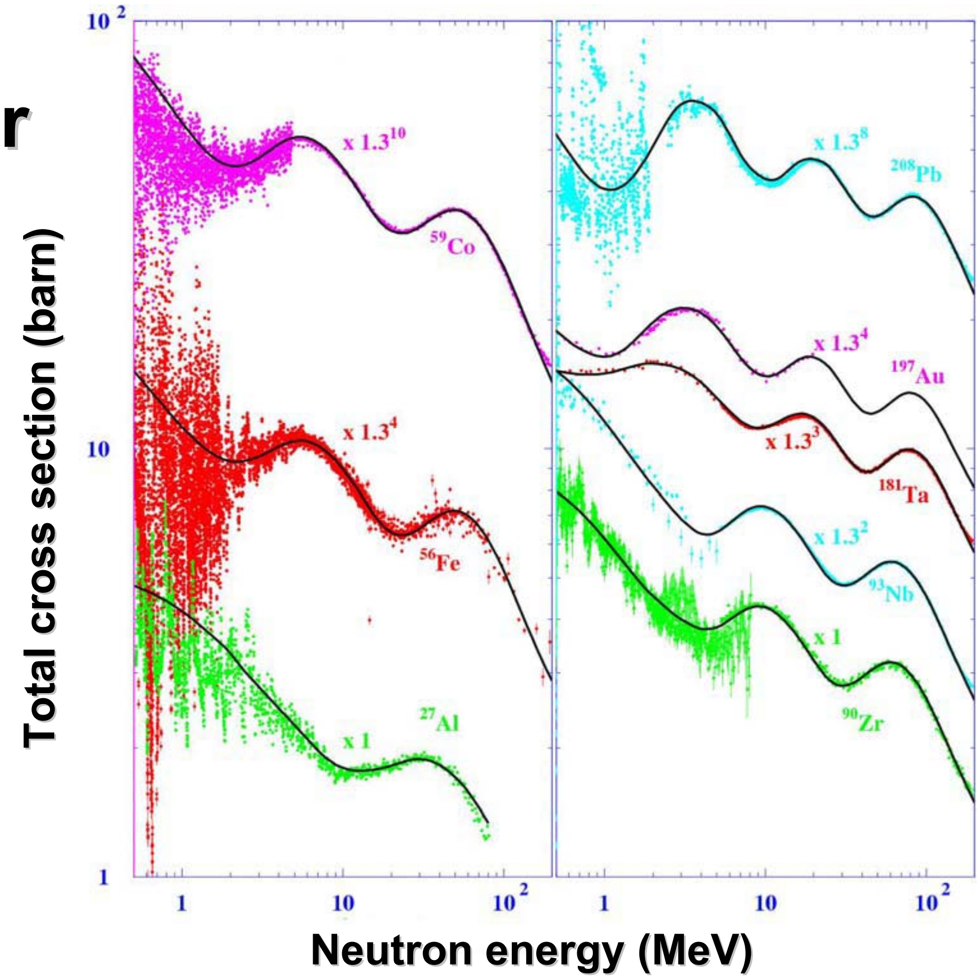


Total cross sections



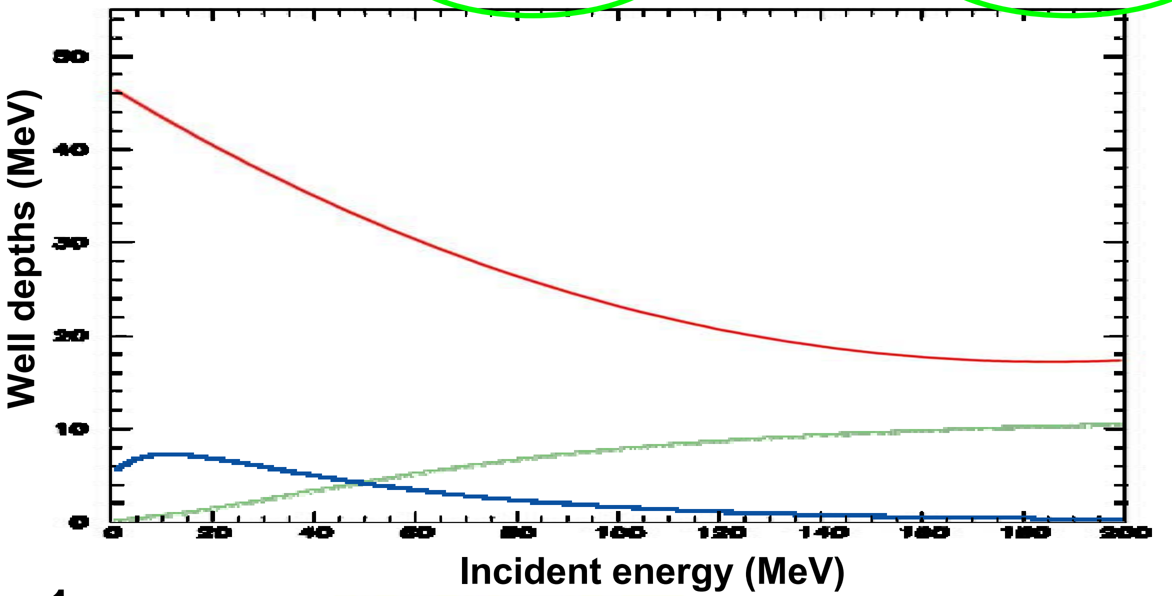
Phenomenologic optical model

- $\approx$ 20 adjusted parameters
- Very precise (1%)
- Weak predictive power

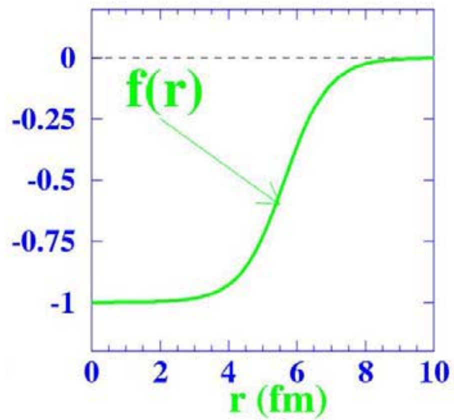


Phenomenologic optical model

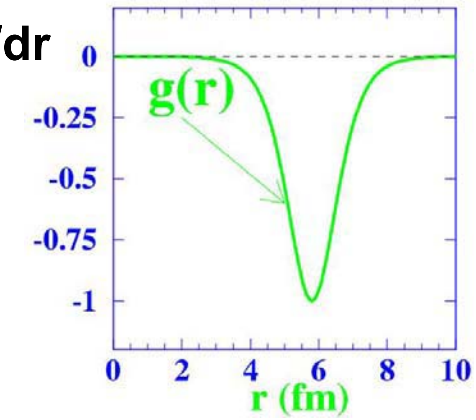
$$U(r,E) = \left[V_V(E)\, f(r,R_V,a_V) + V_S(E)\, g(r,R_S,a_S) \right]$$
$$+\, i \left[W_V(E)\, f(r,R_V,a_V) + W_S(E)\, g(r,R_S,a_S) \right]$$



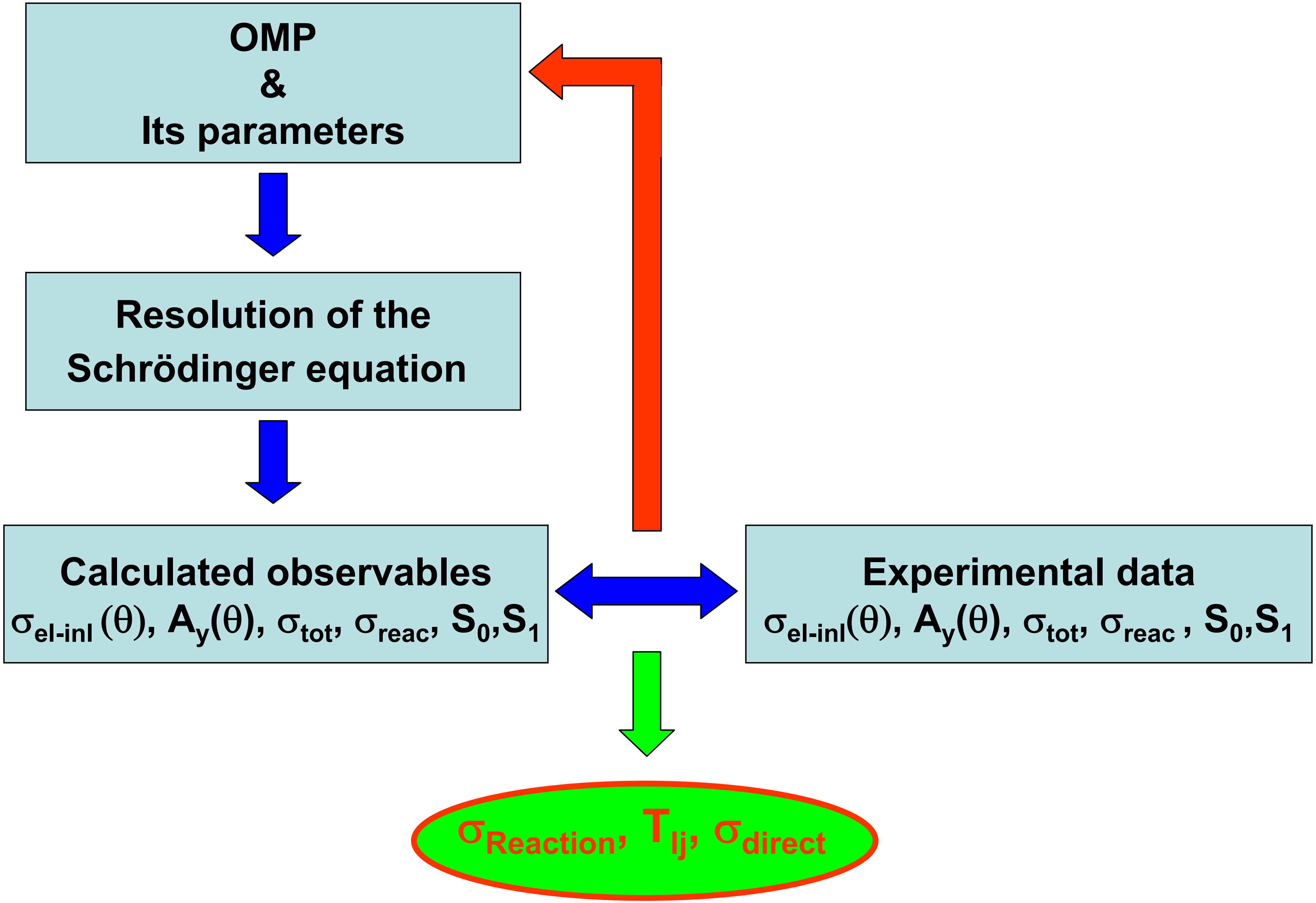
$$f(r,R,a) = \frac{-1}{1+\exp((r-R)/a)}$$



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



Phenomenologic optical model

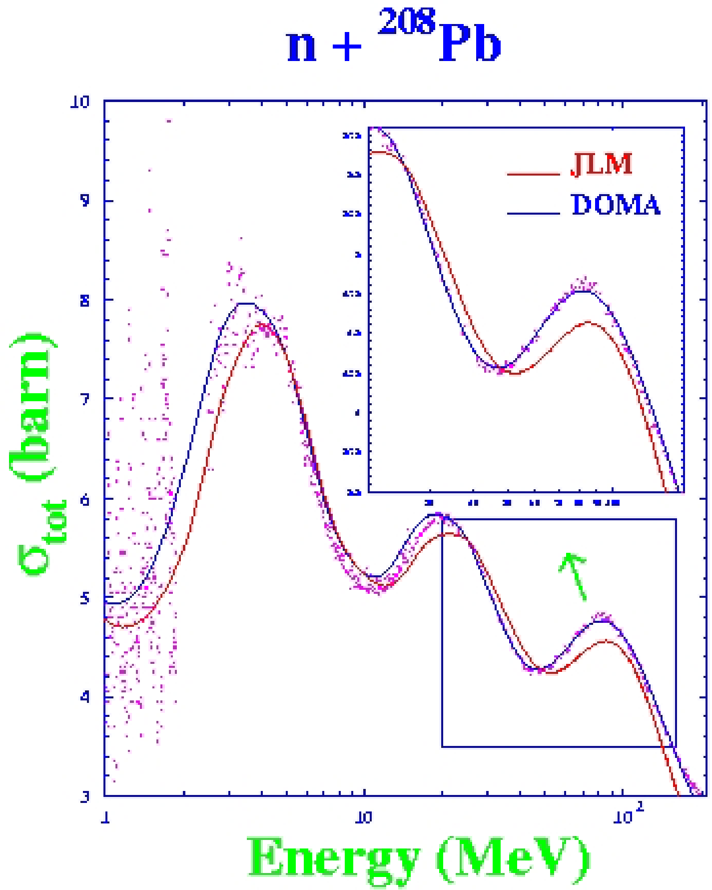


Semi-microscopic optical model

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

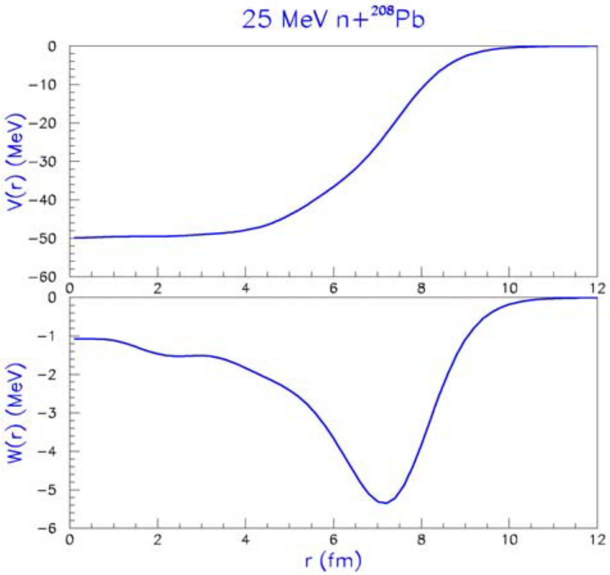
⇒ usable for any nucleus

- **Less precise than the phenomenological approach**



Semi-microscopic optical model

Optical potential = **Effective Interaction** ⊗ **Radial densities**



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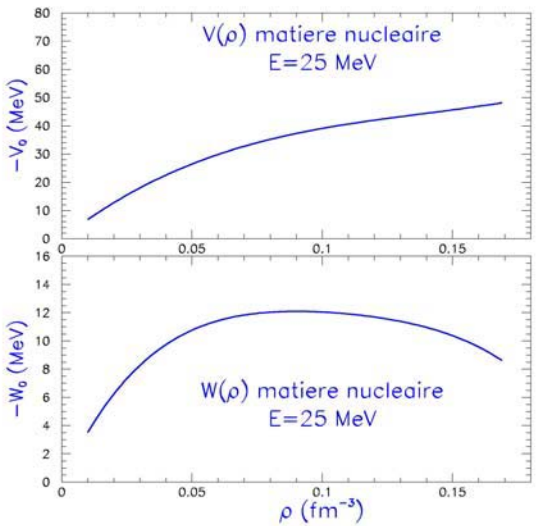
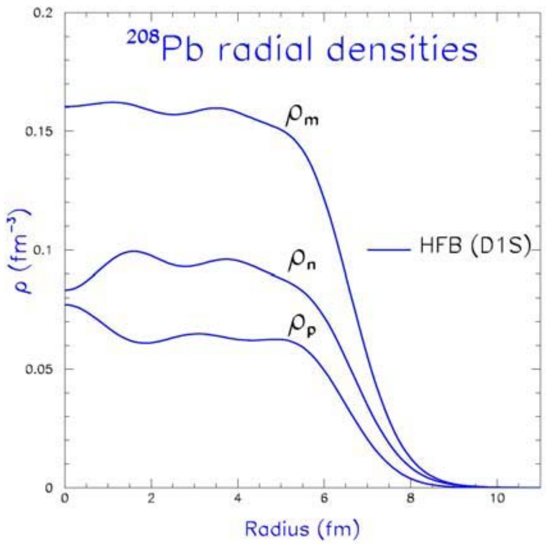


⊗

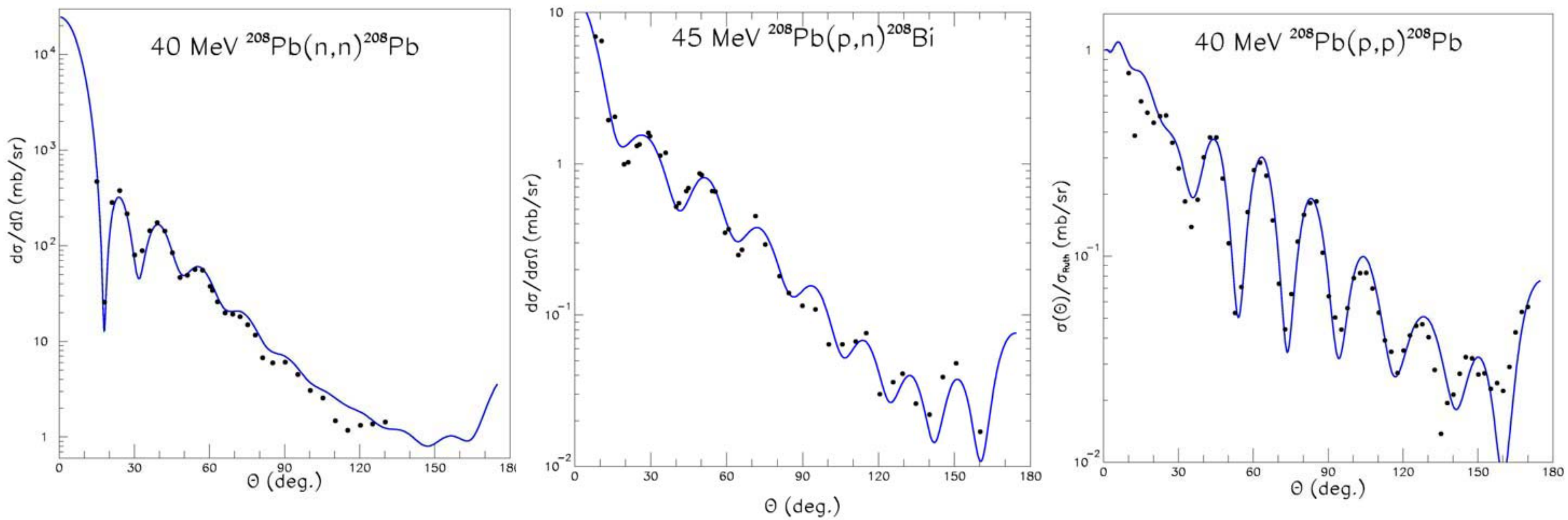


$$\mathbf{U(r,E)} = \frac{\mathbf{U(\rho(r'),E)}}{\mathbf{\rho(r')}} \otimes \mathbf{\rho(r)}$$

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

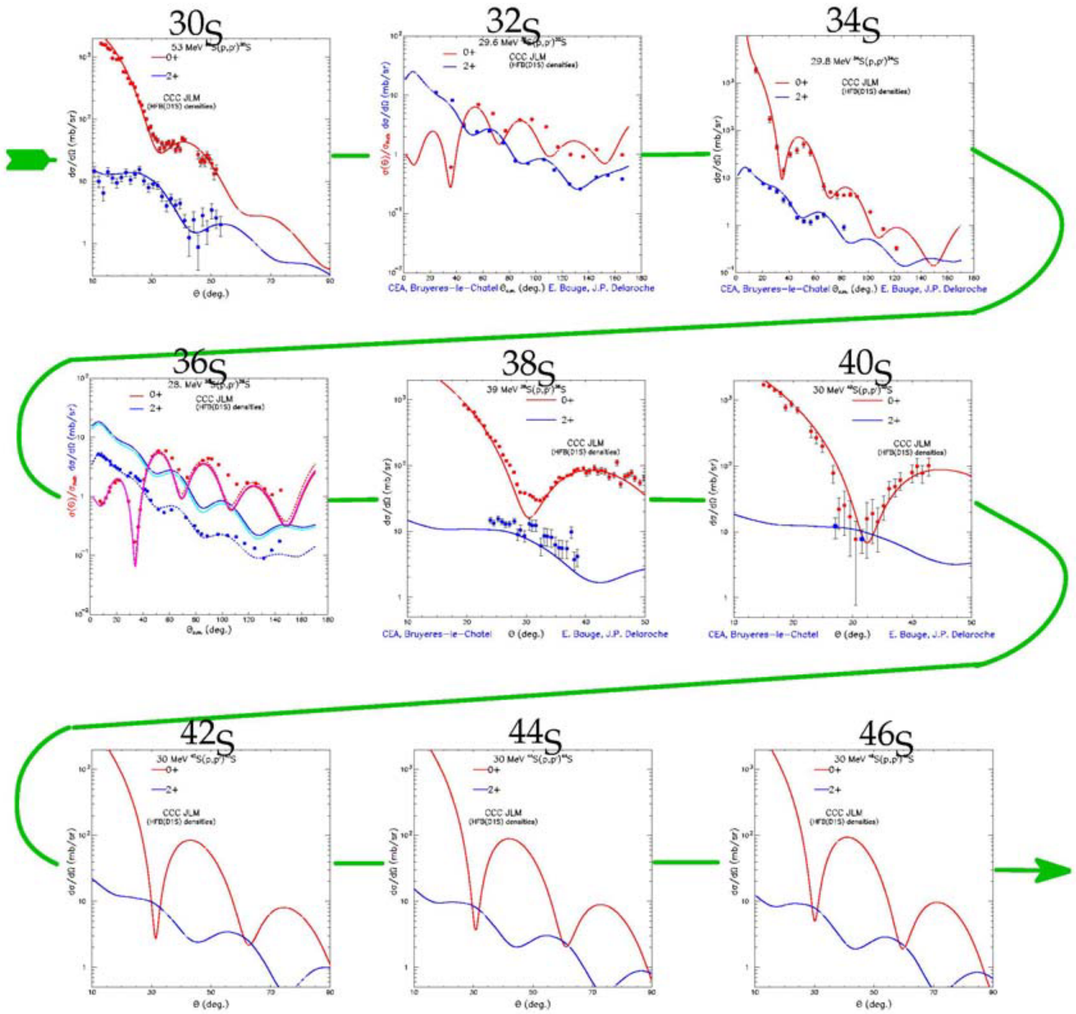
Semi-microscopic optical model

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

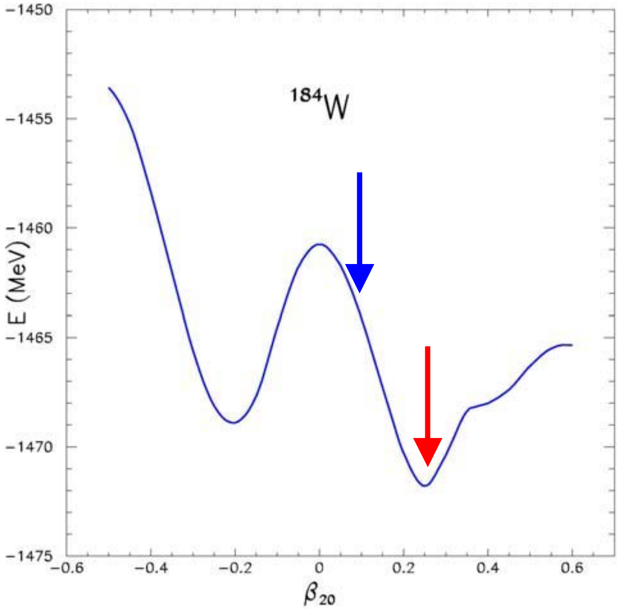


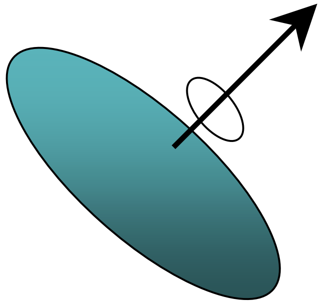
Semi-microscopic optical model

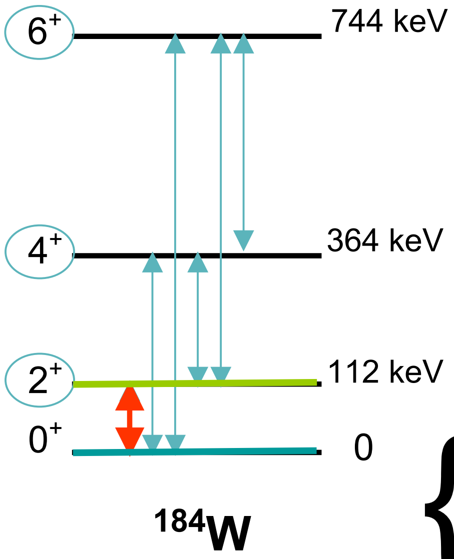
Enables to perform predictions for very exotic nuclei for which There exist no experimental data

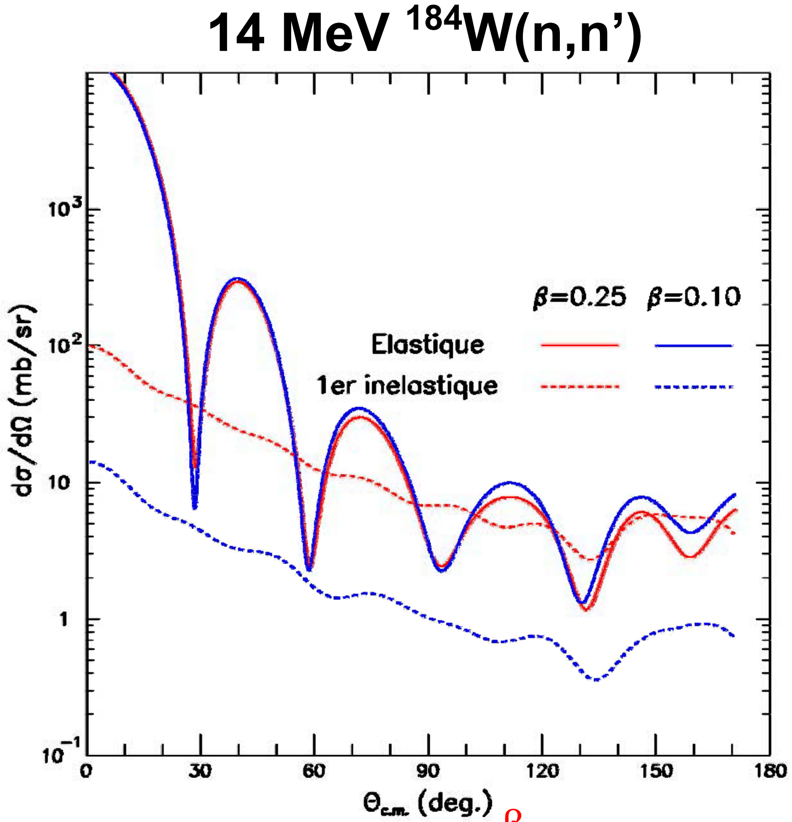


Impact of coupled channels



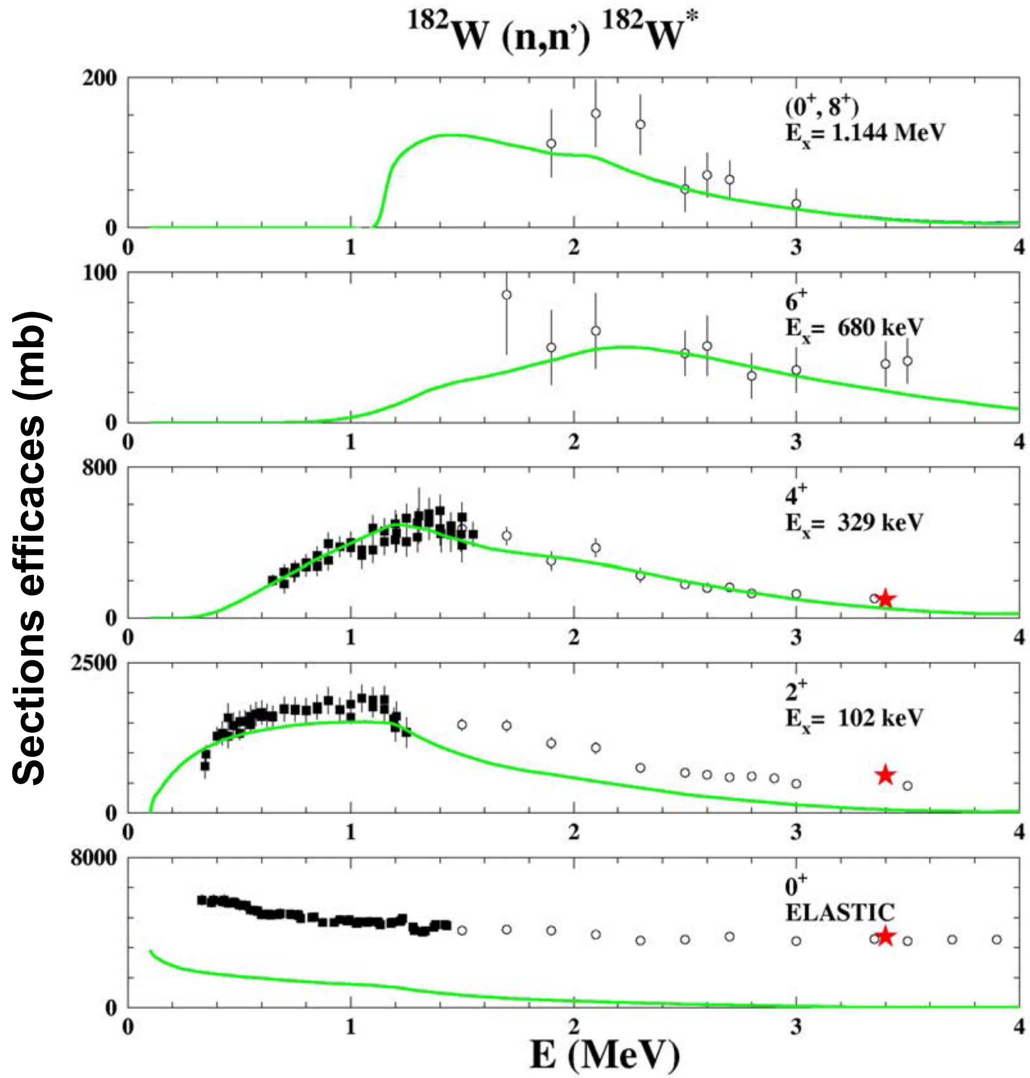




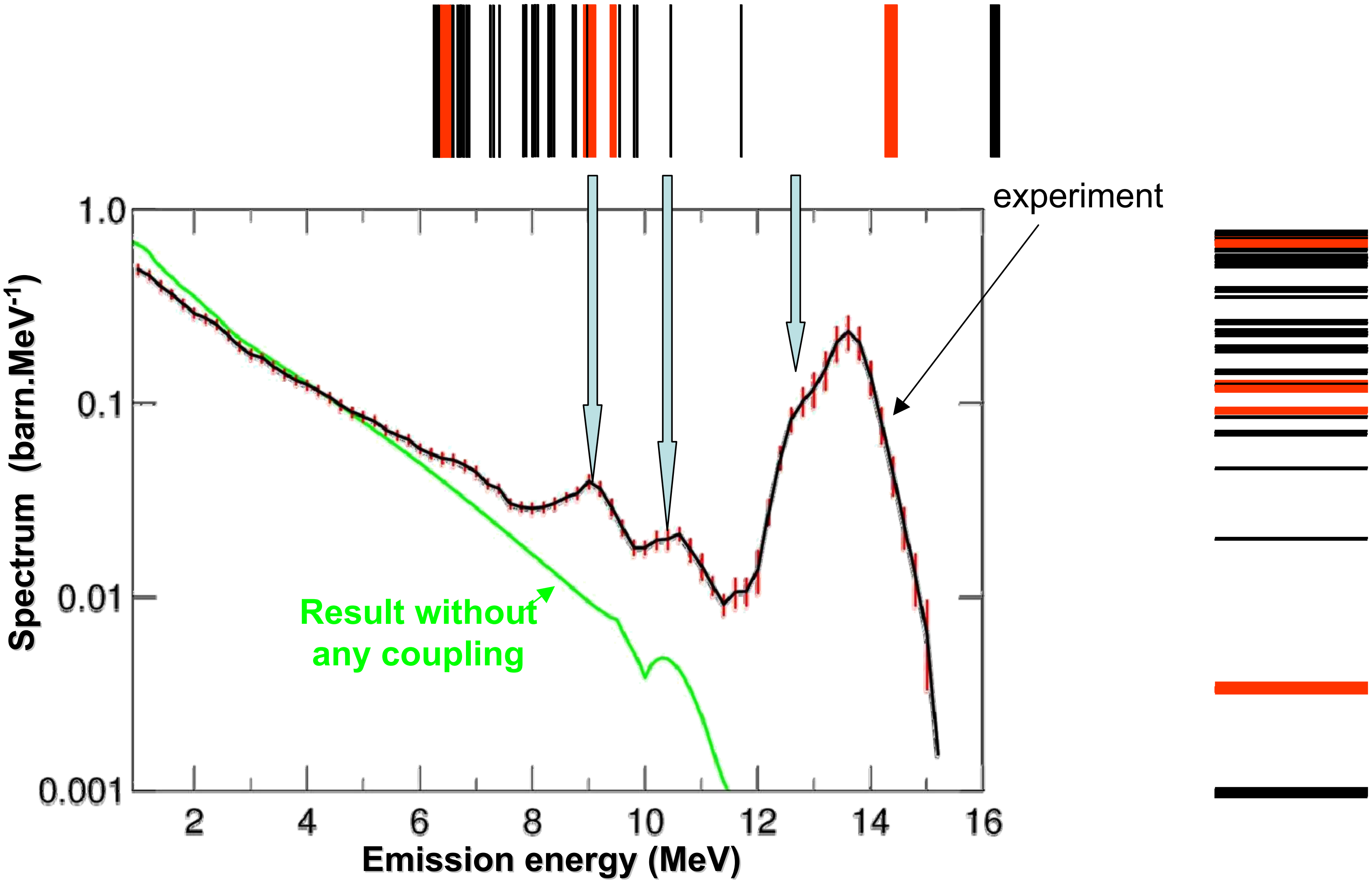


$$\begin{cases} (T+V_{00}-E)\,\Psi_0 = \overset{\beta}{V_{02}}\,\Psi_2 \\ (T+V_{22}-E)\,\Psi_2 = V_{20}\,\Psi_0 \end{cases}$$

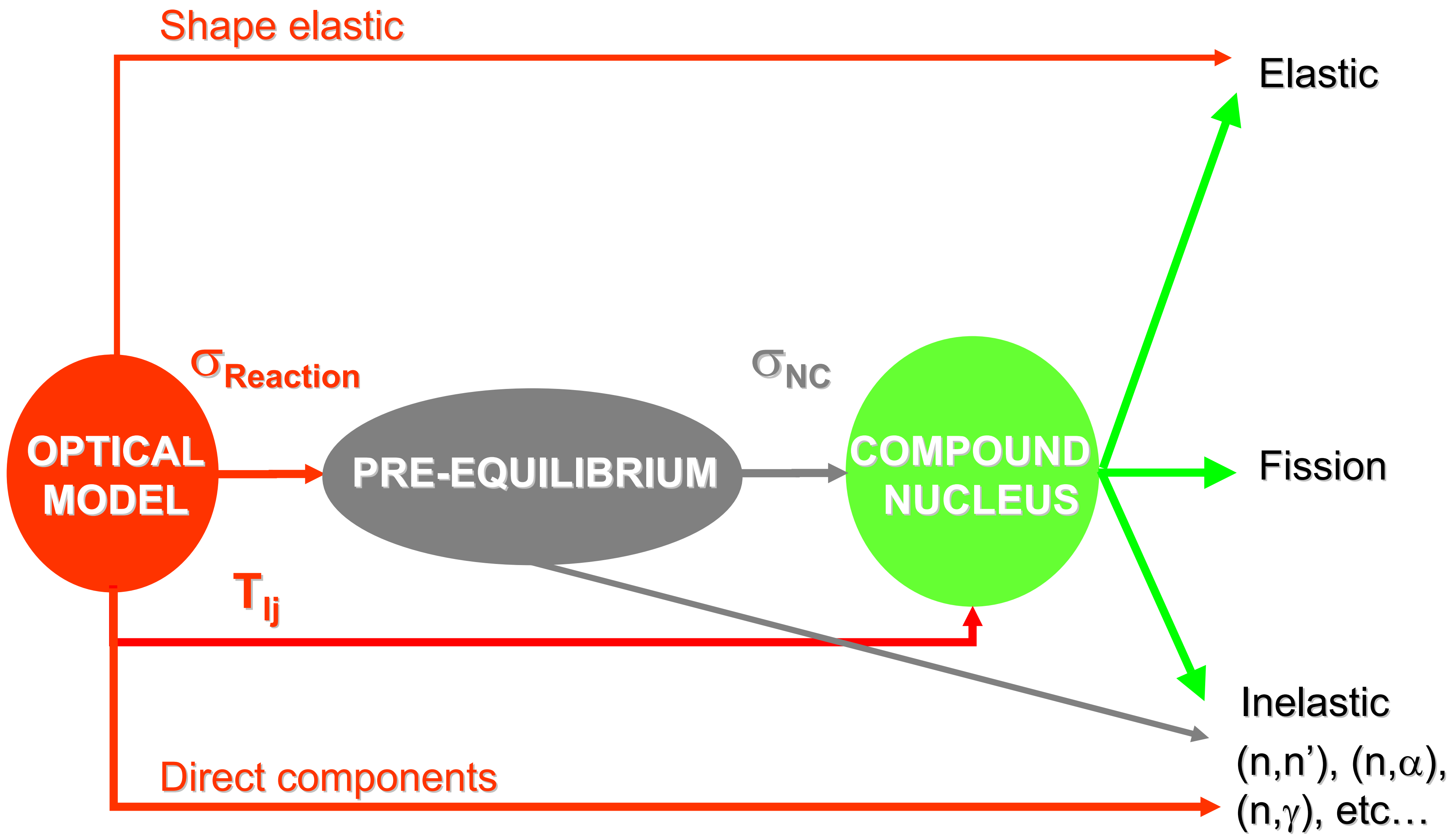
Impact of coupled channels



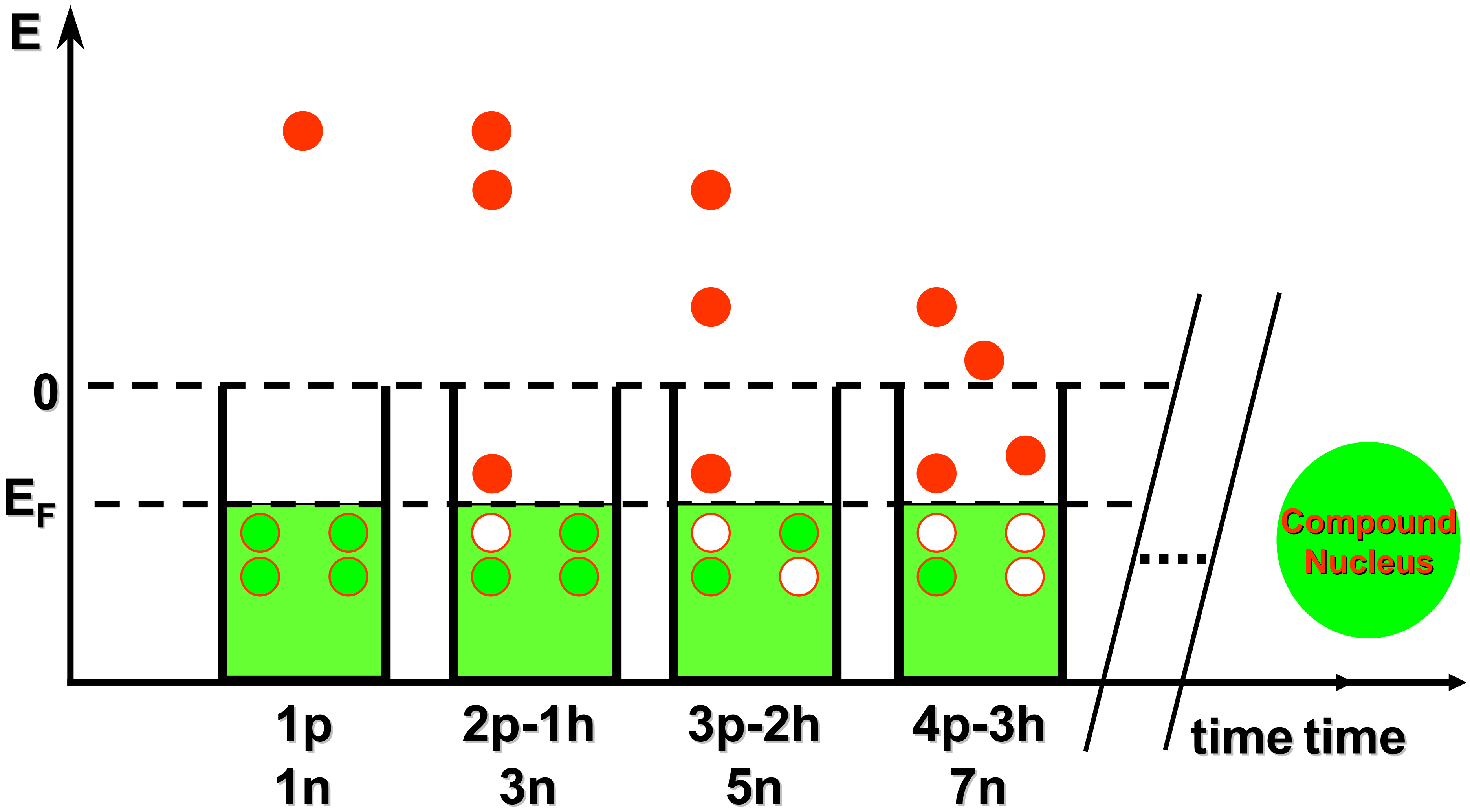
Impact of coupled channels



Models sequence



Pre-equilibrium model



Pre-equilibrium model

(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

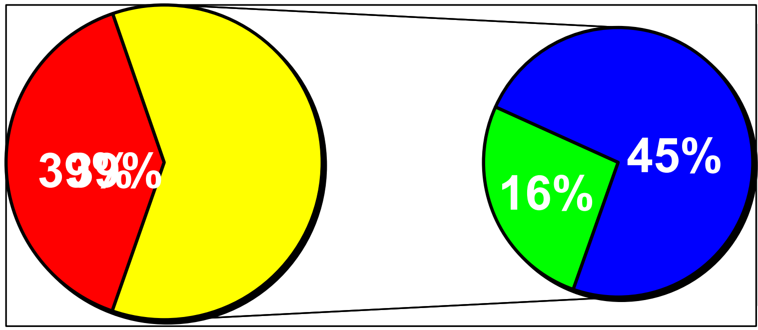
$$\frac{dP(n,E,t)}{dt} = P(n-2, E, t)\,\lambda_{n-2,\,n}(E) + P(n+2, E, t)\,\lambda_{n+2,\,n}(E) - P(n, E, t)\left[\lambda_{n,\,n+2}(E) + \lambda_{n,\,n-2}(E) + \lambda_{n,\,emiss}(E)\right]$$

Emission cross section in channel c

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

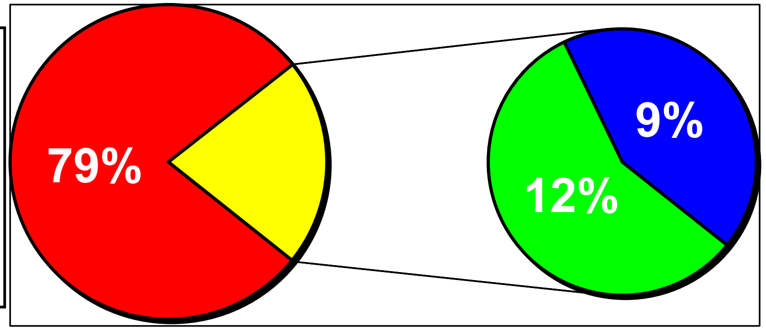
Pre-equilibrium model

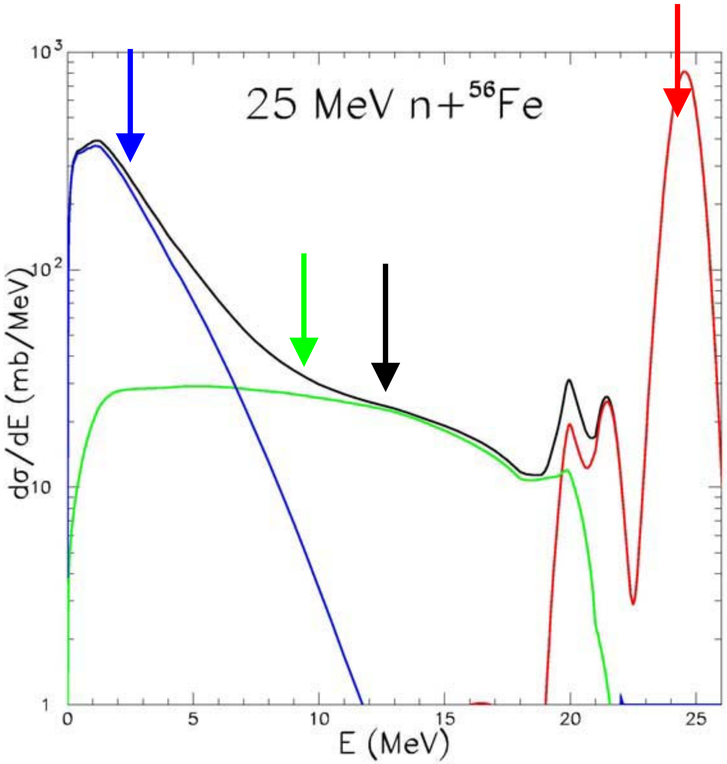
Cross section



Total
Direct
Pre-equilibrium
Statistical

Outgoing energy





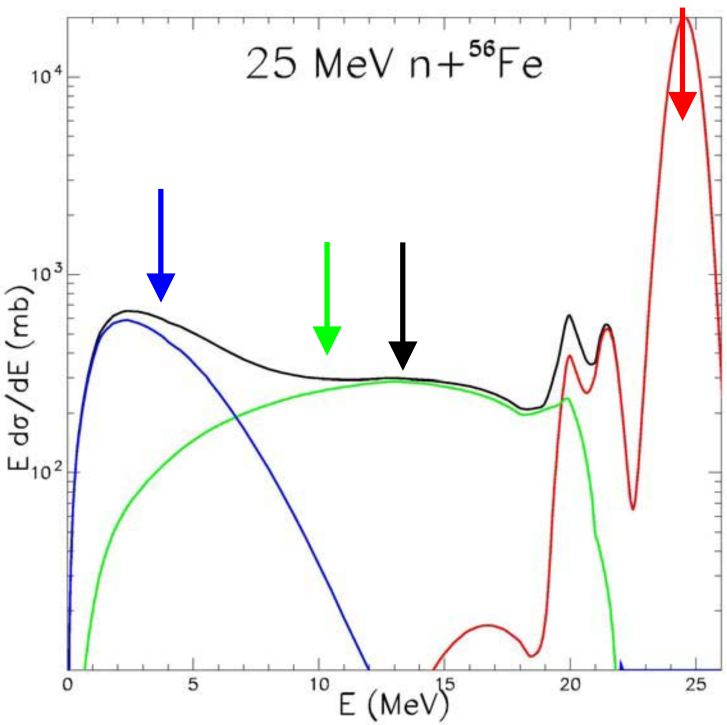
$\langle E_{Tot} \rangle$= 12.1

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

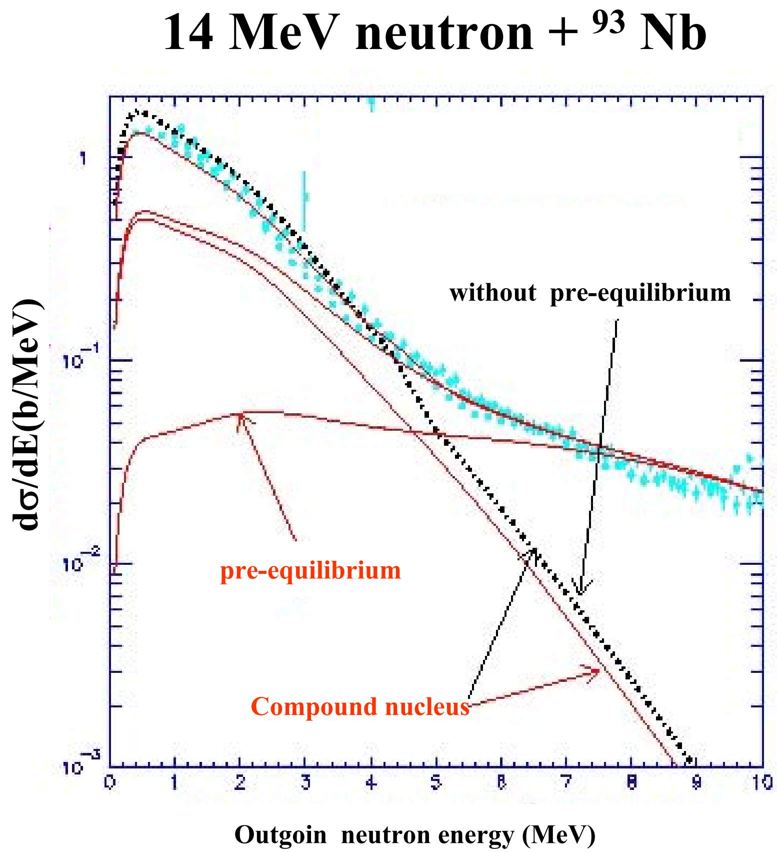
$\langle E_{PE} \rangle$= 9.32

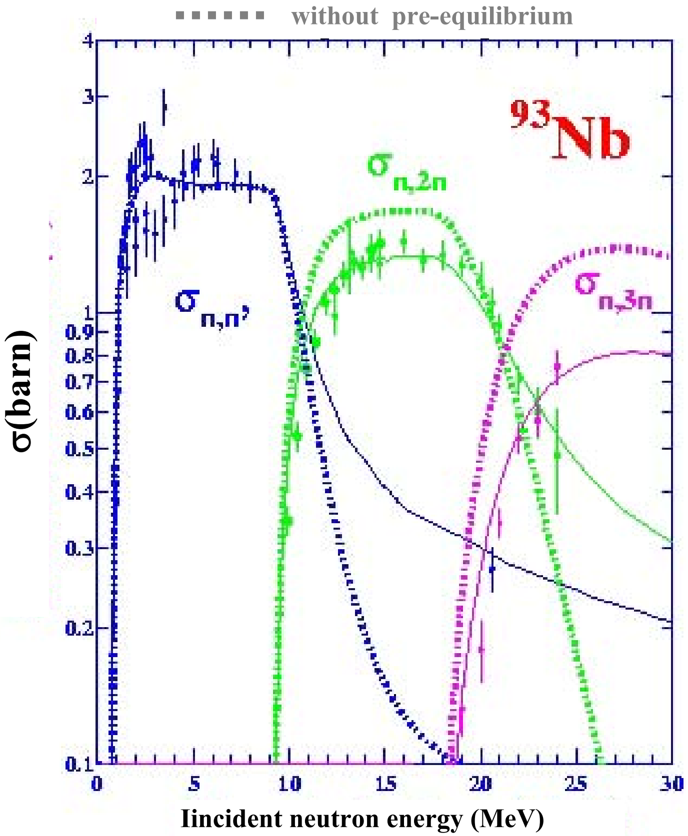
$\langle E_{Sta} \rangle$= 2.5

(MeV)

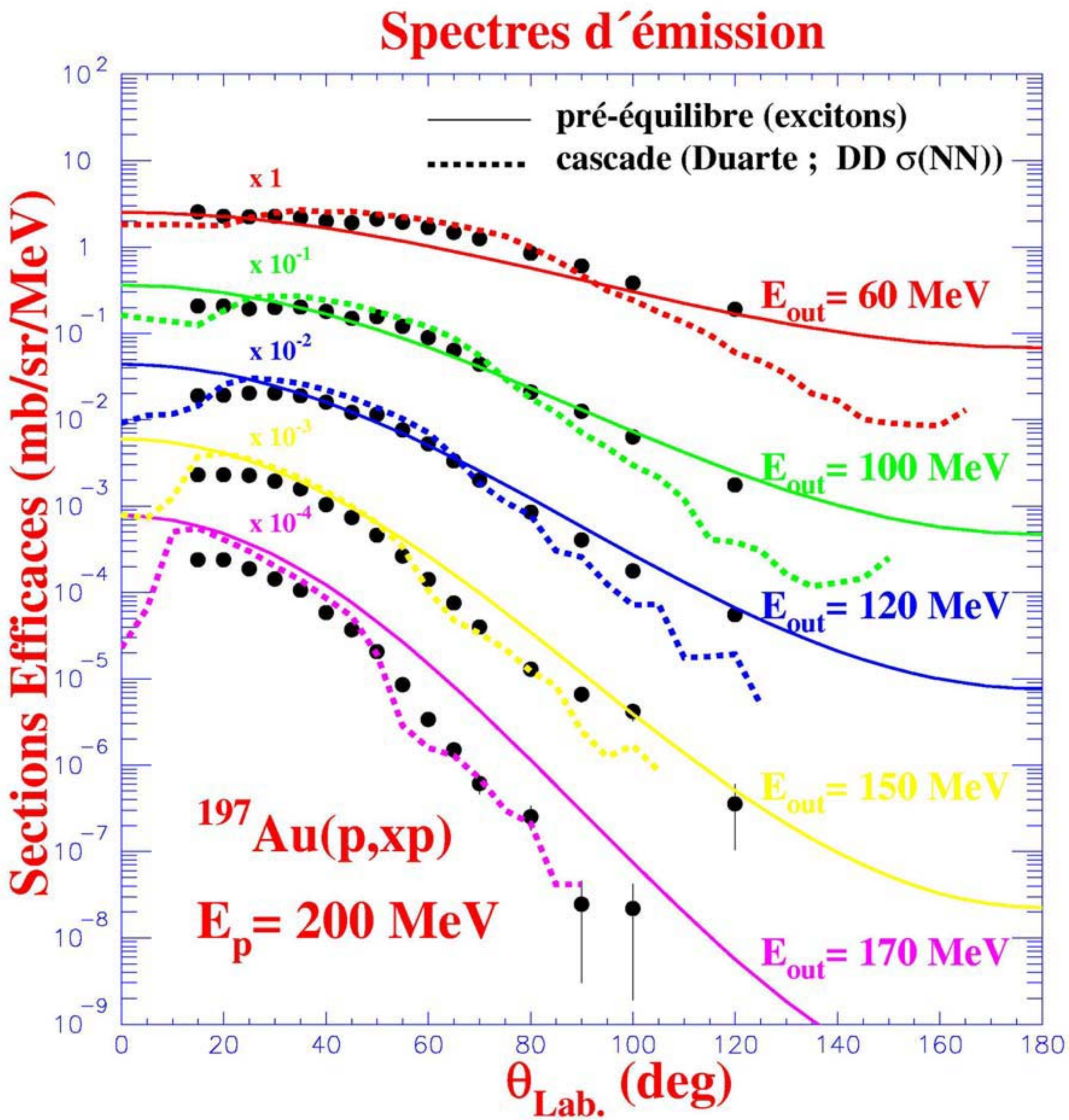


Pre-equilibrium model

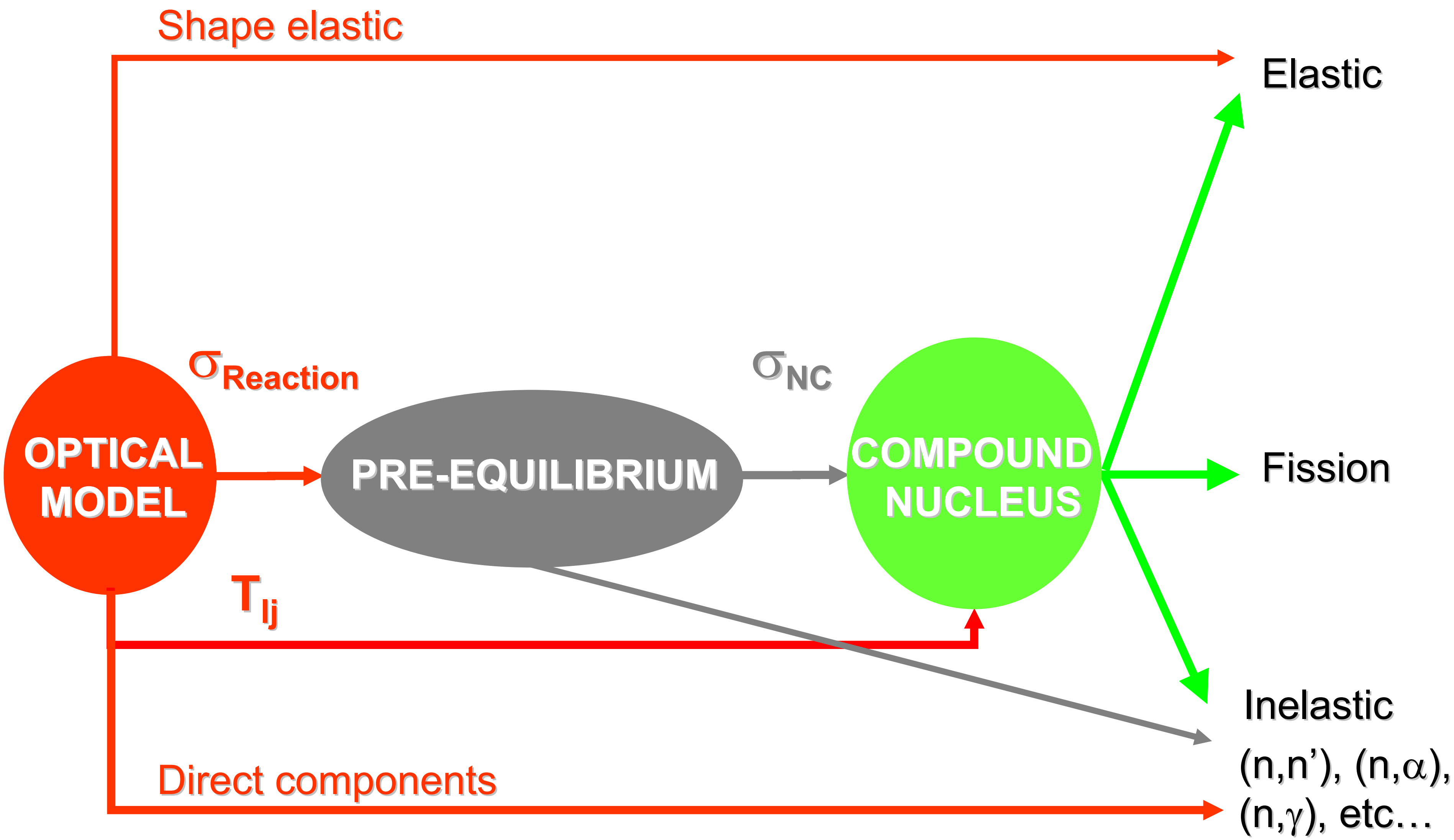




Link with high energy models (Intranuclear cascade)



Models sequence

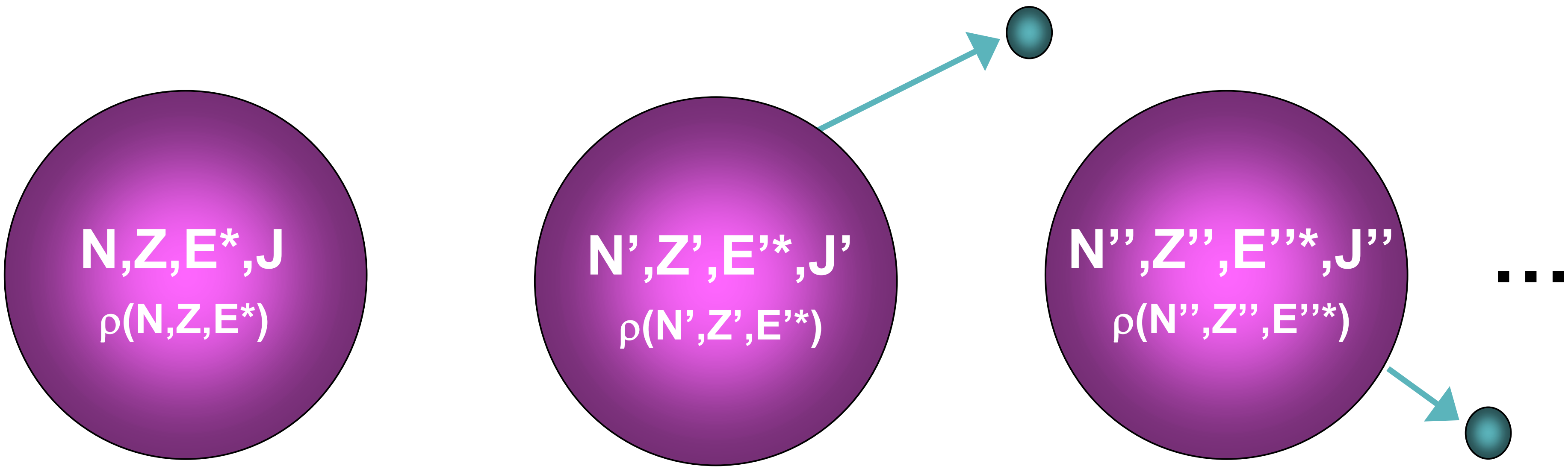


Compound nucleus model

After direct and pre-equilibrium emission

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

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	$J_0-dJ_D-dJ_{PE}$	$= J$



Compound nucleus model

Compound nucleus hypothesys

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

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

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

$\Rightarrow$ **Hauser- Feshbach formula**

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

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

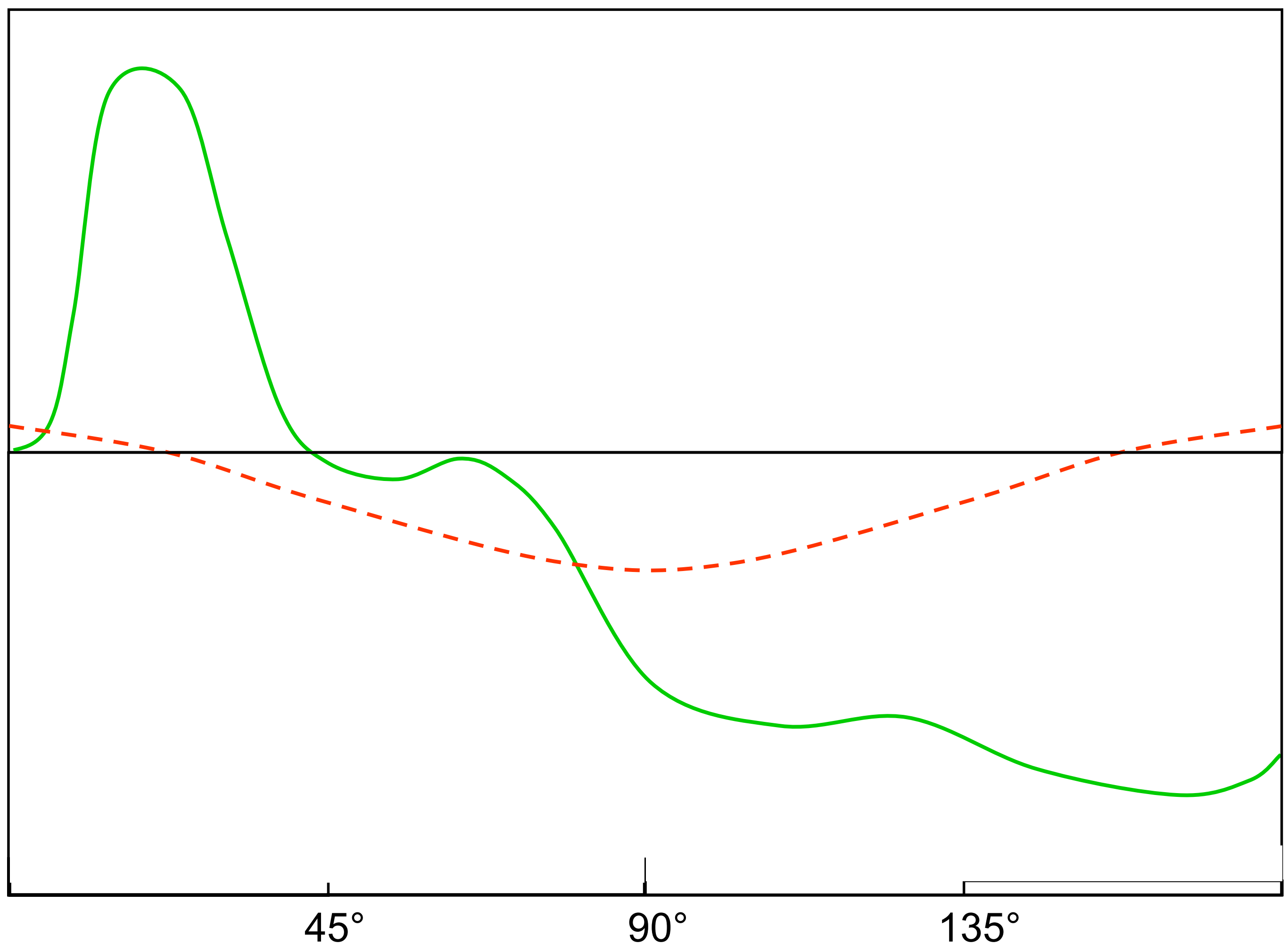
$$\sigma_{ab} = \frac{\pi}{k_a^2} \sum_{J=|I_A - s_a|}^{I_A + s_a + l_a^{max}} \sum_{\pi=\pm} \frac{(2J+1)}{(2I_A+1)\,(2s_a+1)}$$

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

$$\delta_\pi(a)\,\delta_\pi(b)\,\frac{T^{J\pi}_{a,l_a,j_a}\;T^{J\pi}_{b,l_b,j_b}}{\sum_c T^{J\pi}_{c,l_c,j_c}}\;W^{J\pi}_{a,l_a,j_a,b,l_b,j_b}$$

Angular distributions

Compound angular distribution & direct angular distributions



Width fluctuations

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

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

Or $T_\alpha \approx \dfrac{2\pi \langle \Gamma_\alpha \rangle}{D}$

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

Expressions for W_{ab}

- 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

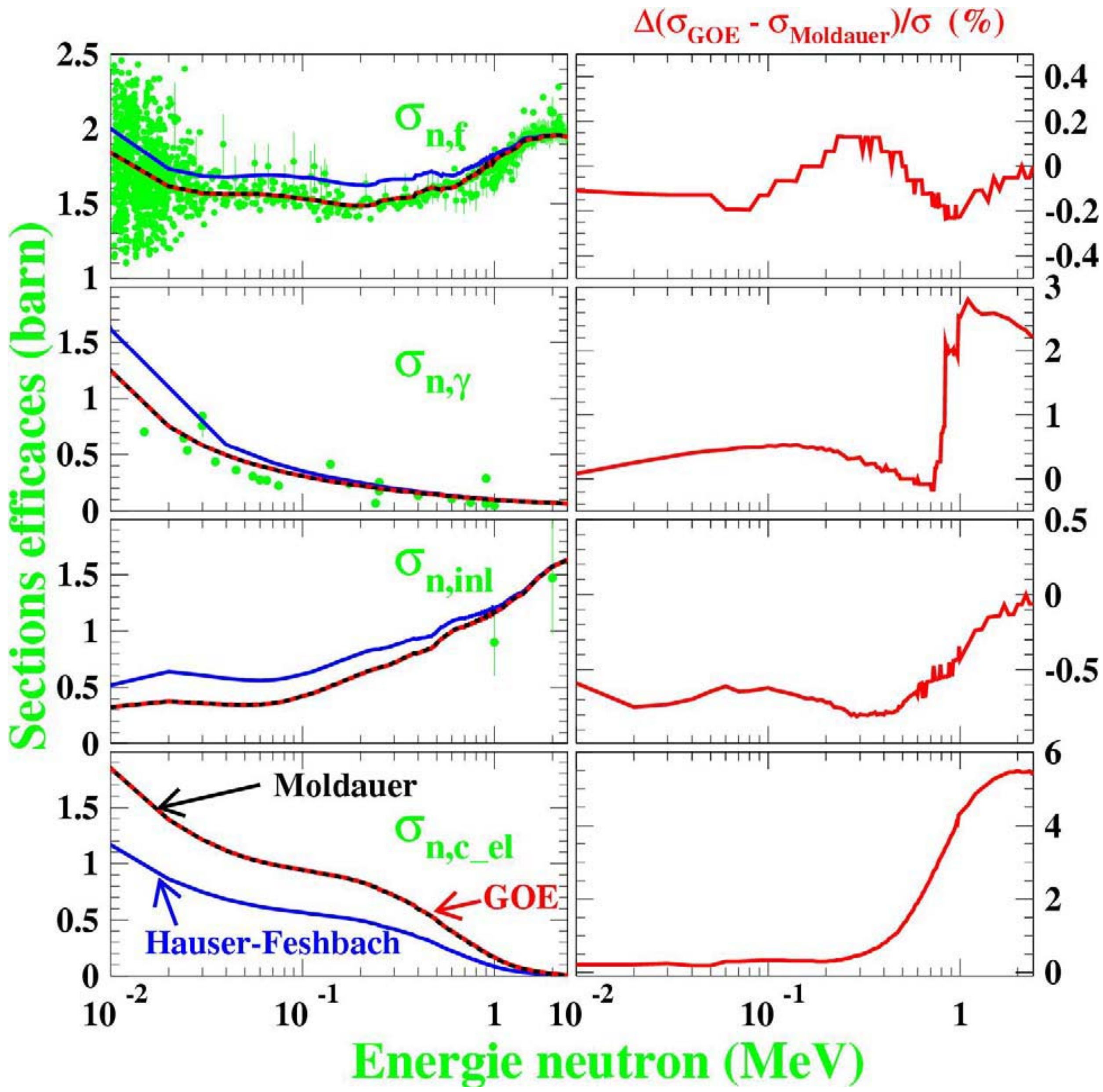
$$W_{a,l_a,j_a,b,l_b,j_b} = \int_0^{+\infty} d\lambda_1 \int_0^{+\infty} d\lambda_2 \int_0^1 d\lambda \; \frac{\lambda(1-\lambda)|\lambda_1 - \lambda_2|}{\sqrt{\lambda_1(1+\lambda_1)\lambda_2(1+\lambda_2)}(\lambda+\lambda_1)^2(\lambda+\lambda_2)^2}$$

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

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

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

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



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

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

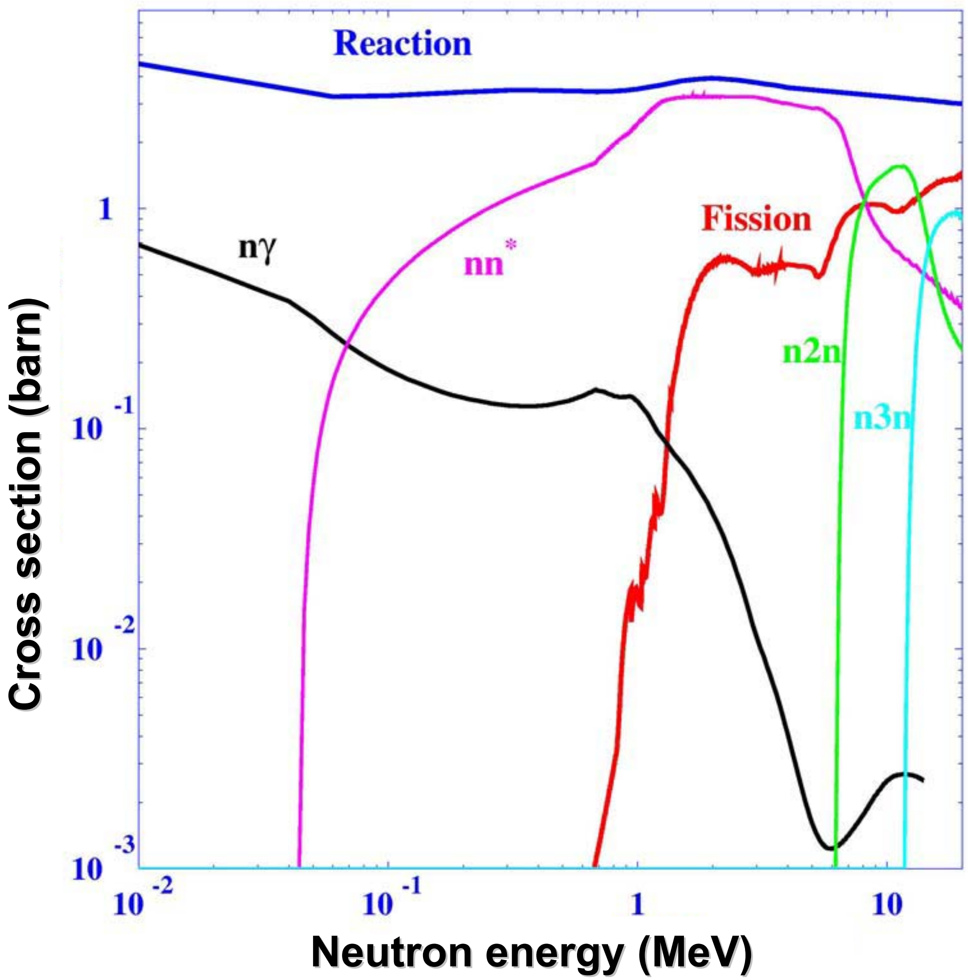
$$\sigma_{ab} = \frac{\pi}{k_a^2} \sum_{J,\pi} \sum_{\alpha,\beta} \frac{(2J+1)}{(2s+1)(2I+1)} T_{lj}^{J\pi}(\alpha) \frac{\left\langle T_b^{J\pi}(\beta) \right\rangle}{\sum_{\delta} \left\langle T_d^{J\pi}(\delta) \right\rangle} W_{\alpha\beta}$$

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

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

Compound nucleus model

$n + {}^{238}U$

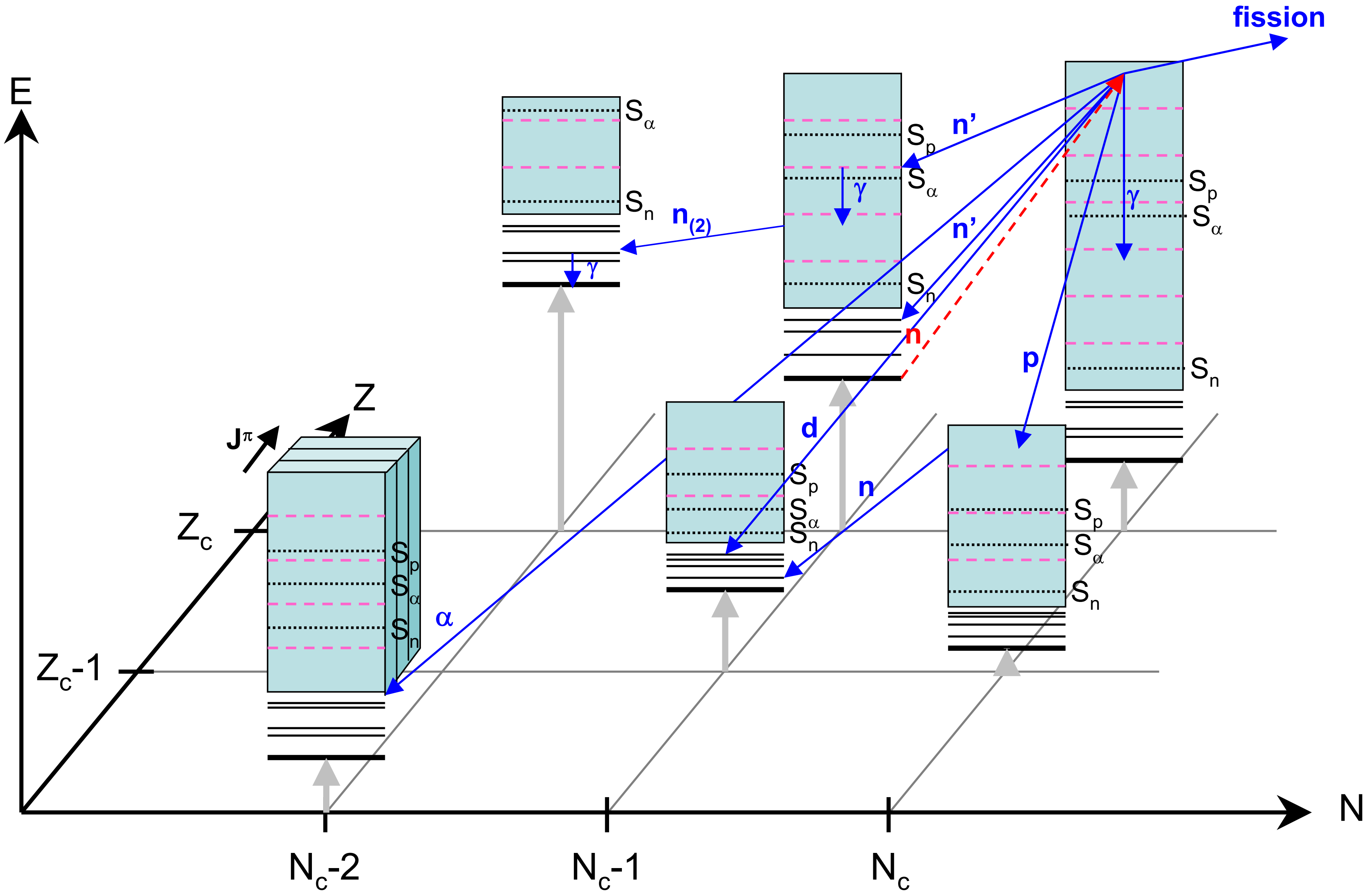


Optical model
+
Statistical model
+
Pre-equilibrium model

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

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

Multiple emission processes



Compound nucleus model

Possible decays

- Emission to a discrete level with energy E_d

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

- Emission in the level continuum

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

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

- Emission of photons, fission

Specific treatment

Gamma transmission coefficients

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

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

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

- k : transition type EM (E ou M)
- λ : transition multipolarity
- ε_γ : outgoing gamma energy

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

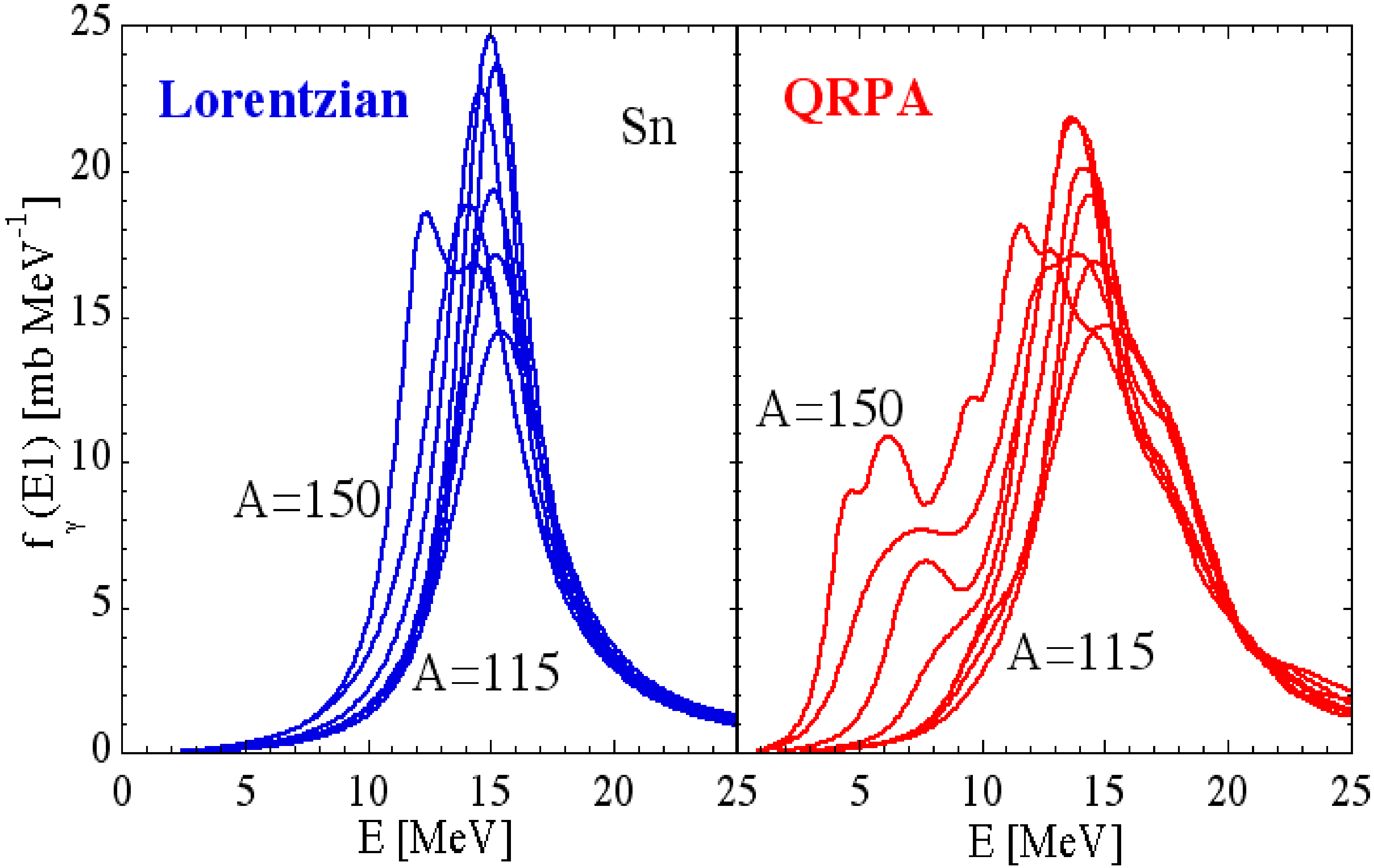
$|J_i-\lambda| \leq J_f \leq J_i+\lambda$

Renormalisation technique for thermal neutrons

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

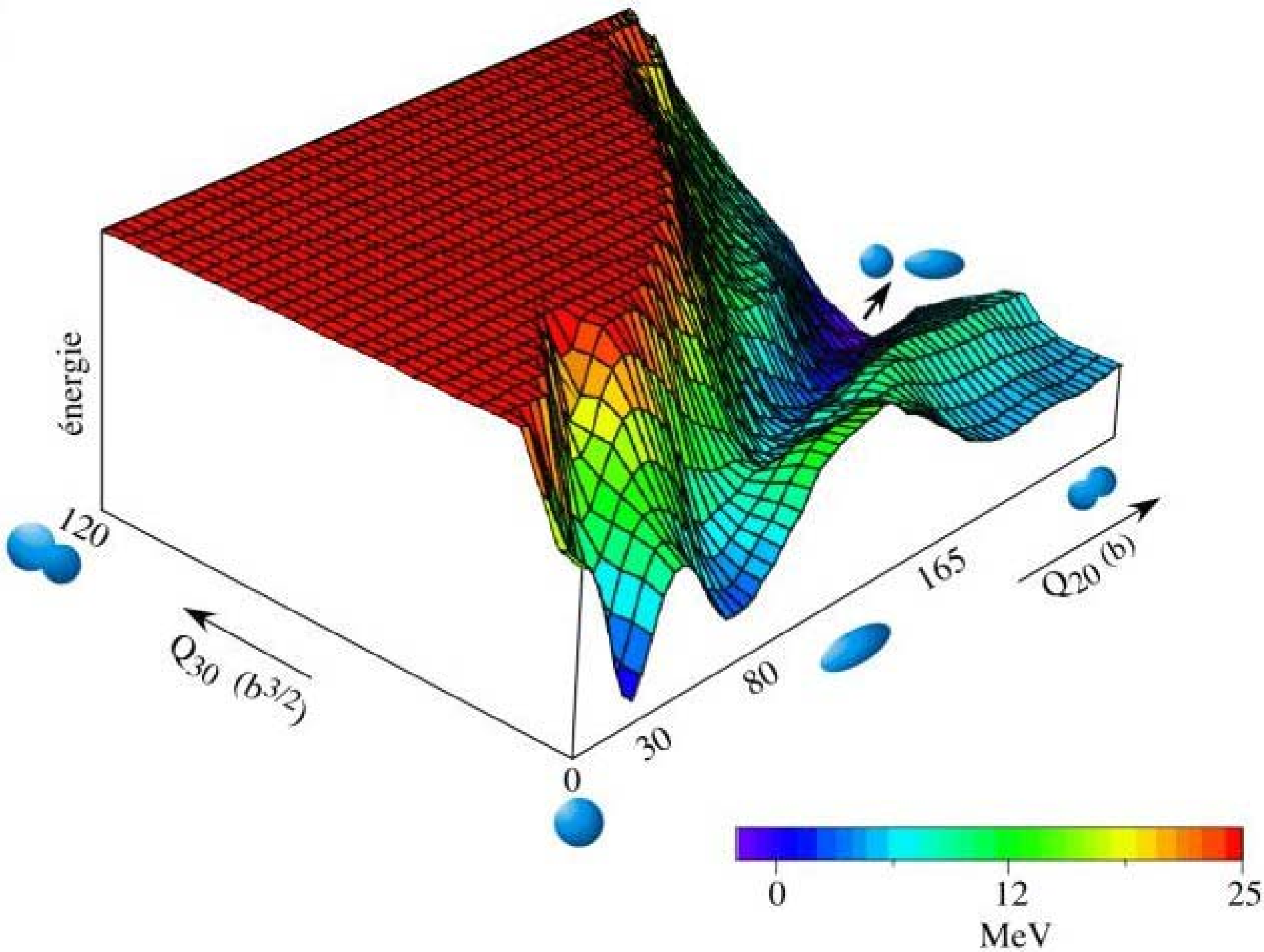
experiment

γ-ray strength functions models

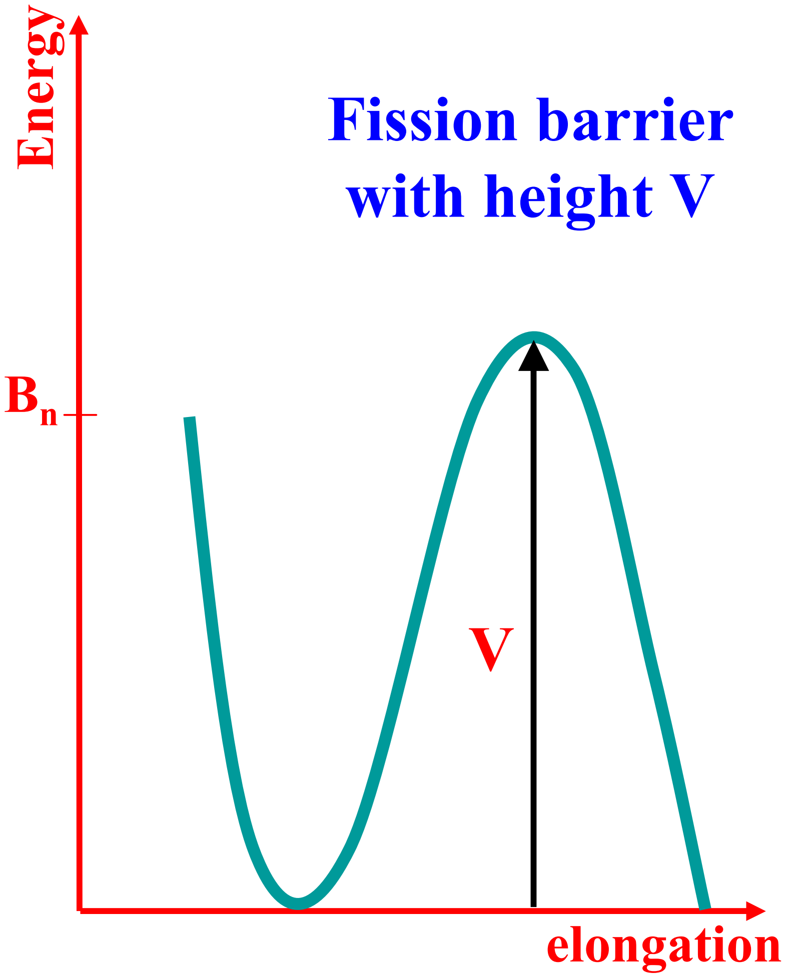


See S. Goriely & E. Khan, NPA 706 (2002) 217.
S. Goriely et al., NPA739 (2004) 331.

Surface ^{238}U

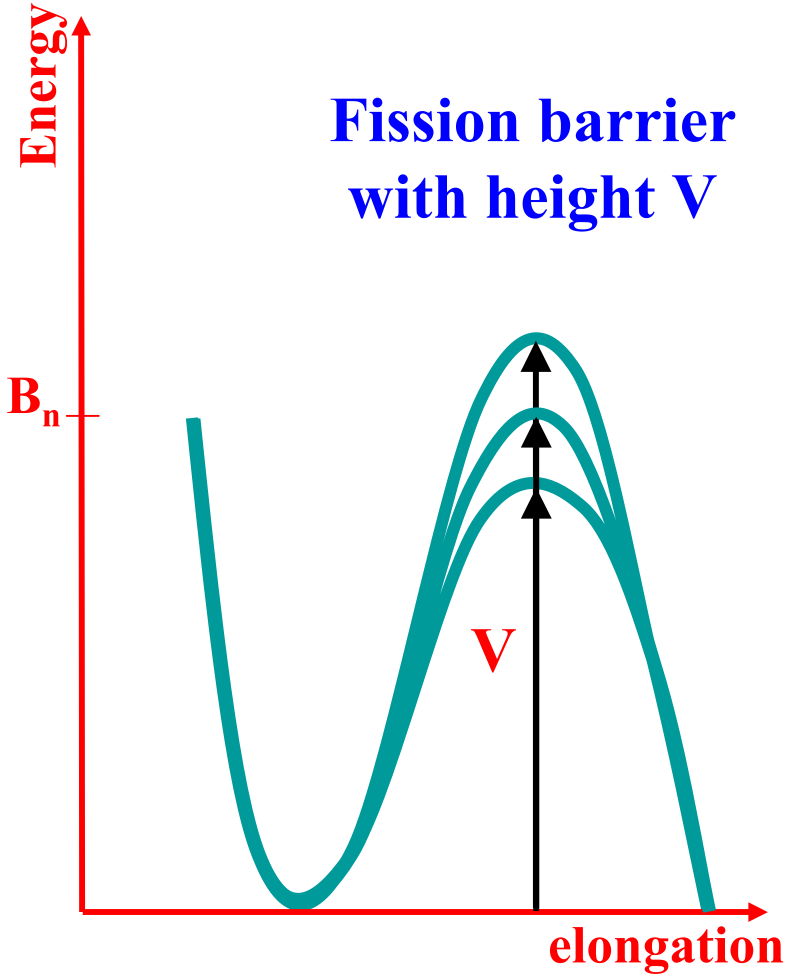


Fissile/Fertile



$B_n < V$

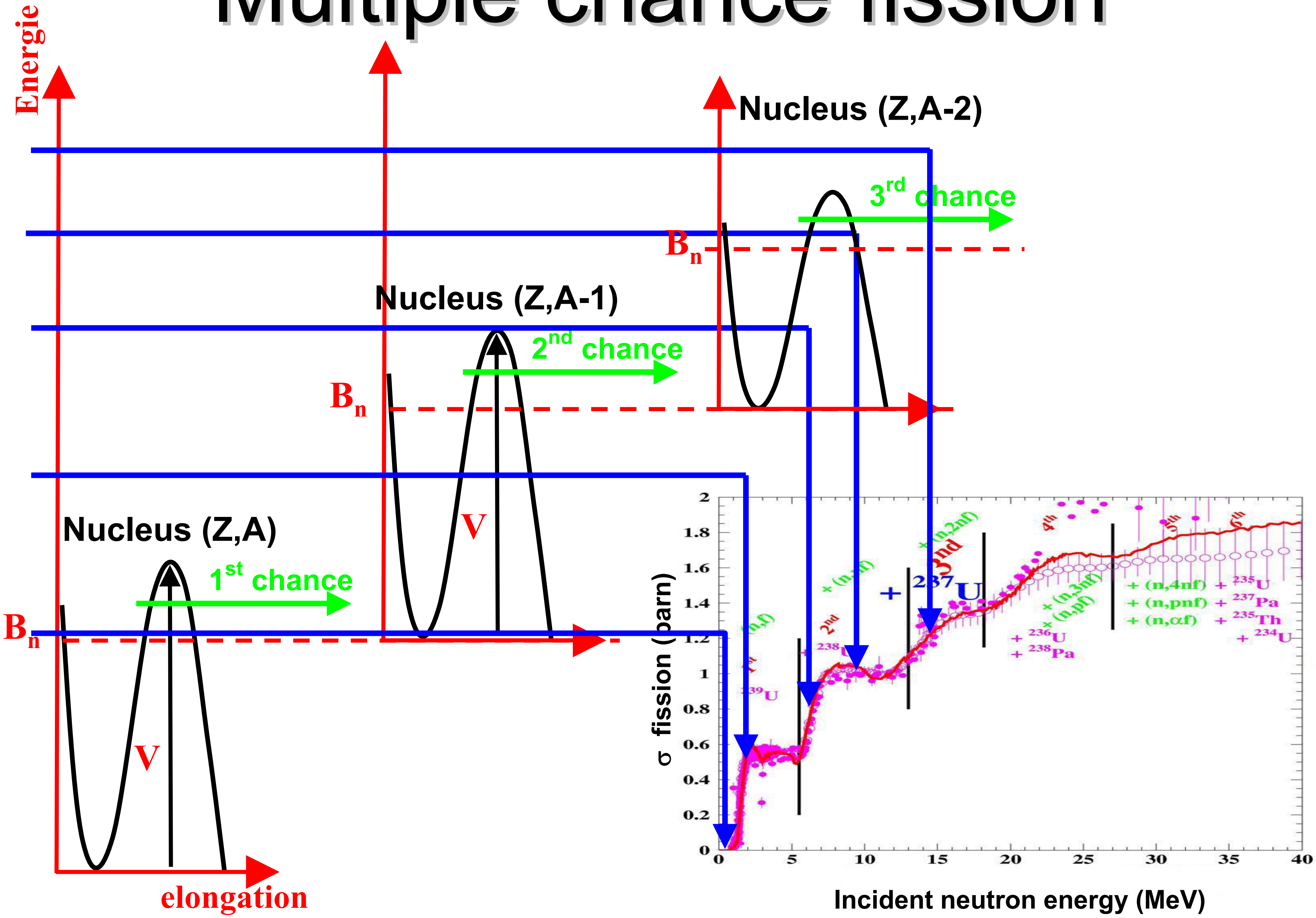
Fertile target (^{238}U)



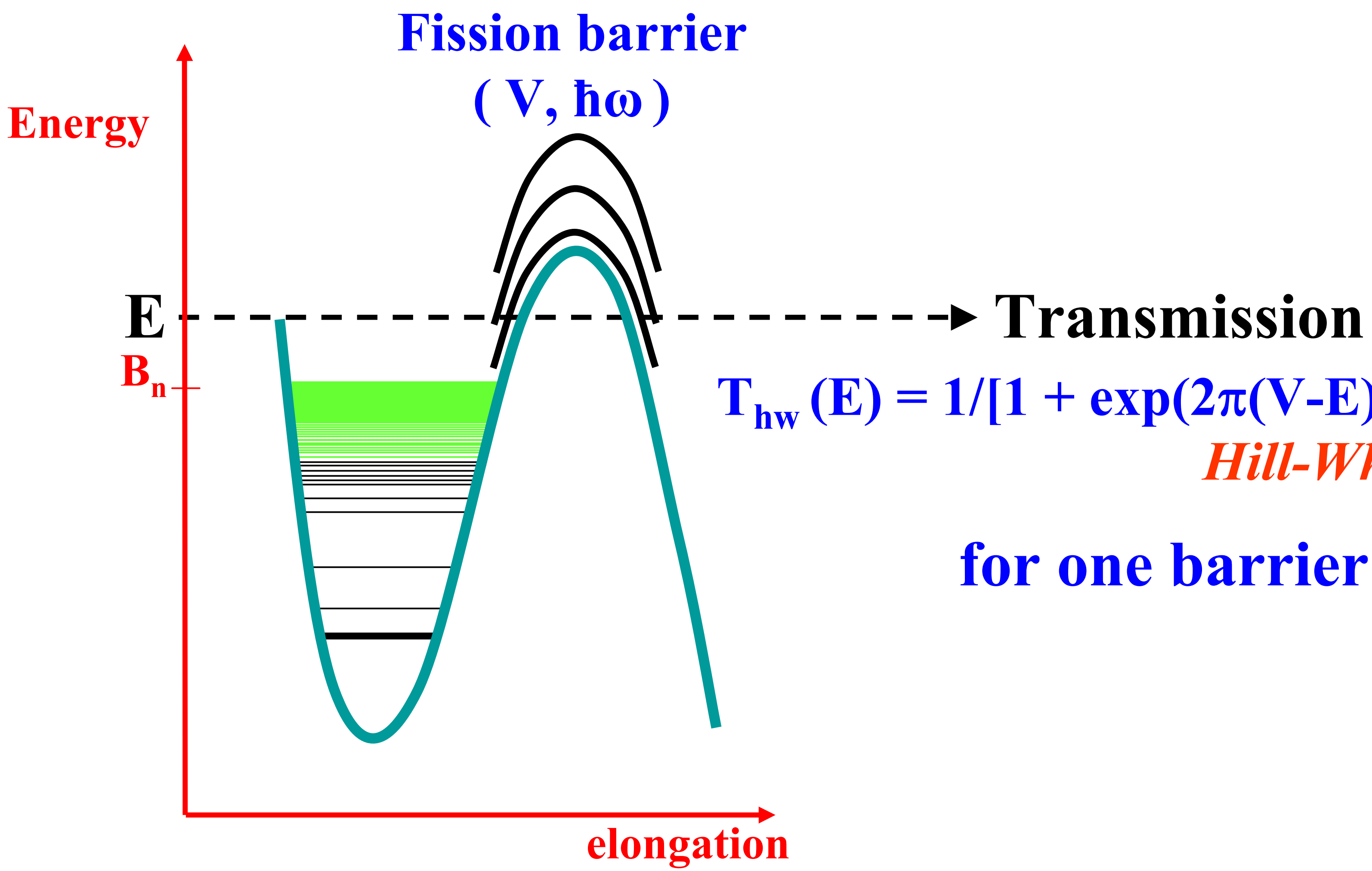
$B_n > V$

Fissile target (^{235}U)

Multiple chance fission



Fission modeling



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

Hill-Wheeler

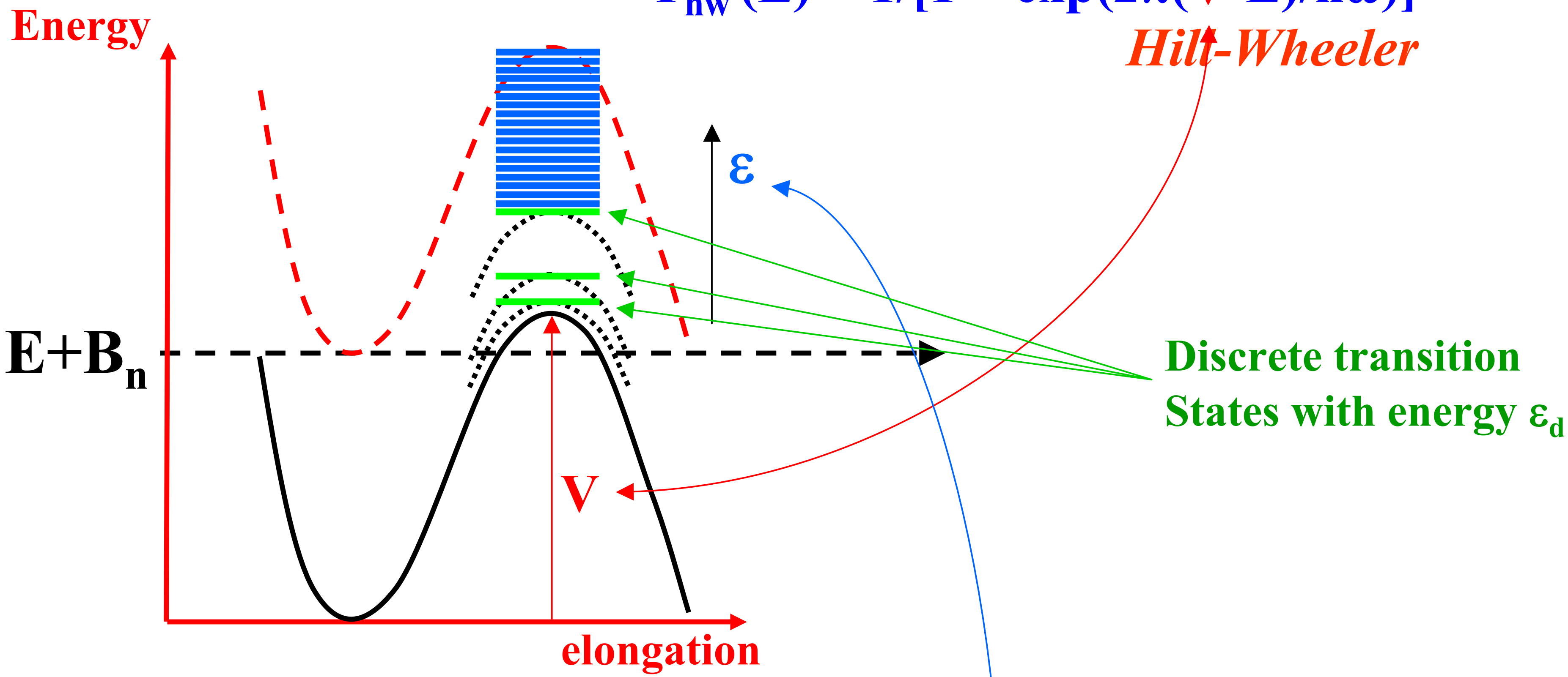
for one barrier !

+ transition state on top of the barrier !

Bohr hypothesys

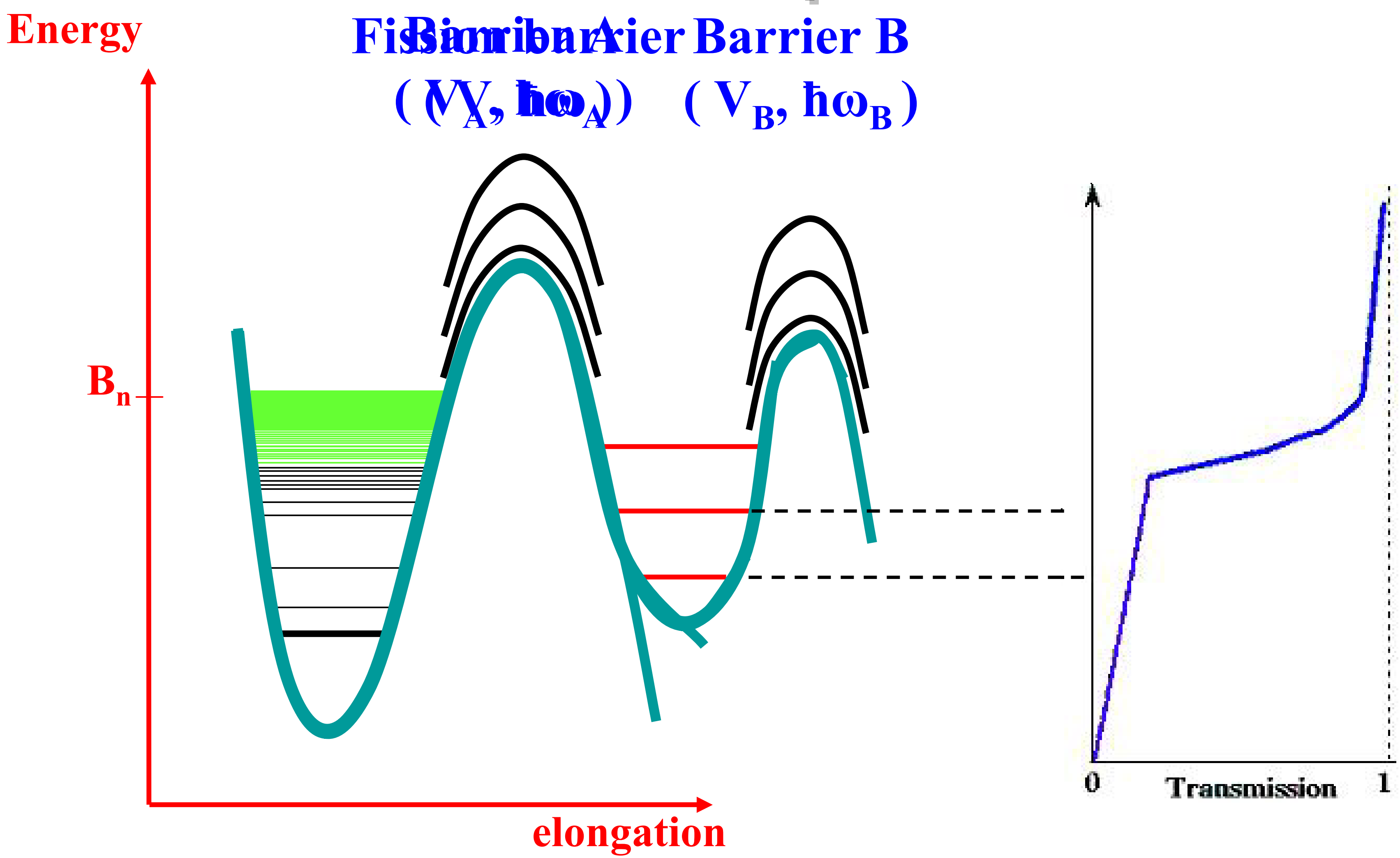
Fission transmission coefficients

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



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

Double-humped barriers



+ transition states on top of the barrier !

+ transition states on top of each barrier !

+ class II states in the intermediate well !

Fission transmission coefficients

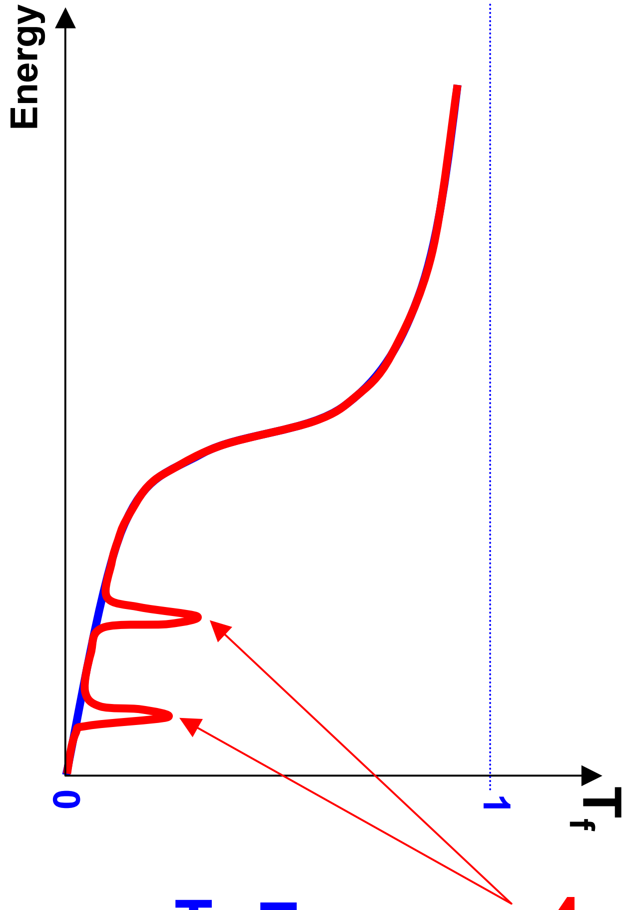
Two barriers A and B

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

Three barriers A, B et C

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

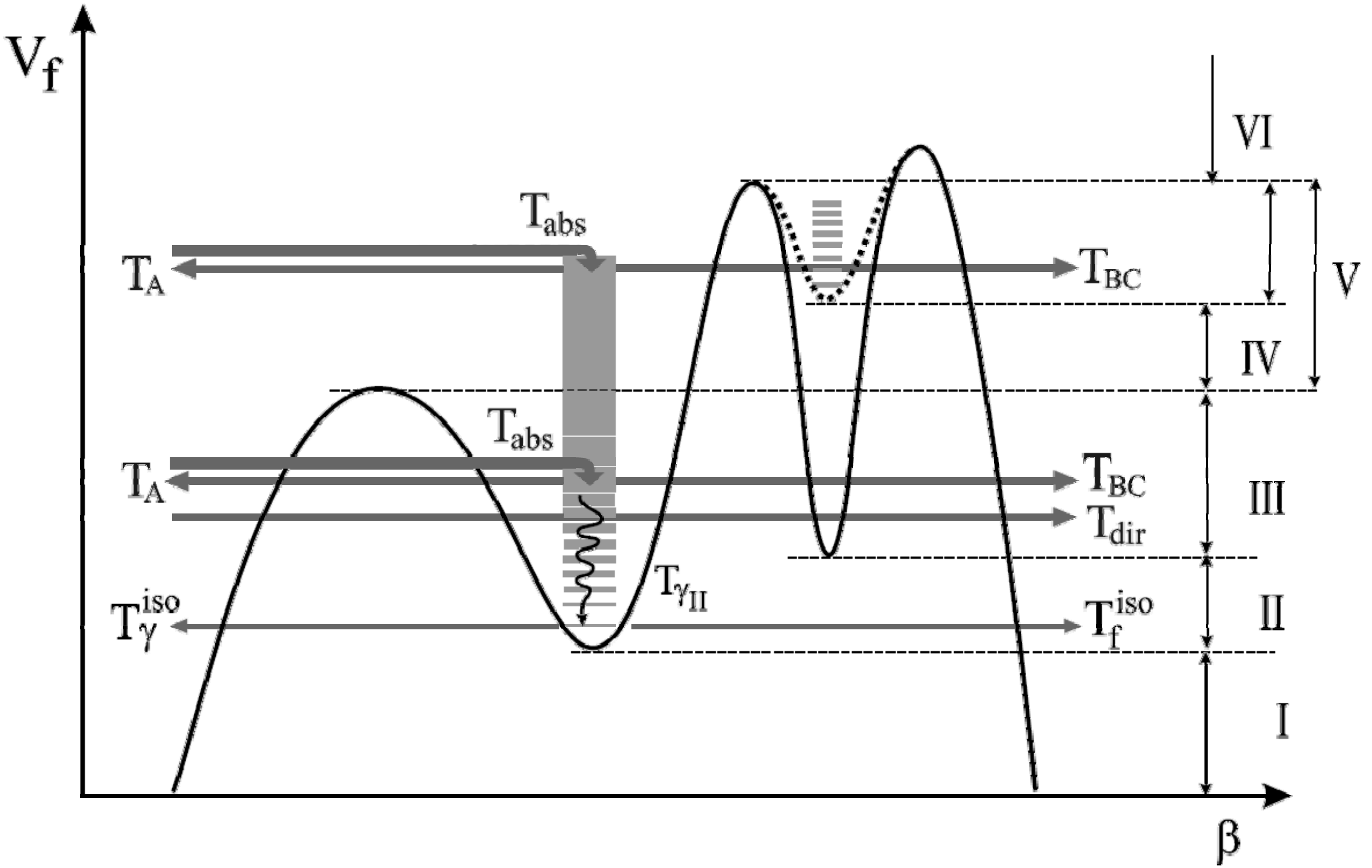
Resonant transmission



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

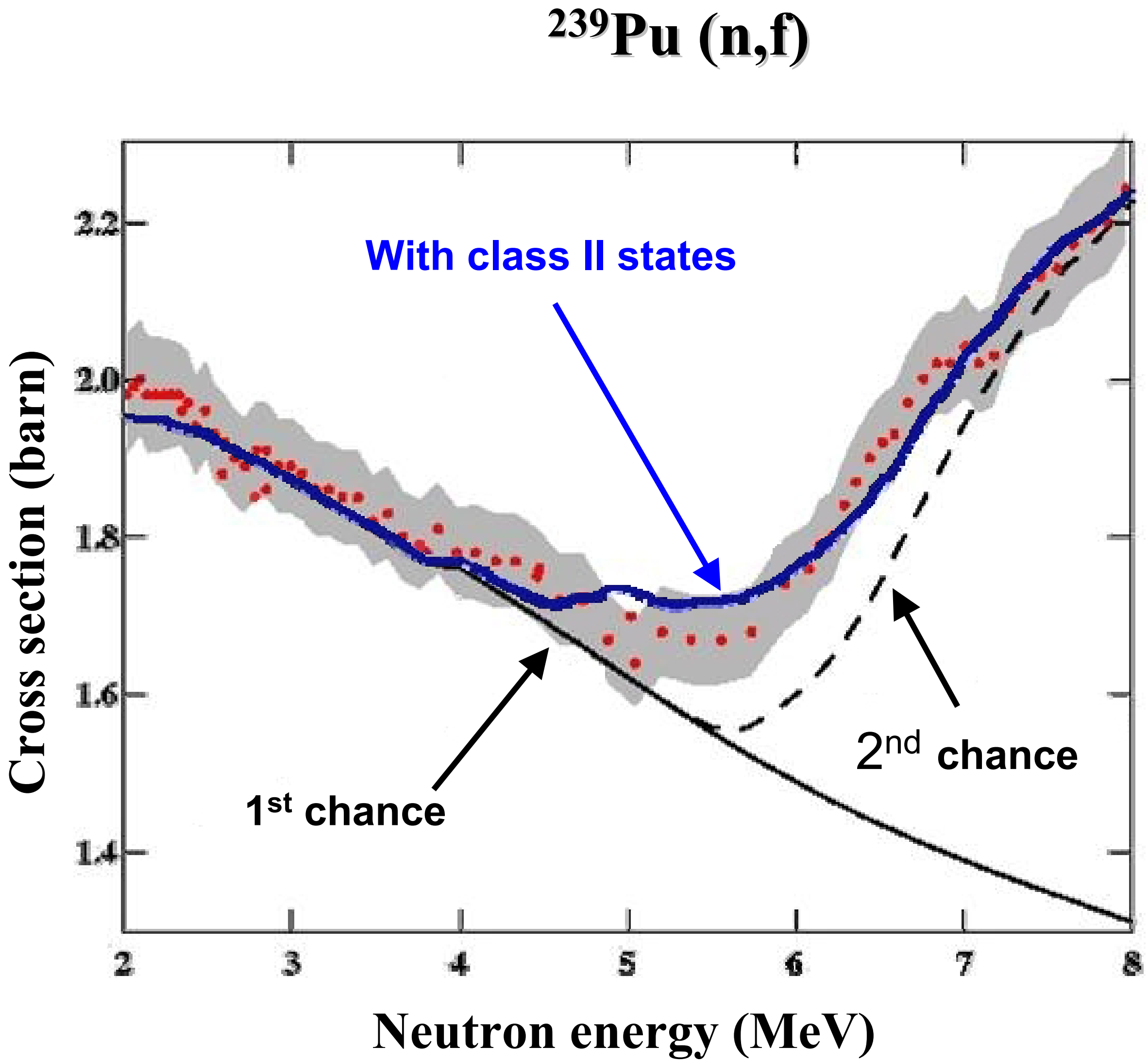
More exact expressions in Sin et al., PRC 74 (2006) 014608

Fission transmission coefficients



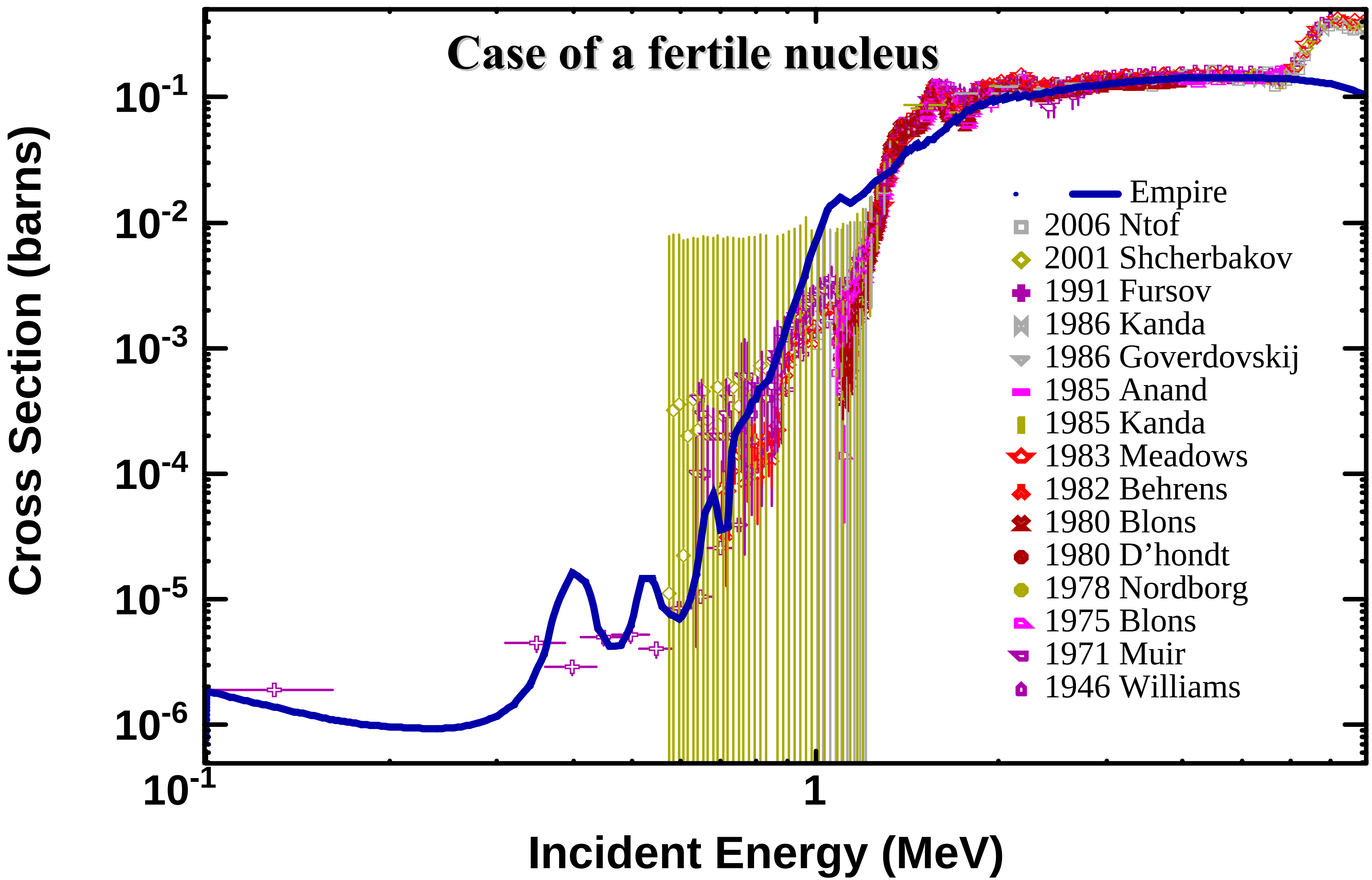
See in Sin et al., PRC 74 (2006) 014608
Bjornholm and Lynn, Rev. Mod. Phys. 52 (1980) 725.

Impact of class II states



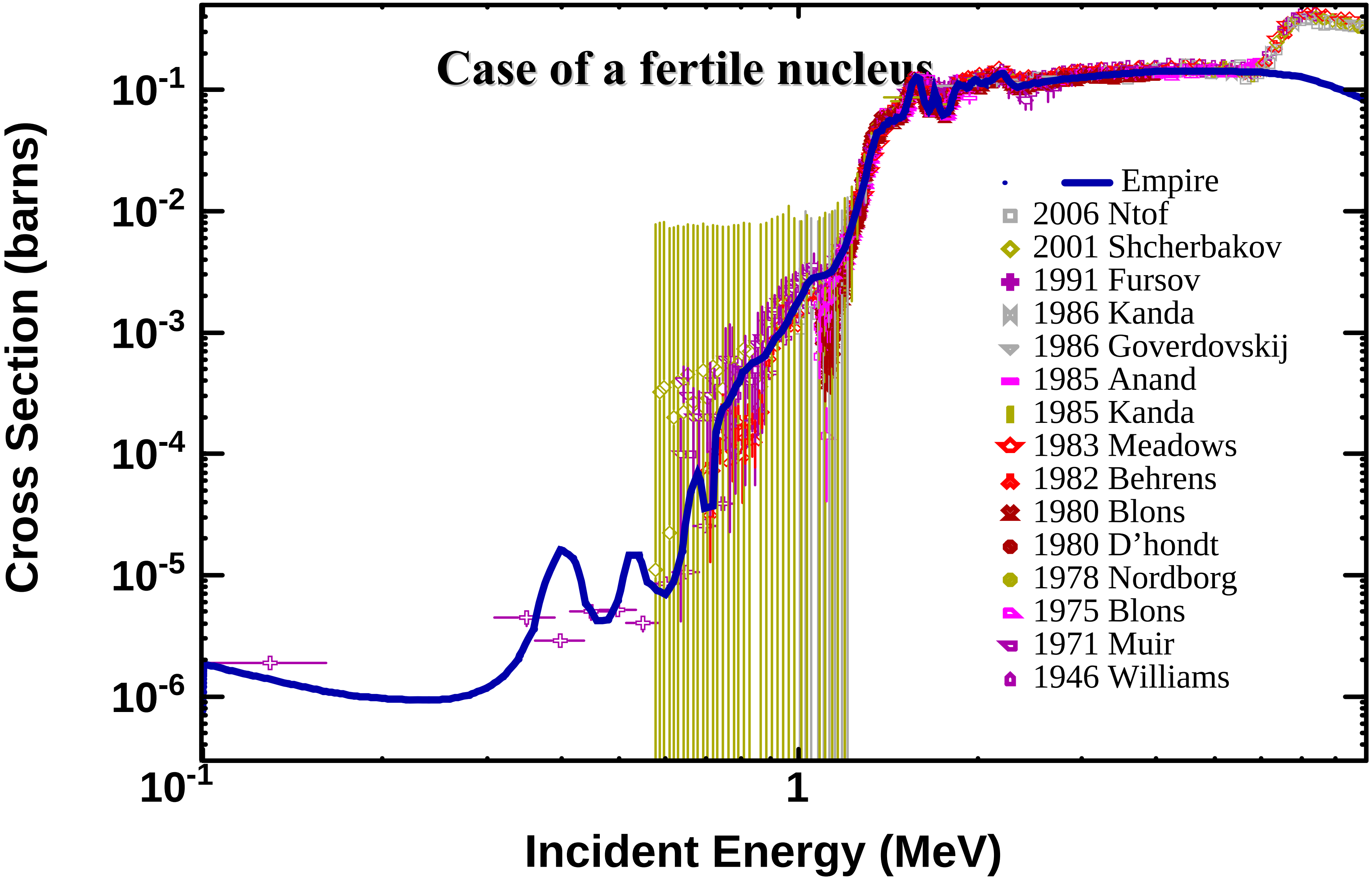
Impact of class II states

Partially damped class II states. No class II states (fully dampe

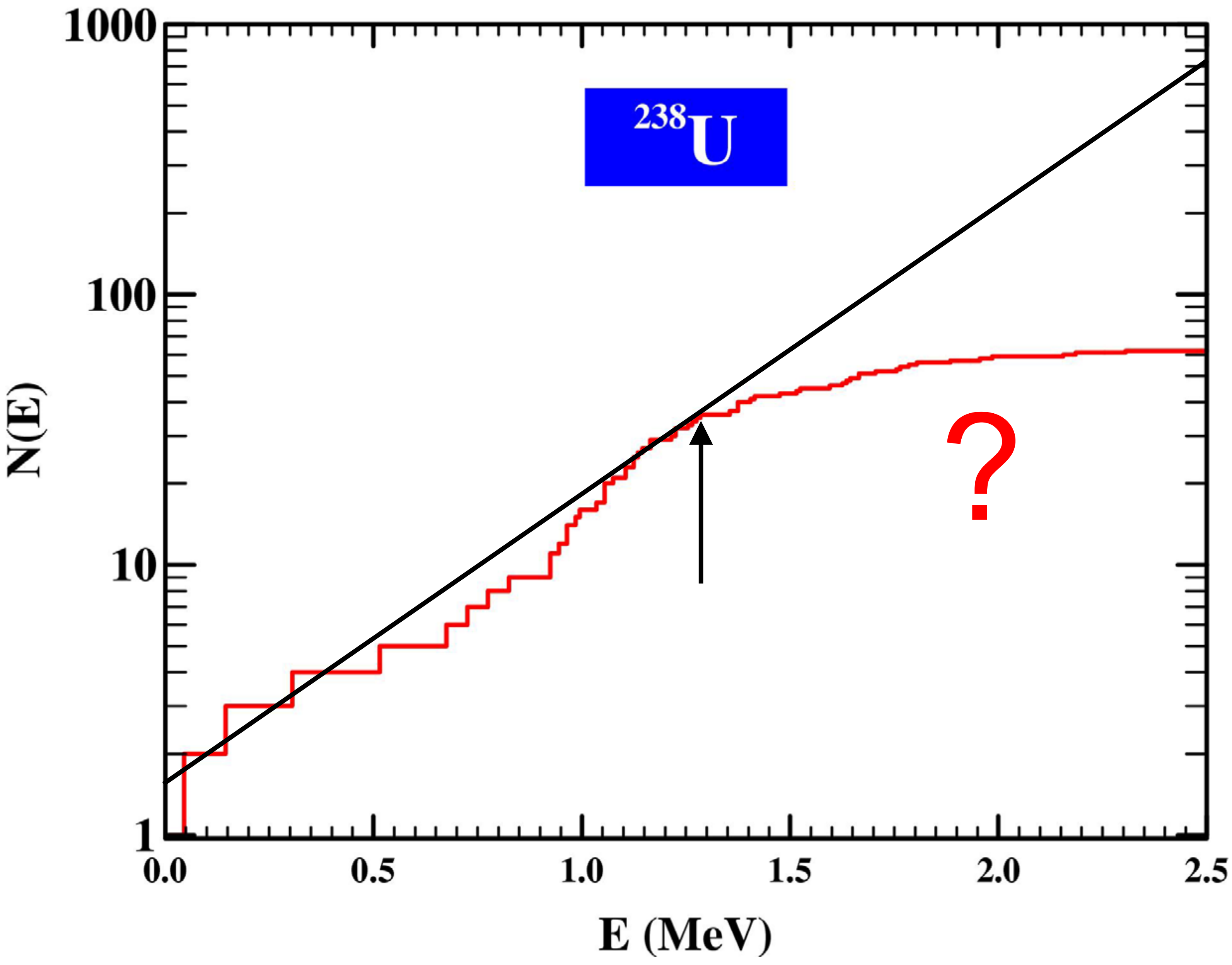


Impact of class II states

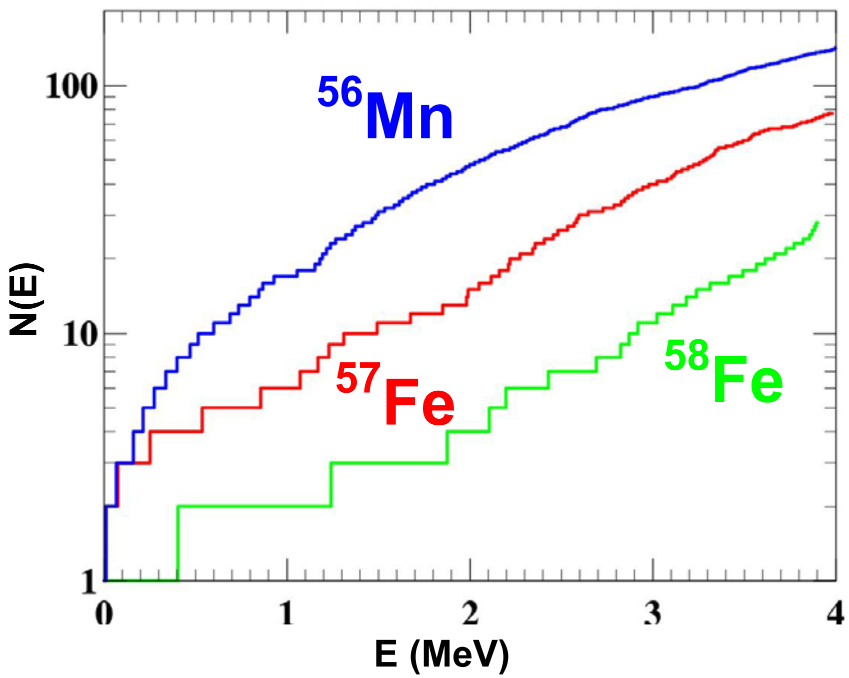
Class I + II states: Partial damping.

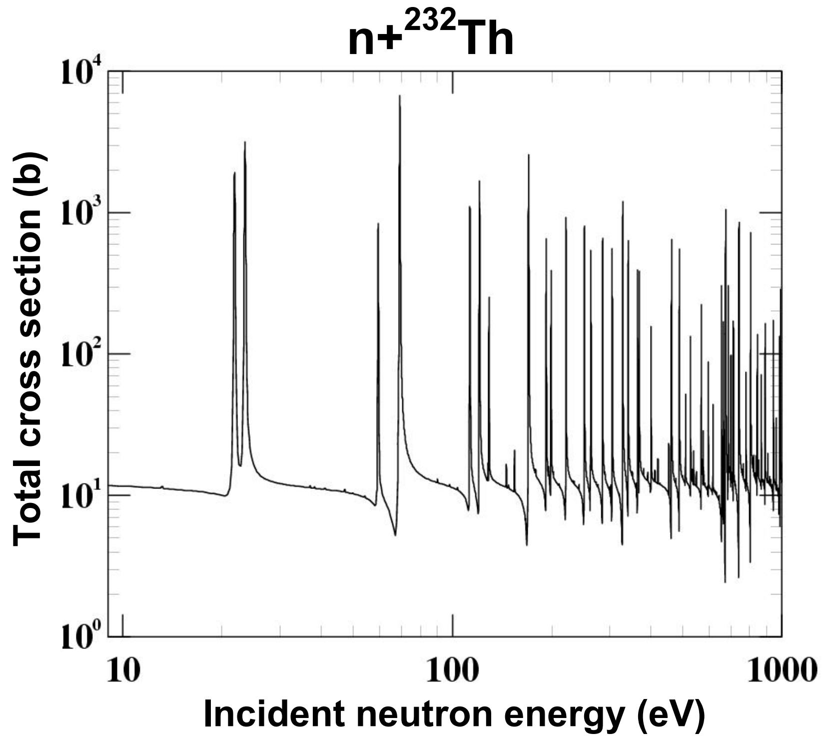


Nuclear level densities



Qualitative aspects





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

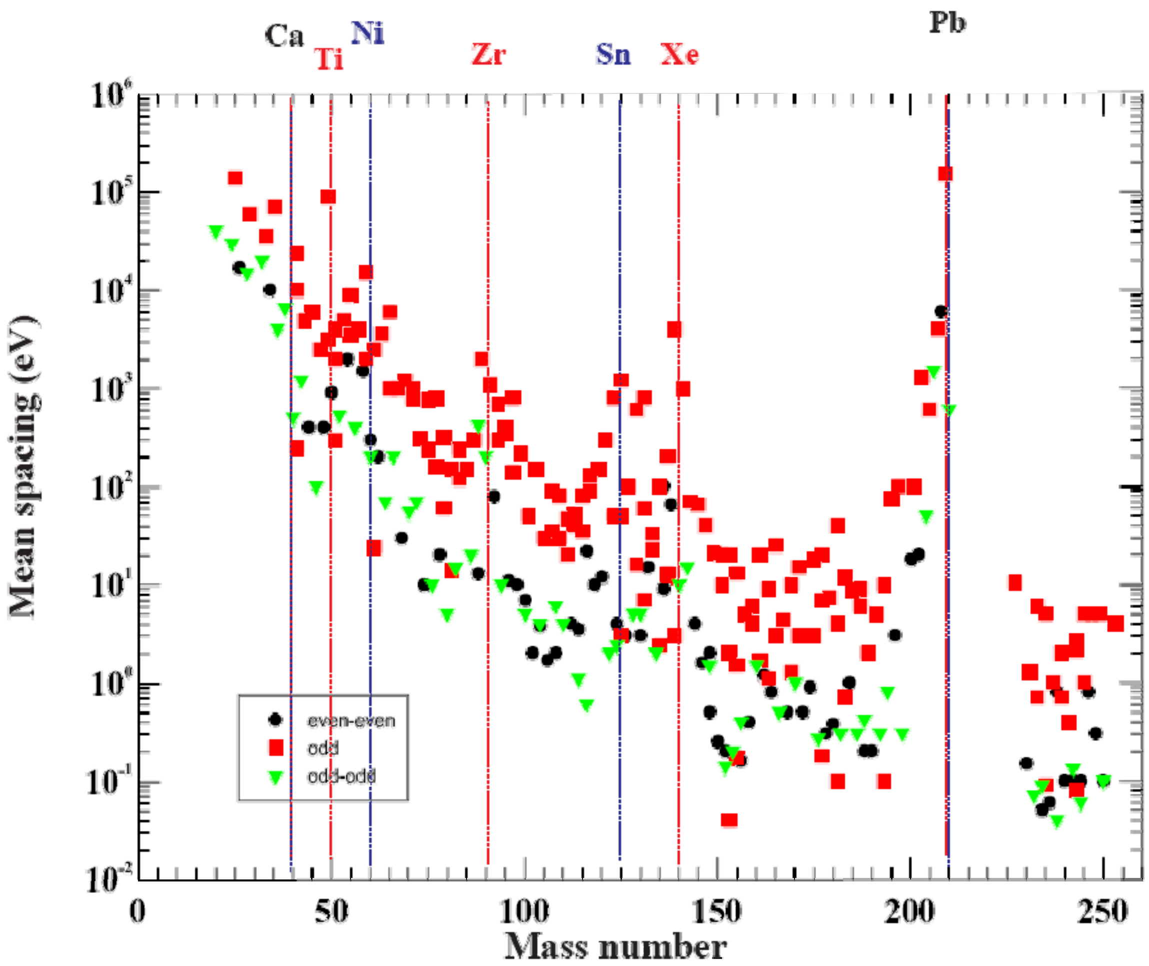
$$\Rightarrow \rho(E) = \frac{dN(E)}{dE} \quad \text{Increases exponentially}$$

$\Rightarrow$ 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

Mean spacing of s-wave neutron resonances at B_n



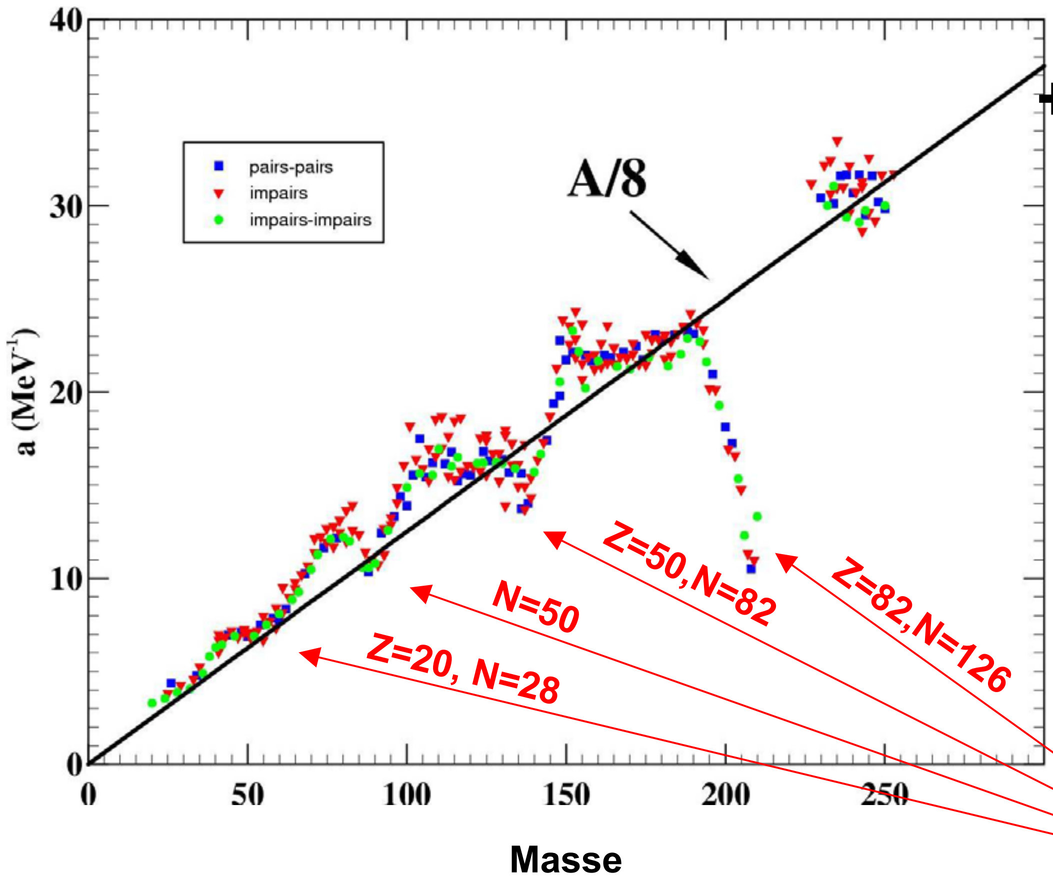
Iljinov et al., NPA 543 (1992) 517.

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

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

Quantitative analysis of mean s-wave resonances spacings at B_n

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



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

Odd-even effects accounted for

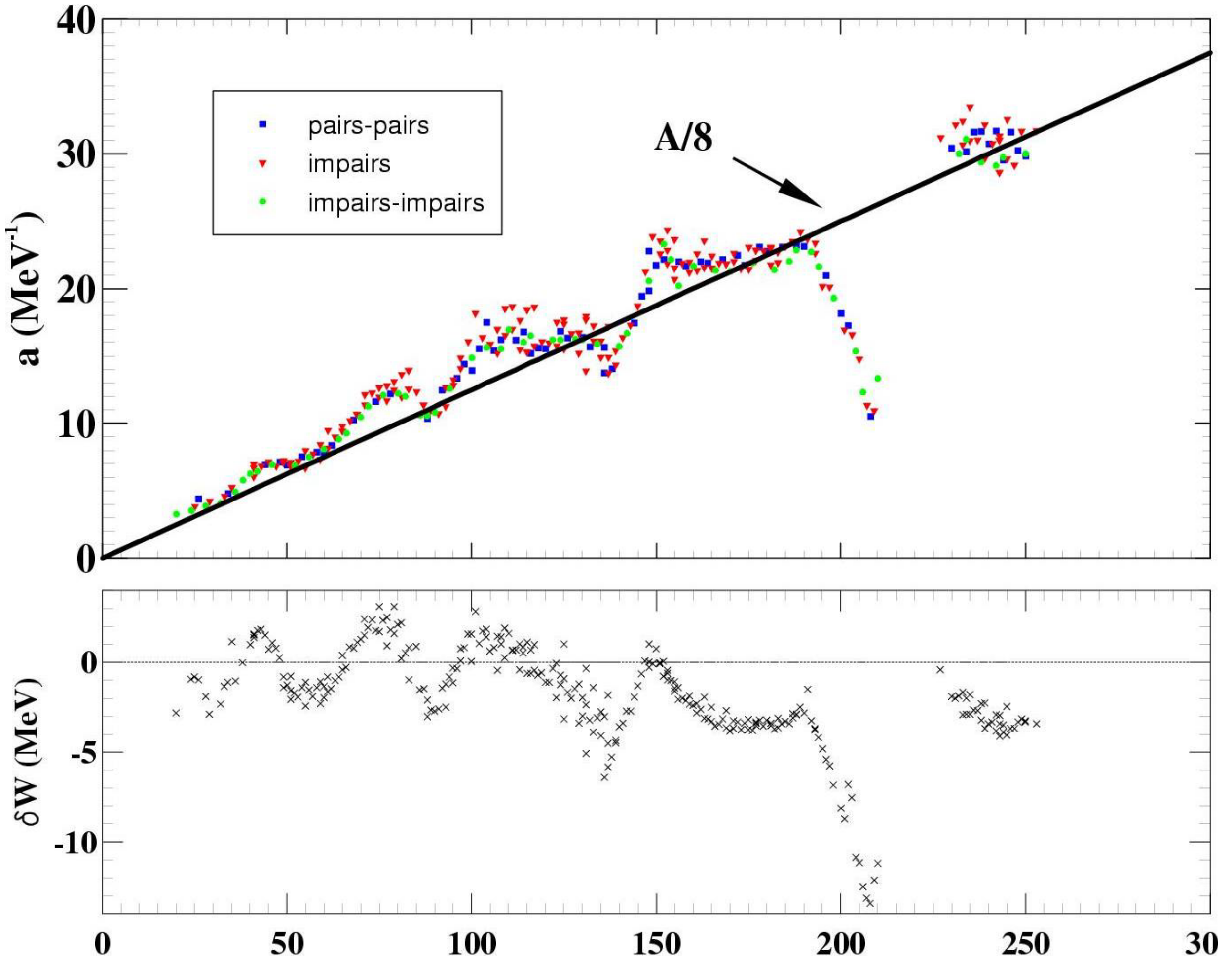
$$U \rightarrow U^* = U - \Delta$$

⇒ odd-even effects

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

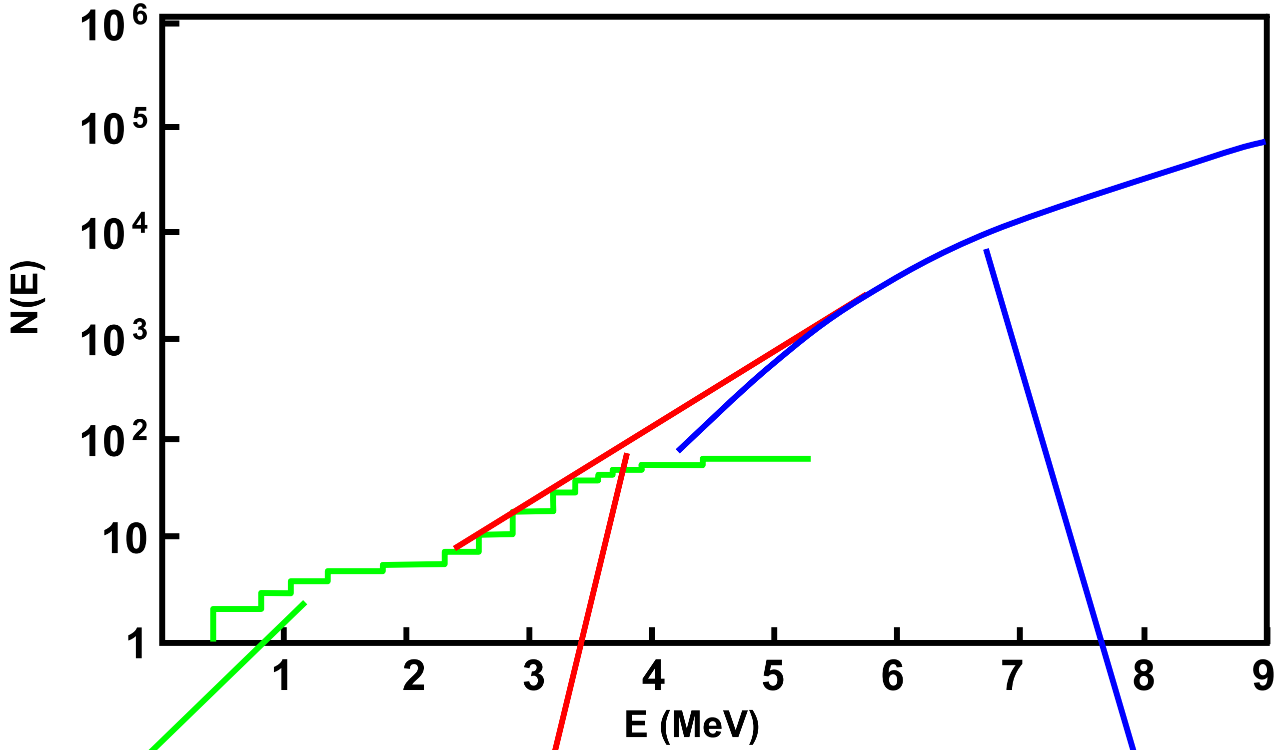
Shell effects

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 nuclear level densities



Discrete levels (spectroscopy)

Temperature law

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

Fermi gaz (adjusted at B_n)

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

Other methods

- **Superfluid model and Generalized Superfluid model**
  Ignatyuk et al., PRC 47 (1993) 1504 & RIPL2 Tecdoc (IAEA)

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

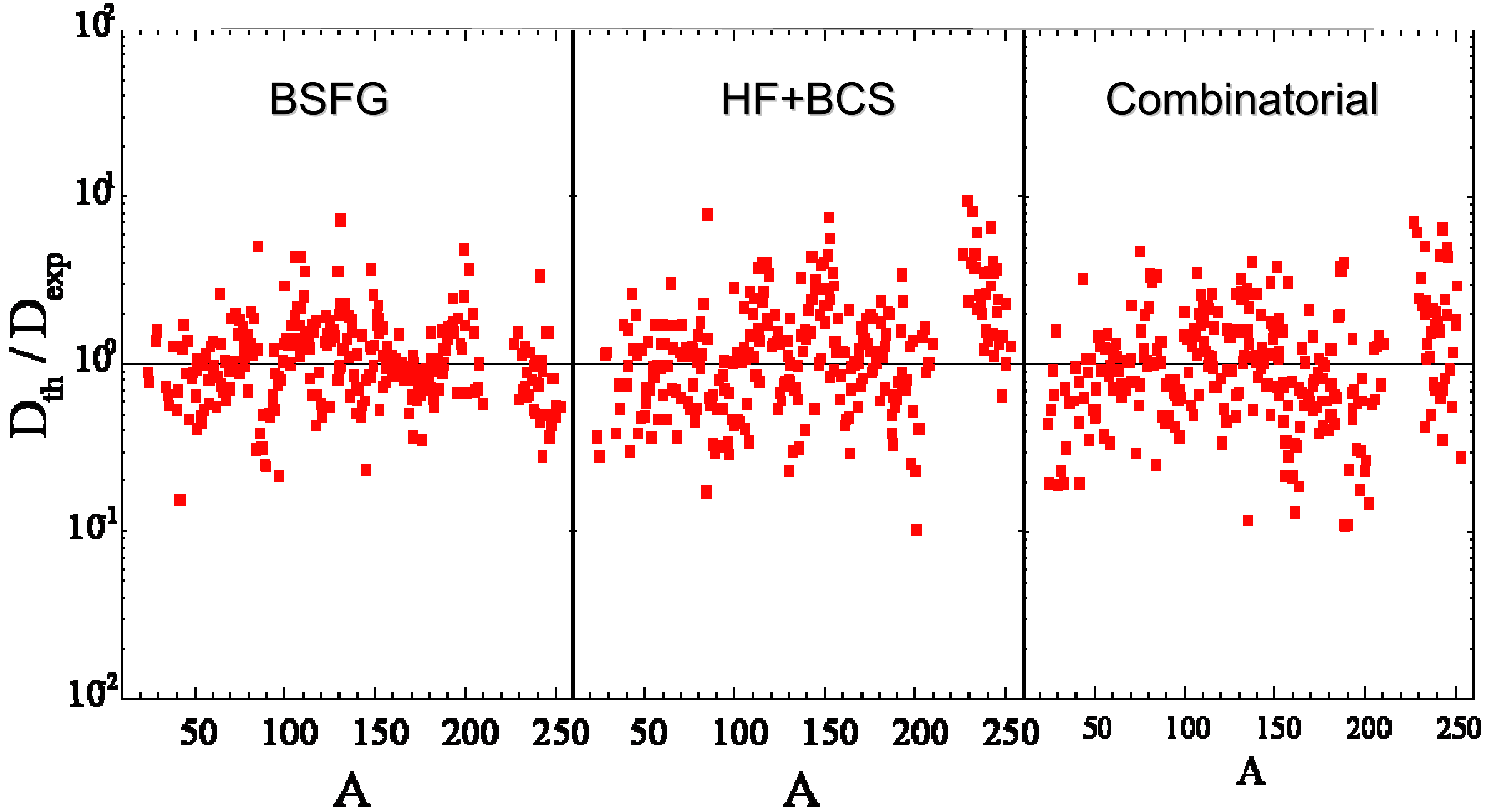
- **Shell Model Monte Carlo method**
  Agrawal et al., PRC 59 (1999) 3109 and references therein

  ⇒ More realistic hamiltonians
  ⇒ Time consuming & not of practical use

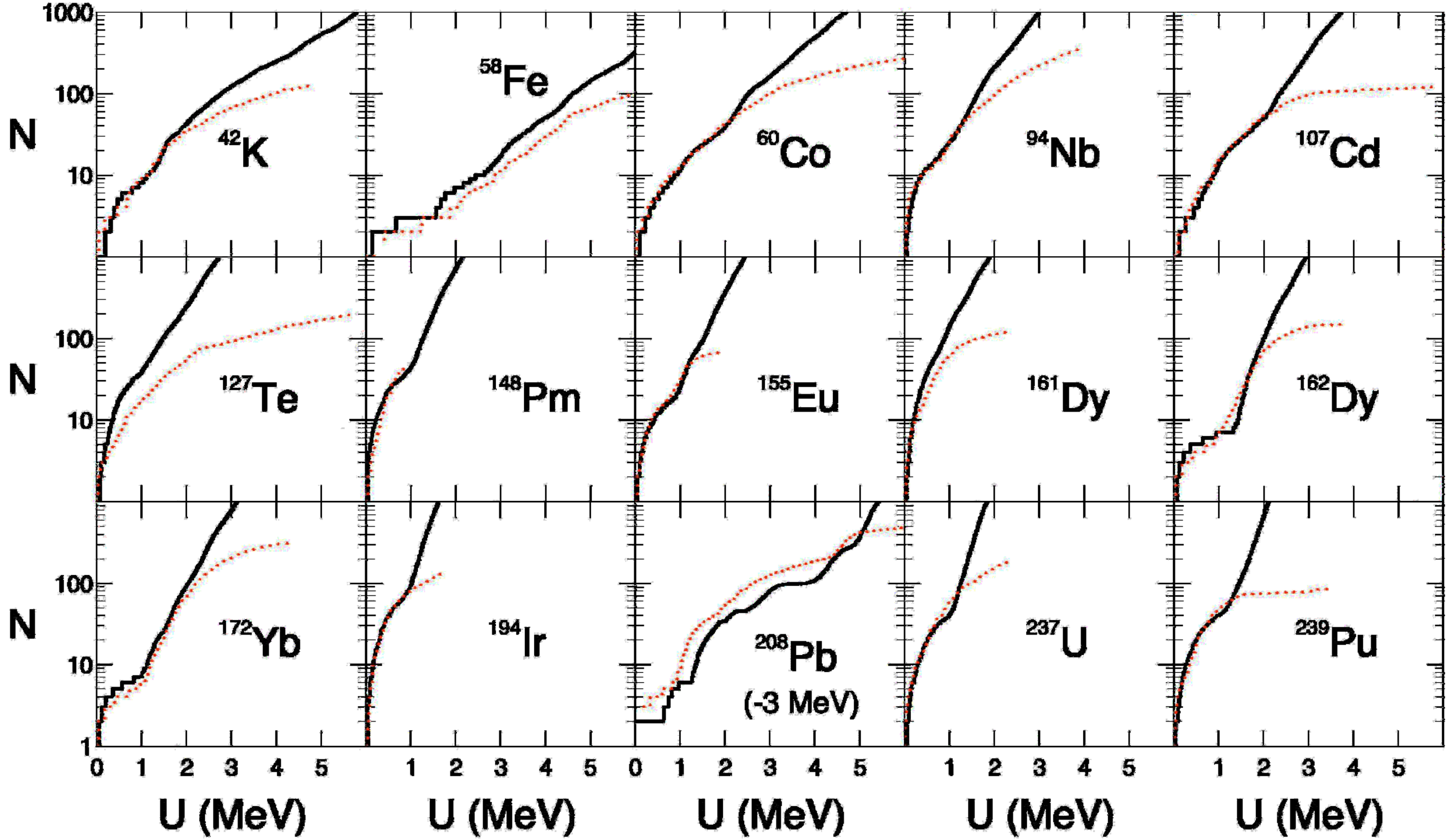
- **Combinatorial approach**
  S. Hilaire & S. Goriely, NPA 779 (2006) 63 and references therein

  ⇒ Direct counting method of both partial and total level densities
  ⇒ Access to non statistical effects

Combinatorial method



Combinatorial method



Particle-hole level densities (pure ESM)

Hilaire et al., NPA 632 (1998) 417 and references therein

- **Ericson (1960) : No Pauli principle**
  $\Rightarrow$ **global overestimation**

- **Williams (1971) : Pauli principle but finite well depth neglected**
  $\Rightarrow$ **unphysical holes and thus overestimation over a few tens of MeV**

- **Běták and Doběs (1976) : Finite well depth accounted for**
  $\Rightarrow$ **no more unphysical holes but overestimation because of mathematical approximations**

- **Obložinský (1986) : Finite depth + restricted particle levels**
  $\Rightarrow$ **same mathematical problems as Běták and Doběs**

- **Anzaldo-Meneses (1995) : Mathematical corrections**
  $\Rightarrow$ **Improvement of Williams expressions**

- **Hilaire, Delaroche & Koning (1998) : Generalised corrections**
  $\Rightarrow$ **Analytical expression = exact up to hundreds of MeV**

Particle-hole level densities (improved ESM)

- **C.Y. Fu (1984) : Advanced Pairing correction**
  ⇒ implementation in the usual Williams formula of the Superfluid model pairing in an approximate but easily tractable form
- **Akkermans & Gruppelaar (1985) : Renormalisation funciton**
  ⇒ Ensure that summing p-h densities gives total densities
- **C.Y. Fu (1985) : Advanced Spin cut-off factor**
  ⇒ same as in 1984 but for p-h spin cut-off
- **C. Kalbach (1995) : Shell Shifted ESM**
  ⇒ Inclusion and treatment of a gap in the single particle level scheme
- **Harangozo et al. (1998) : Energy dependent single particle states**

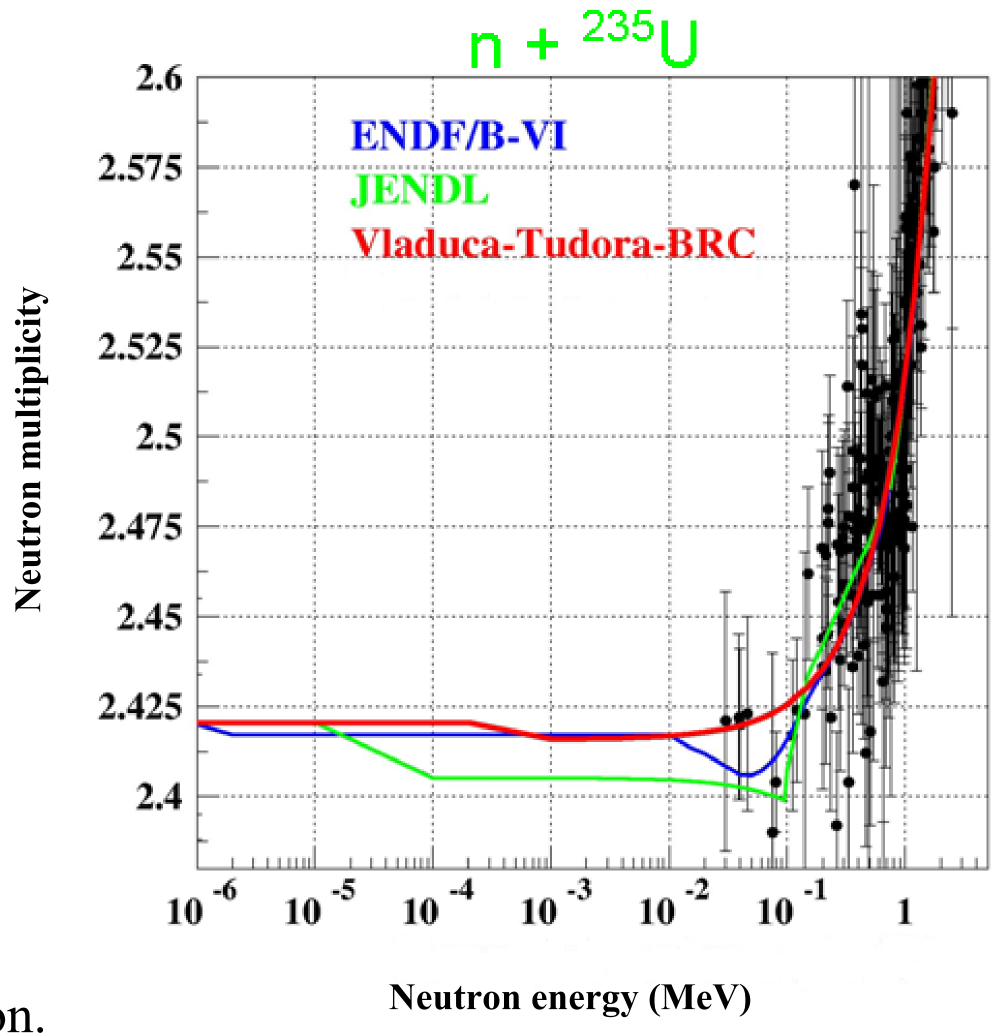
Particle-hole level densities (RIPL III)

Realistic (i.e non statistical) p-h level densities based on the combinatorial model and coherent with the total level densities within the same approach

Neutron multiplicities

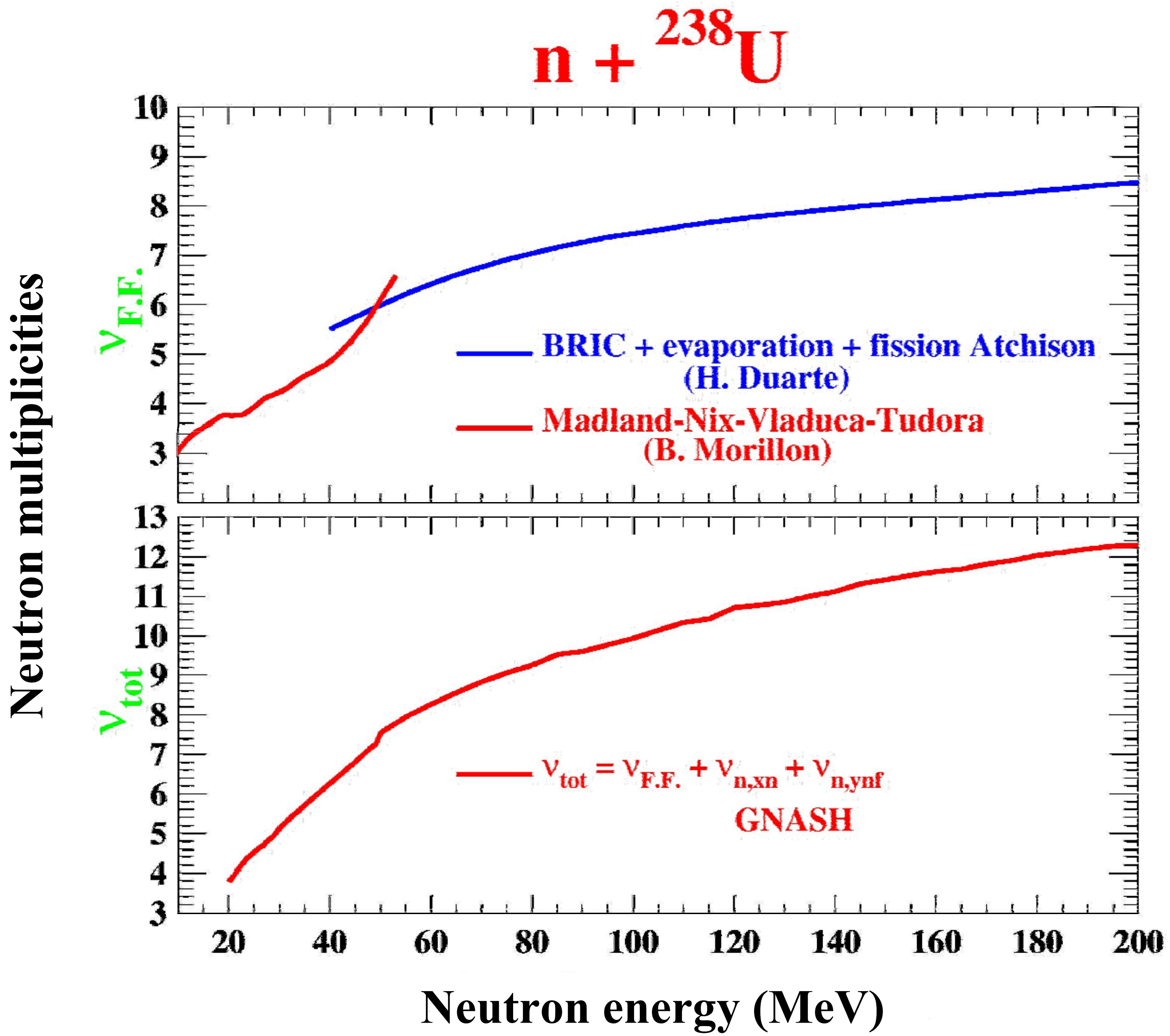
$$\overline{\nu_{p\,i}} = \frac{< E_i^* > - < E_\gamma^{tot}\, i >}{< S_{n\,i} > + < \epsilon_i >}$$

$$\overline{\nu}_p = \sum_{i=1}^{N} \frac{\sigma_{f\,i}}{\sigma_f} \left(i - 1 + \overline{\nu}_{p\,i}\right)$$

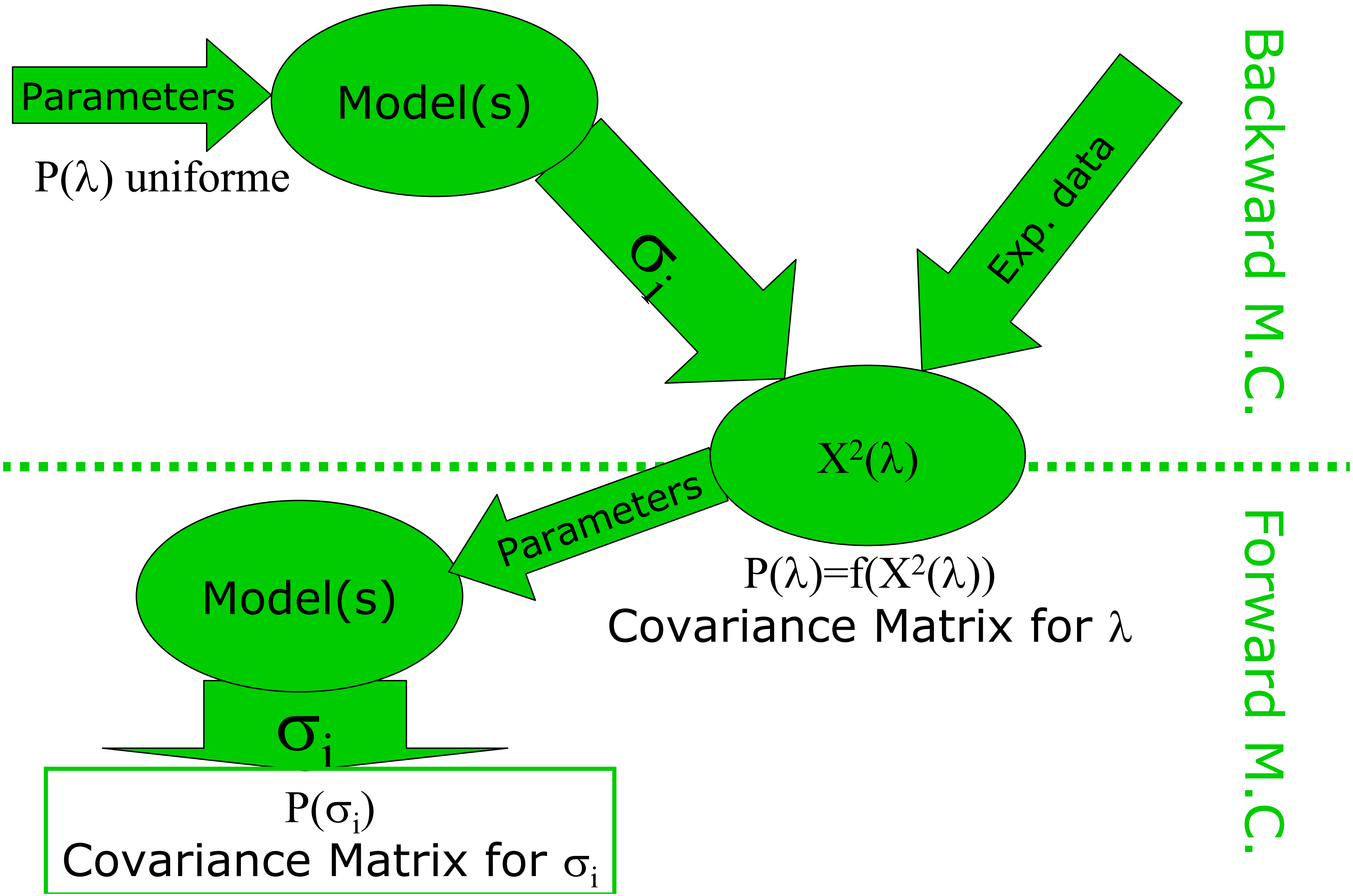


$\sigma_{f\,i}$: i^{th} chance fission cross section.

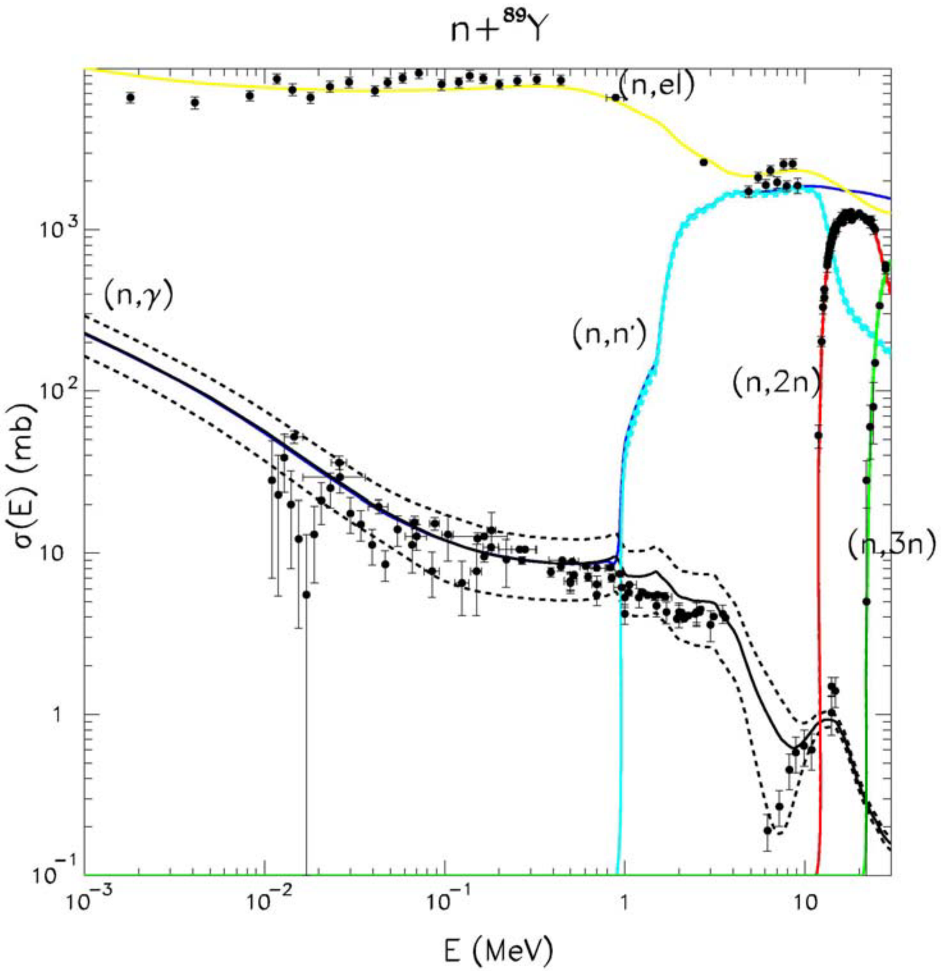
Neutron multiplicities
Connection with a high energy model

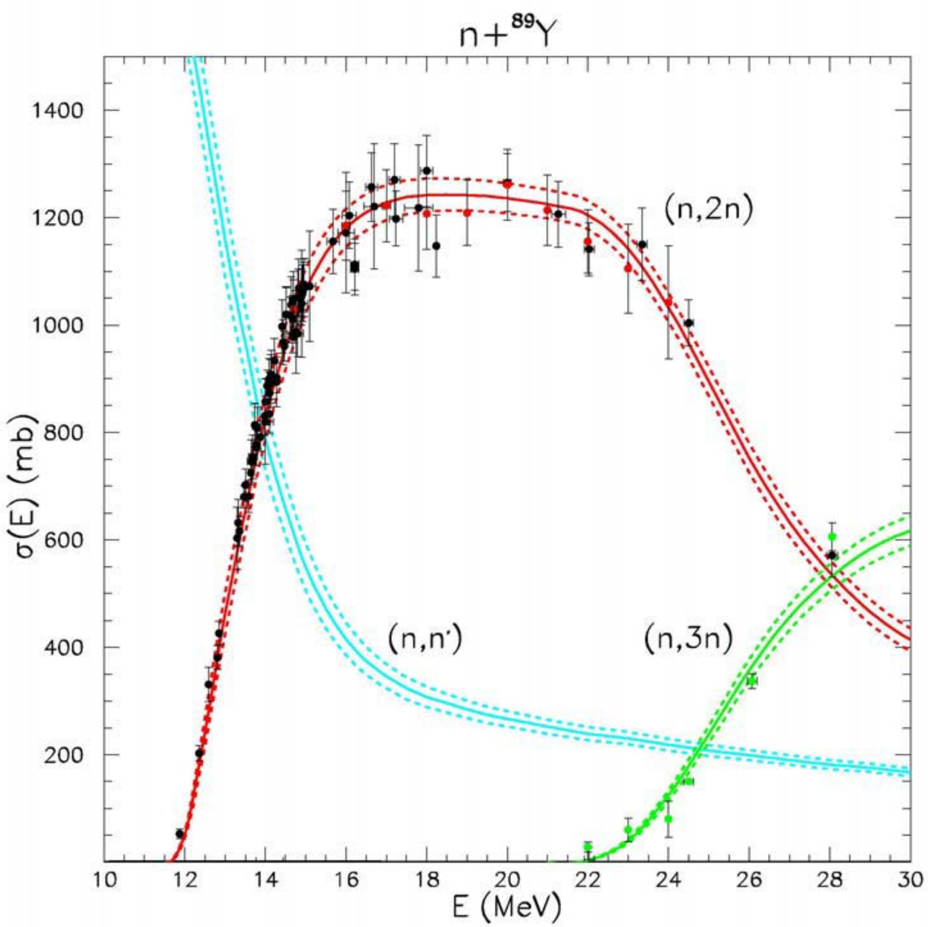


Backward-Forward Monte-Carlo method

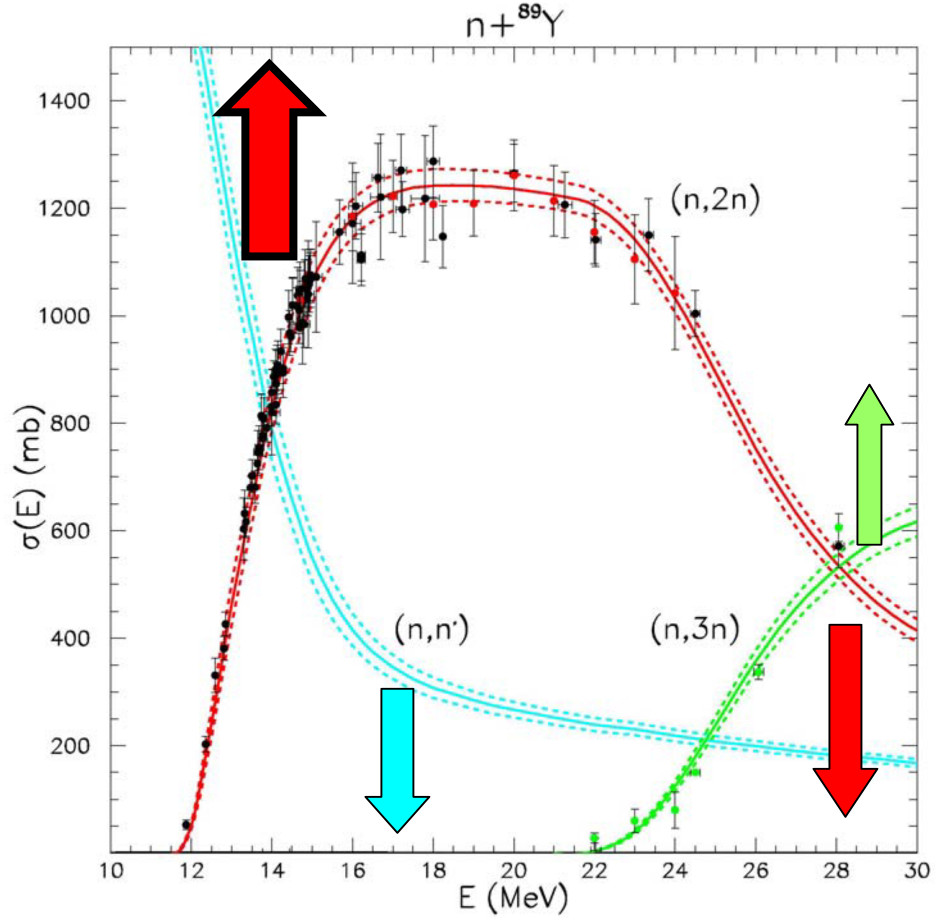


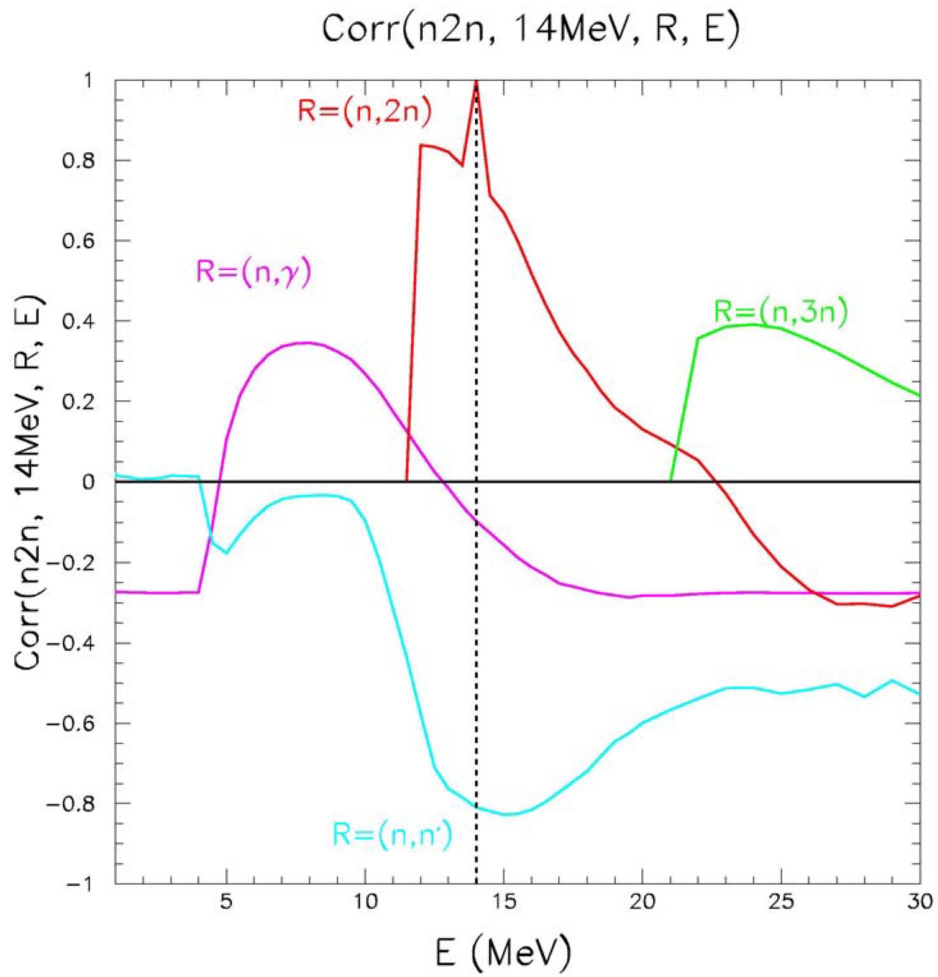
Variance-covariance matrices





Variance-covariance matrices





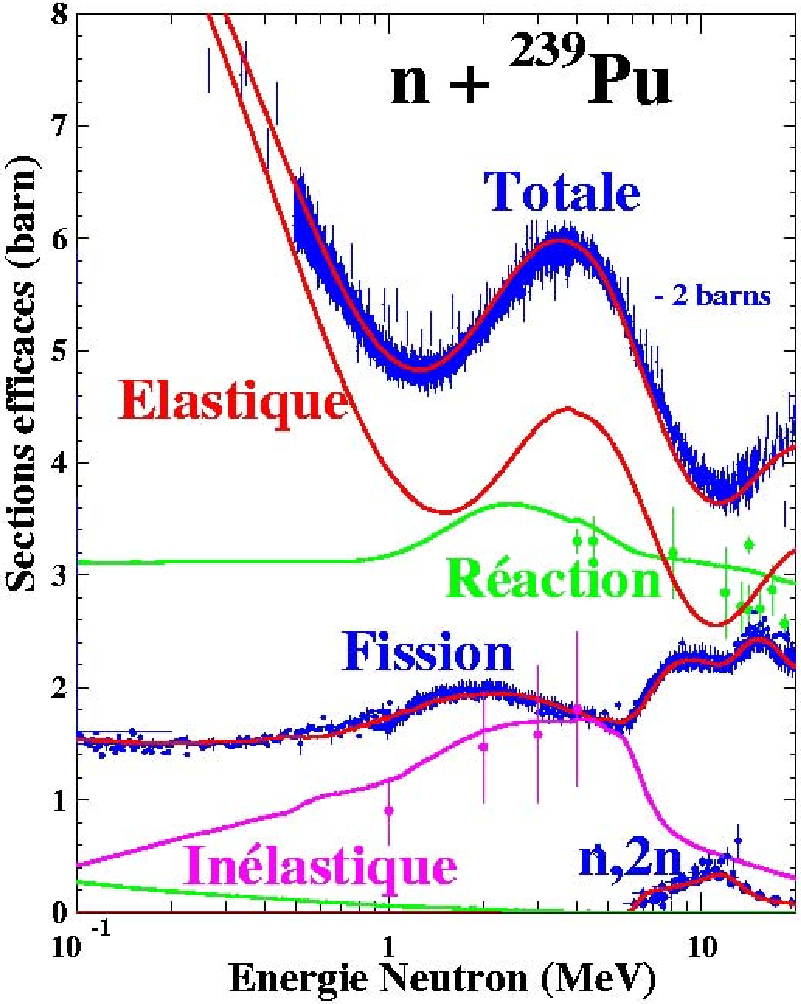
4th PART

Few concrete examples

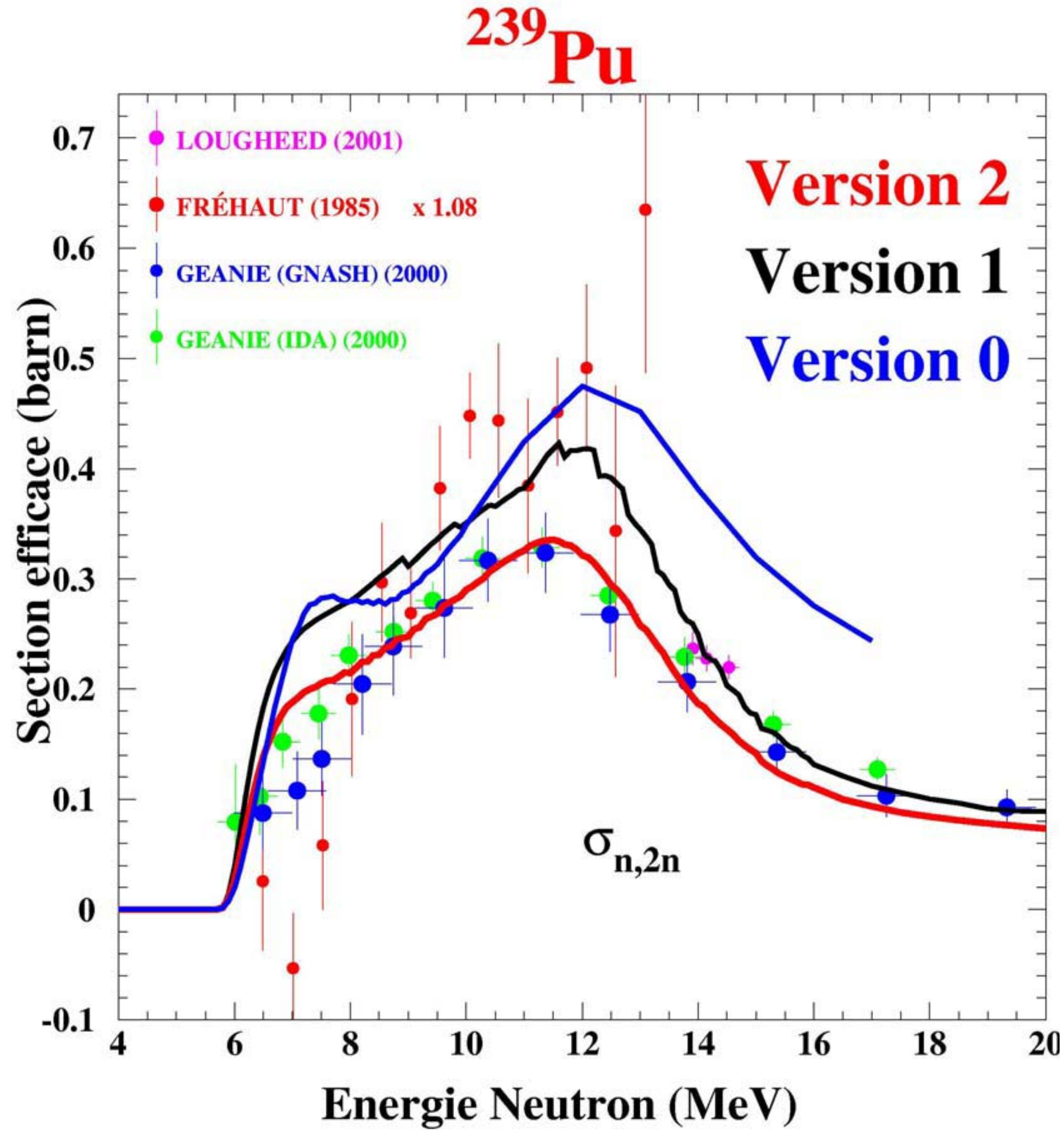
Few concrete examples

- (n,2n) cross section for ^{239}Pu
- Europium neutron cross sections
- Impact of nuclear level densities
- Multiple chance fission & model coherence
- Coupled channel impact
- Problème des sections efficaces expérimentales $^{238}Pu(n,f)$
- Test relatif des évaluations n+^{235}U et n+^{239}Pu
- Validation with integral experiment
- Feedback from integral experiment

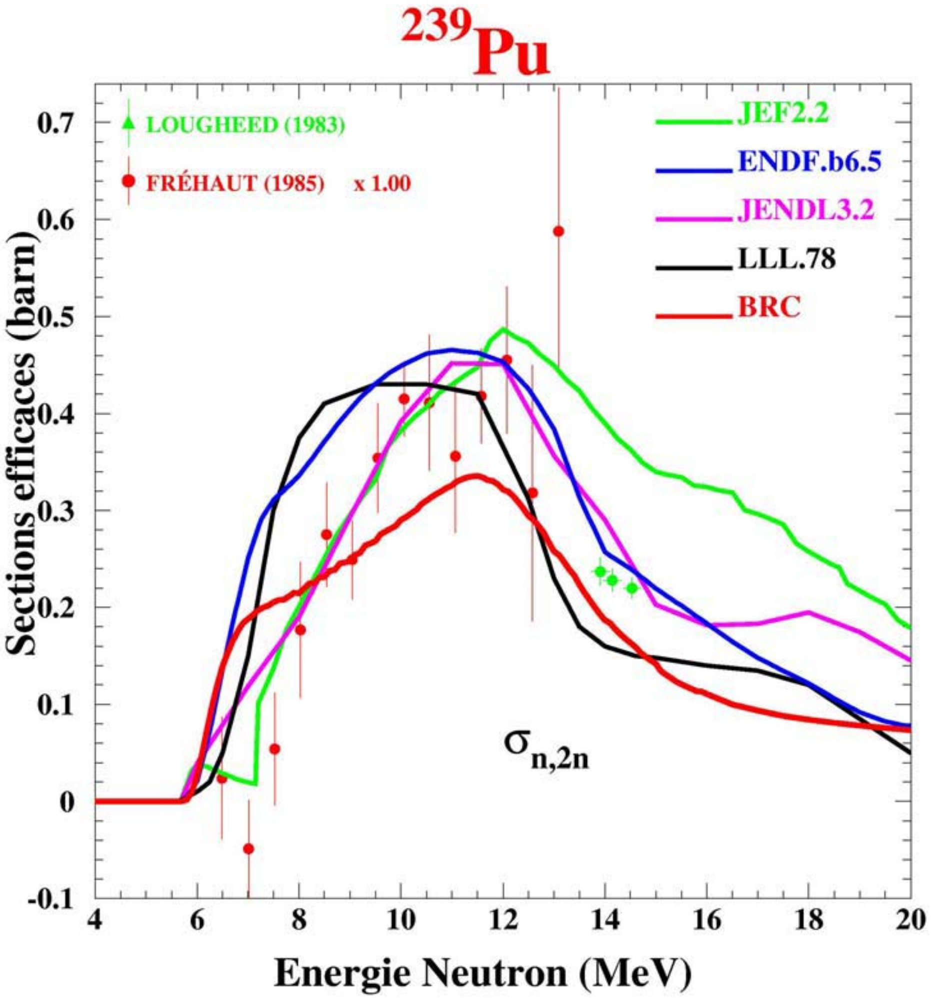
The (n,2n) odyssey



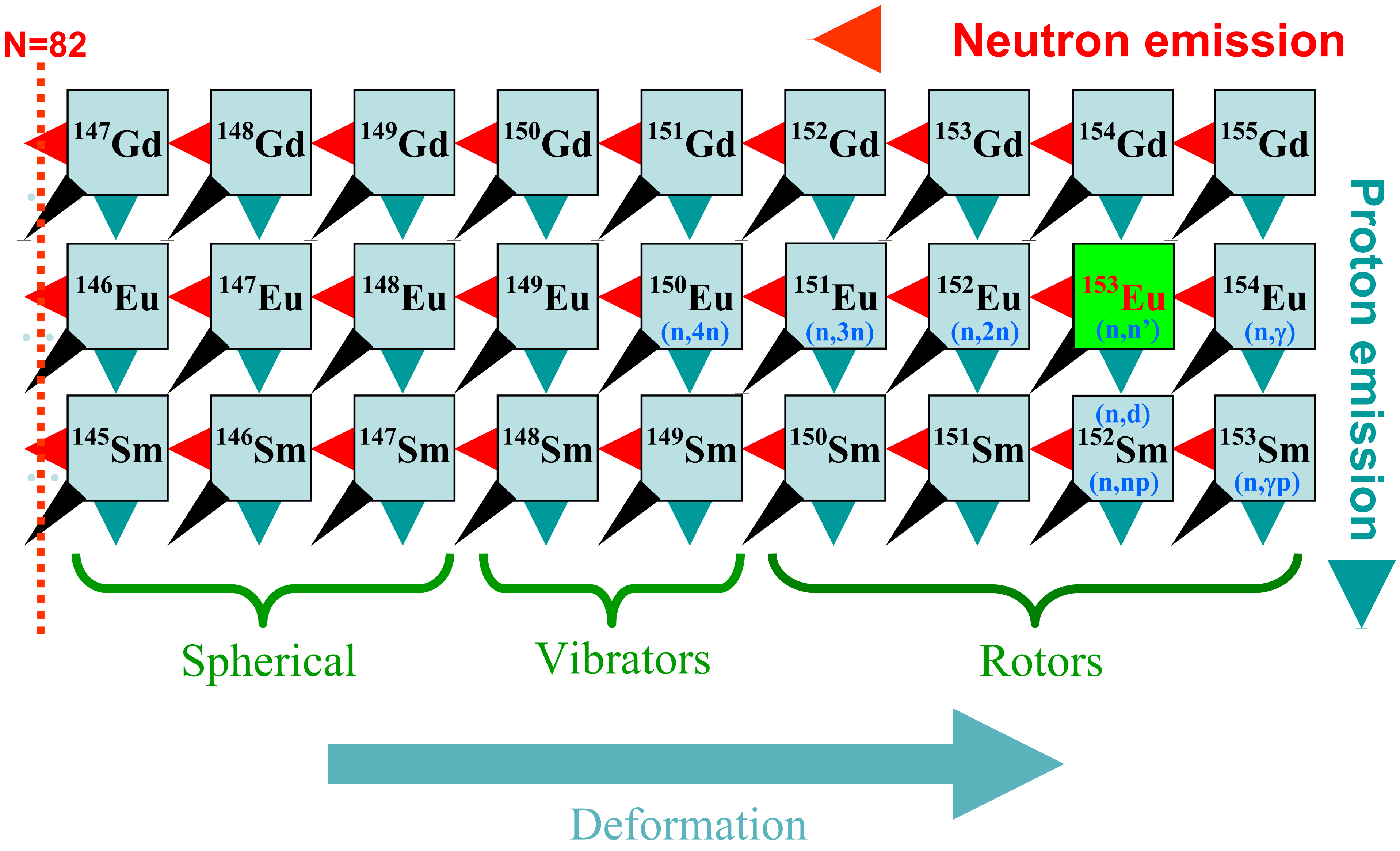
The (n,2n) odyssey



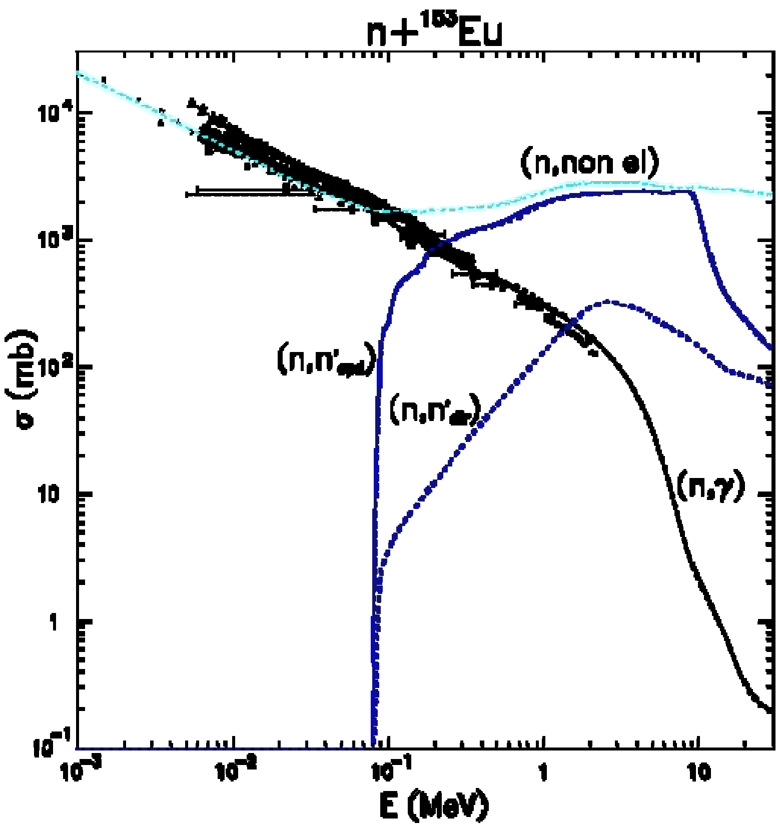
The (n,2n) odyssey



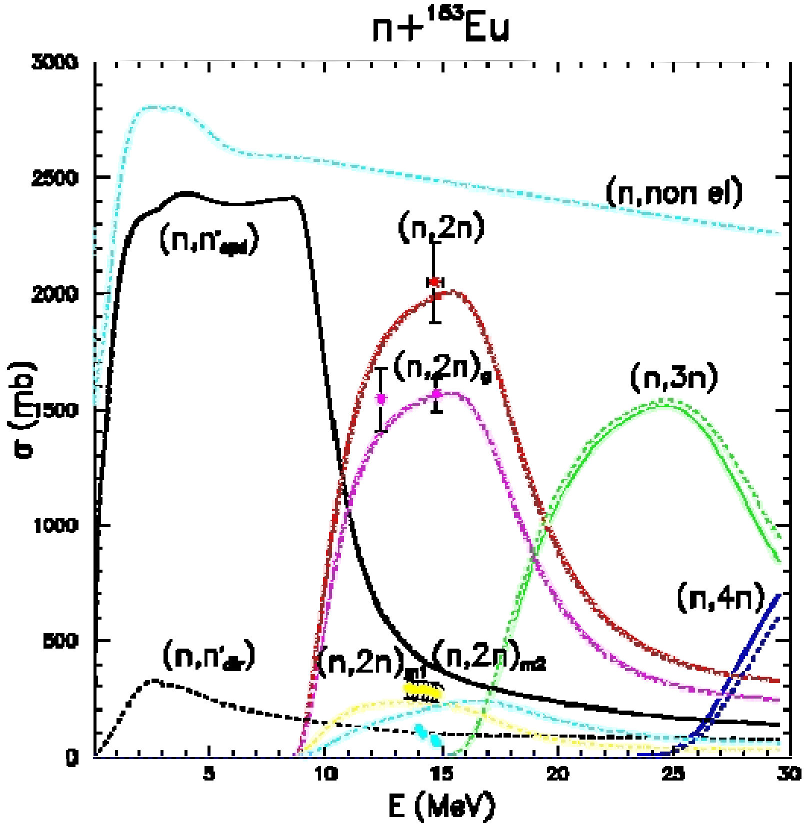
Europiums


N=82
Neutron emission
Proton emission
^{147}Gd ^{148}Gd ^{149}Gd ^{150}Gd ^{151}Gd ^{152}Gd ^{153}Gd ^{154}Gd ^{155}Gd
^{146}Eu ^{147}Eu ^{148}Eu ^{149}Eu ^{150}Eu (n,4n) ^{151}Eu (n,3n) ^{152}Eu (n,2n) ^{153}Eu (n,n’) ^{154}Eu (n,γ)
^{145}Sm ^{146}Sm ^{147}Sm ^{148}Sm ^{149}Sm ^{150}Sm ^{151}Sm (n,d) ^{152}Sm (n,np) ^{153}Sm (n,γp)
Spherical
Vibrators
Rotors
Deformation

Europiums

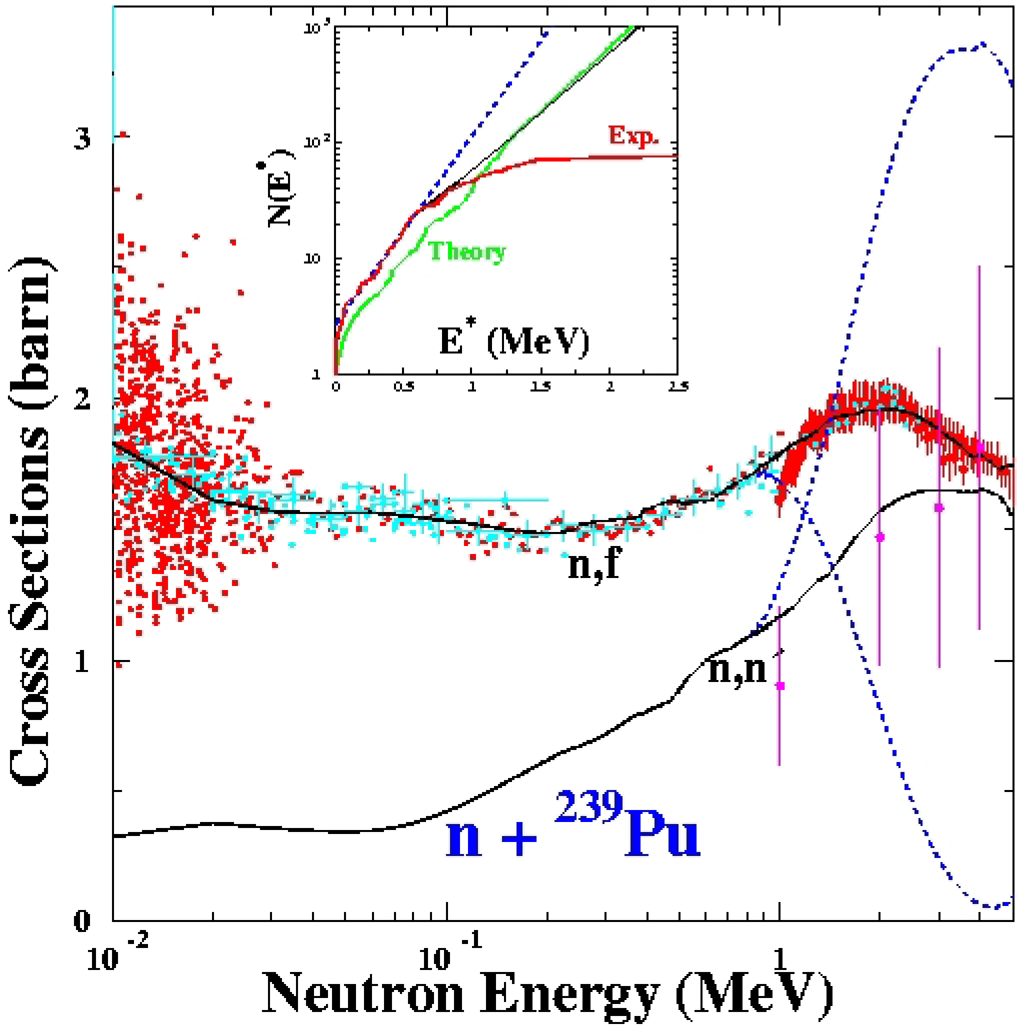


$n+^{153}Eu$
(n,non el)
(n,n'spd)
(n,n'dir)
(n,γ)
σ (mb)
E (MeV)

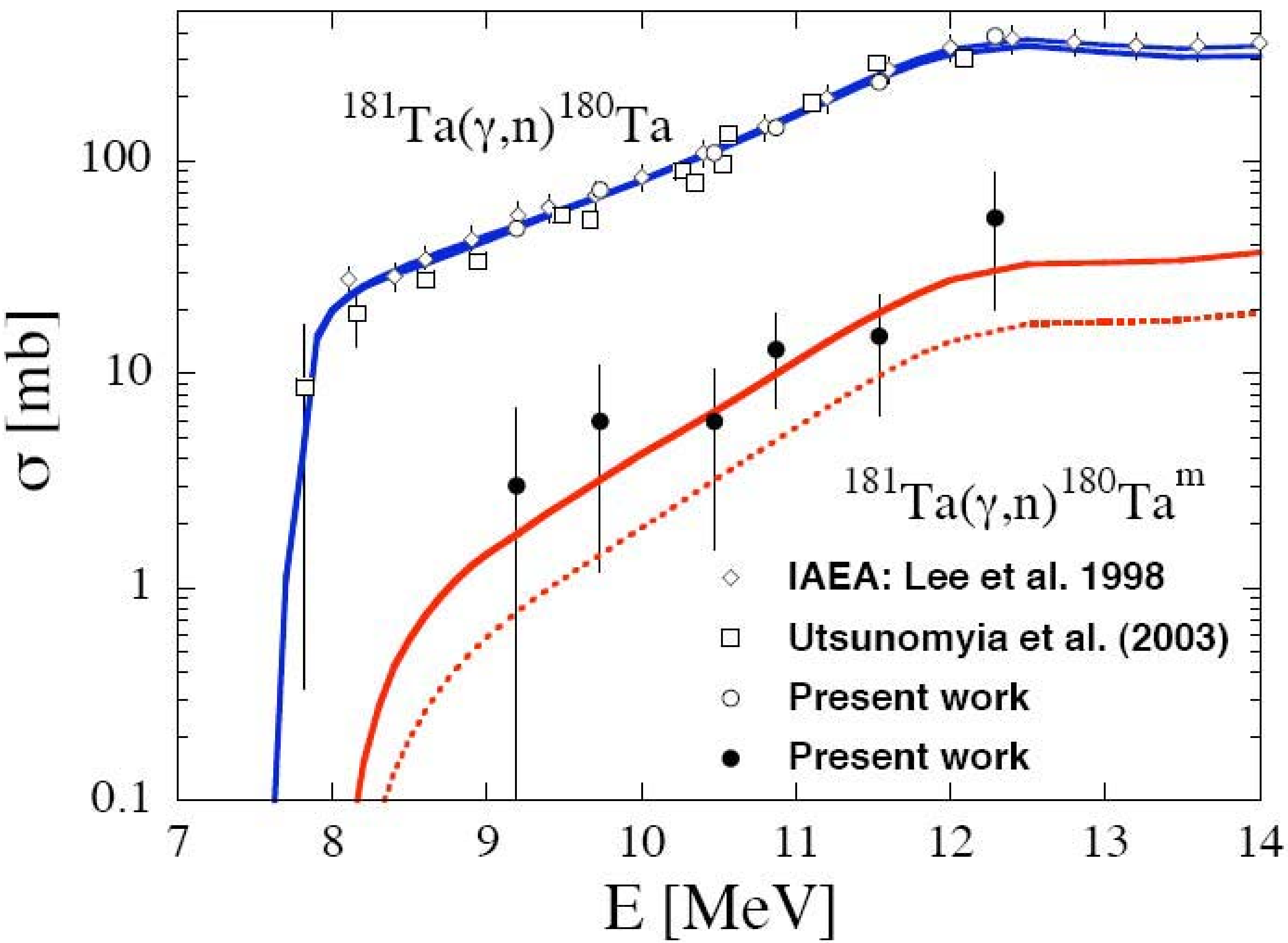


$n+^{153}Eu$
(n,non el)
(n,n'spd)
(n,2n)
(n,2n)g
(n,3n)
(n,4n)
(n,n'dir)
(n,2n)m1
(n,2n)m2
σ (mb)
E (MeV)

Impact of level densities

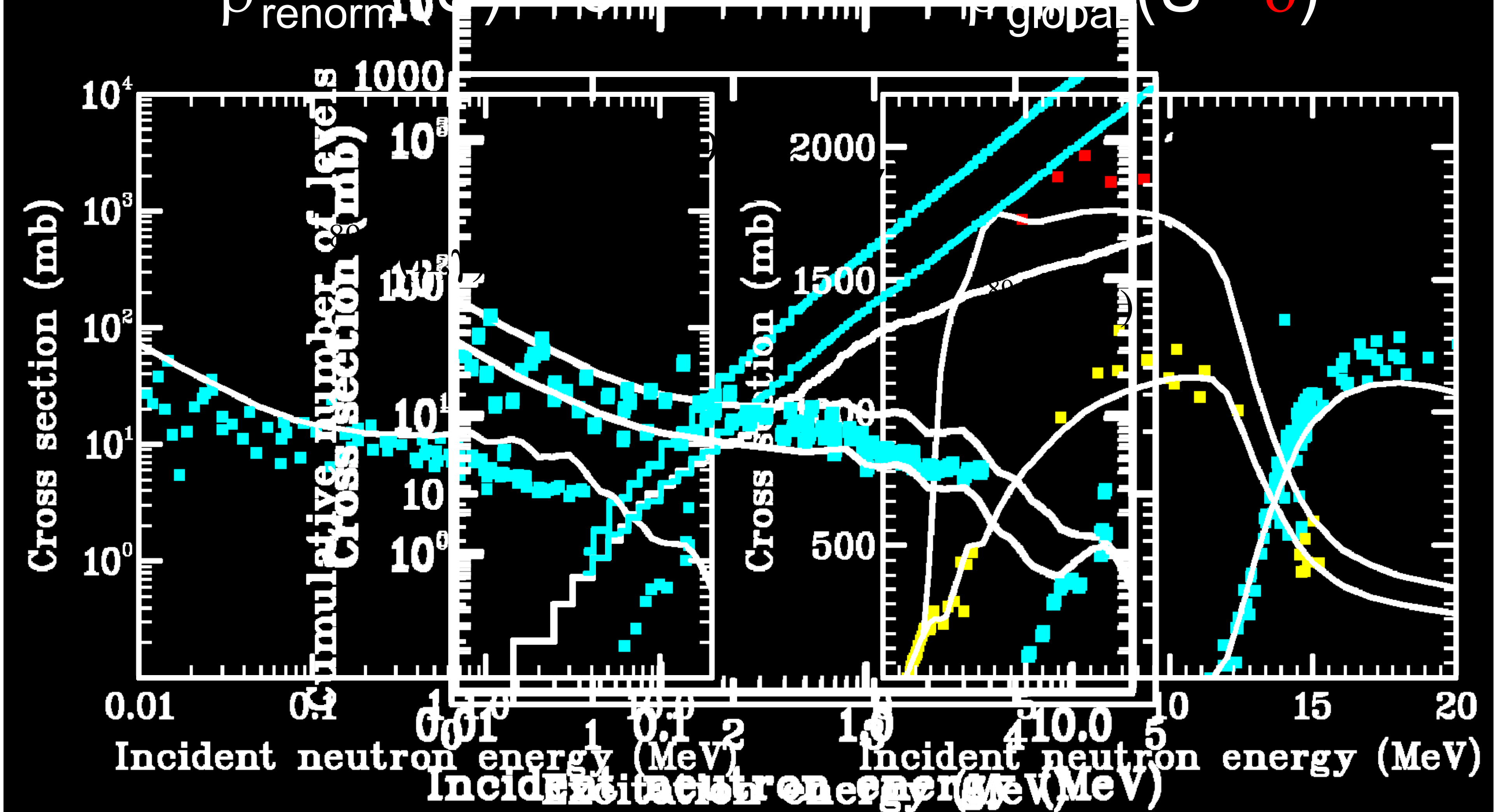


Impact of level densities

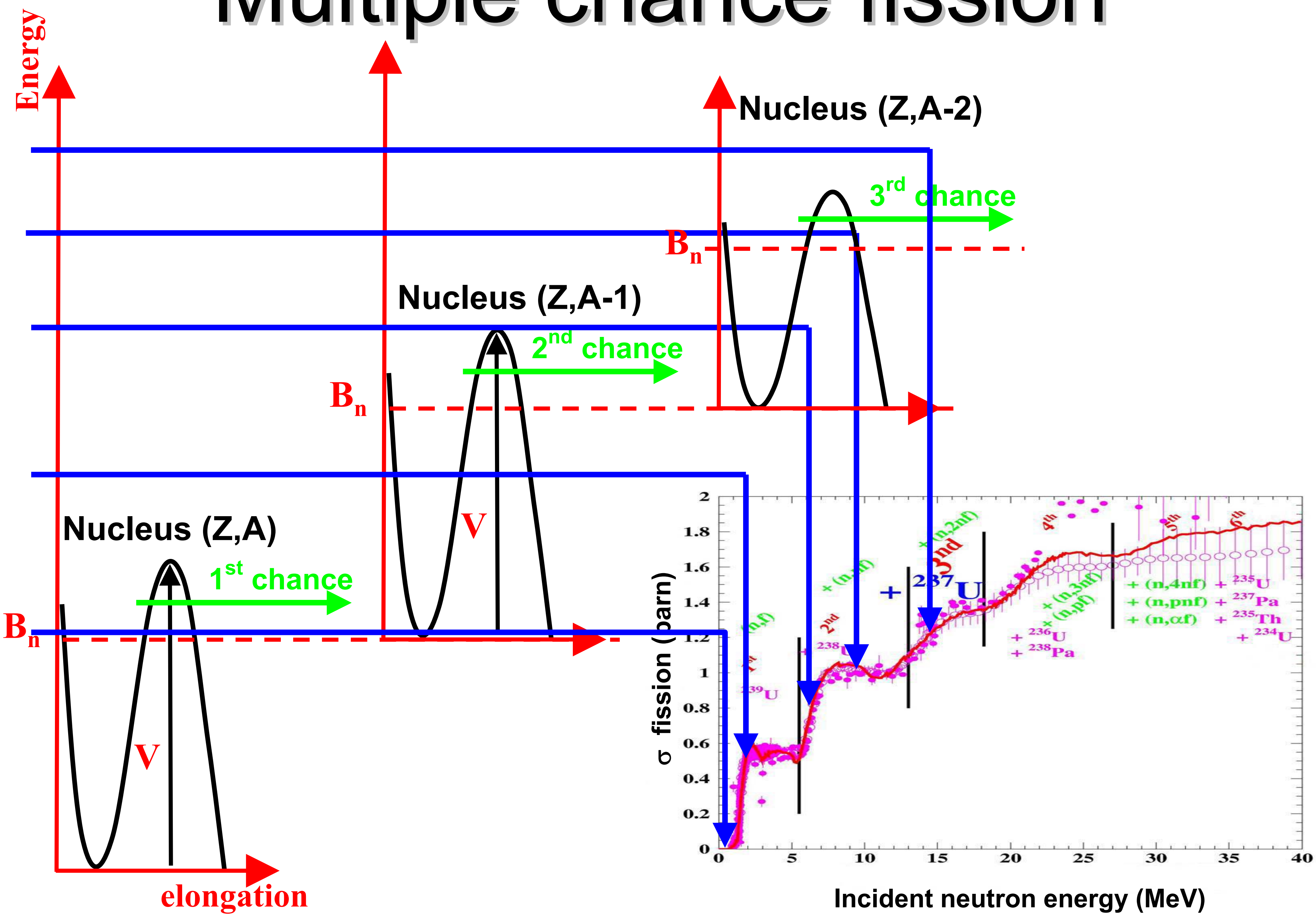


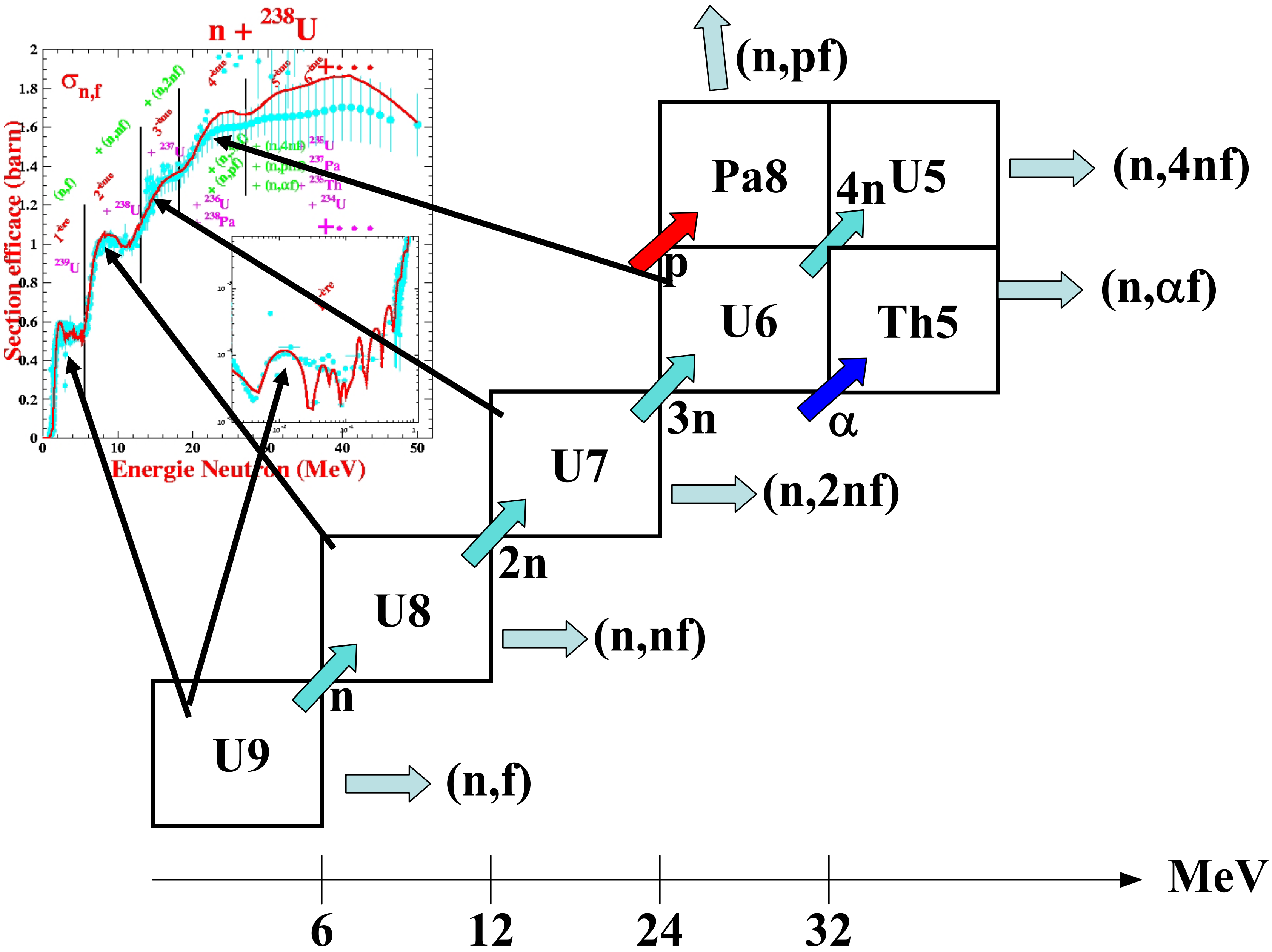
Impact of level densities

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



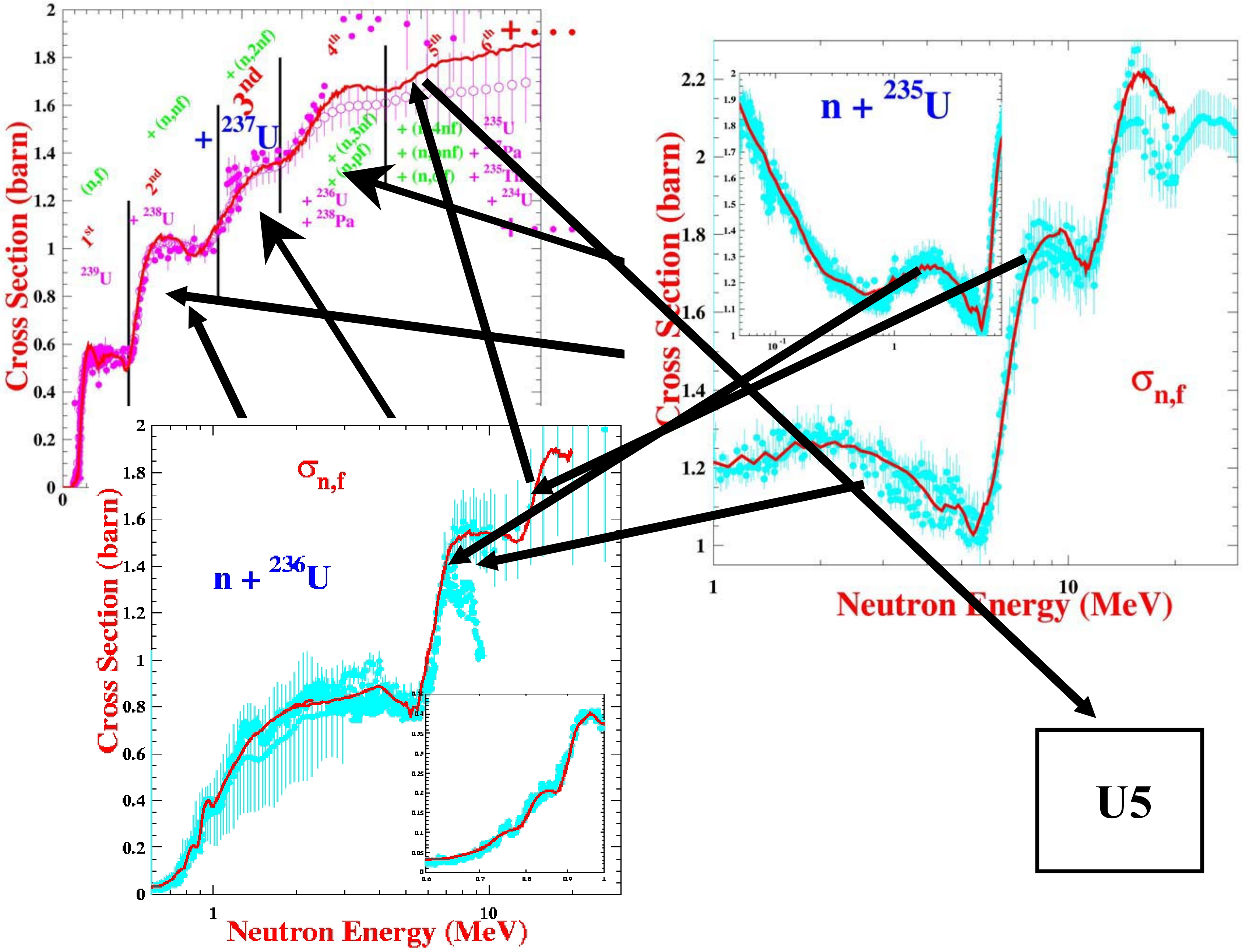
Multiple chance fission



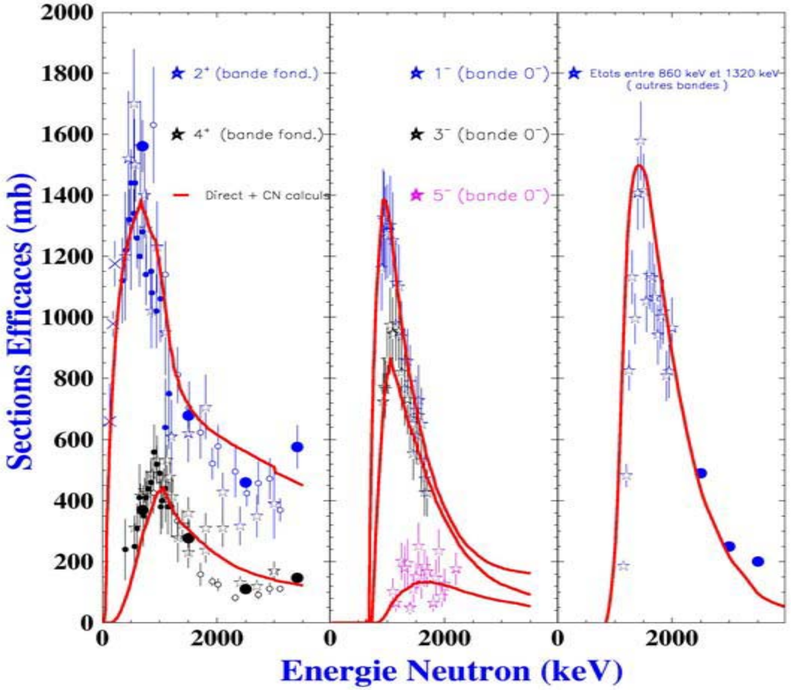


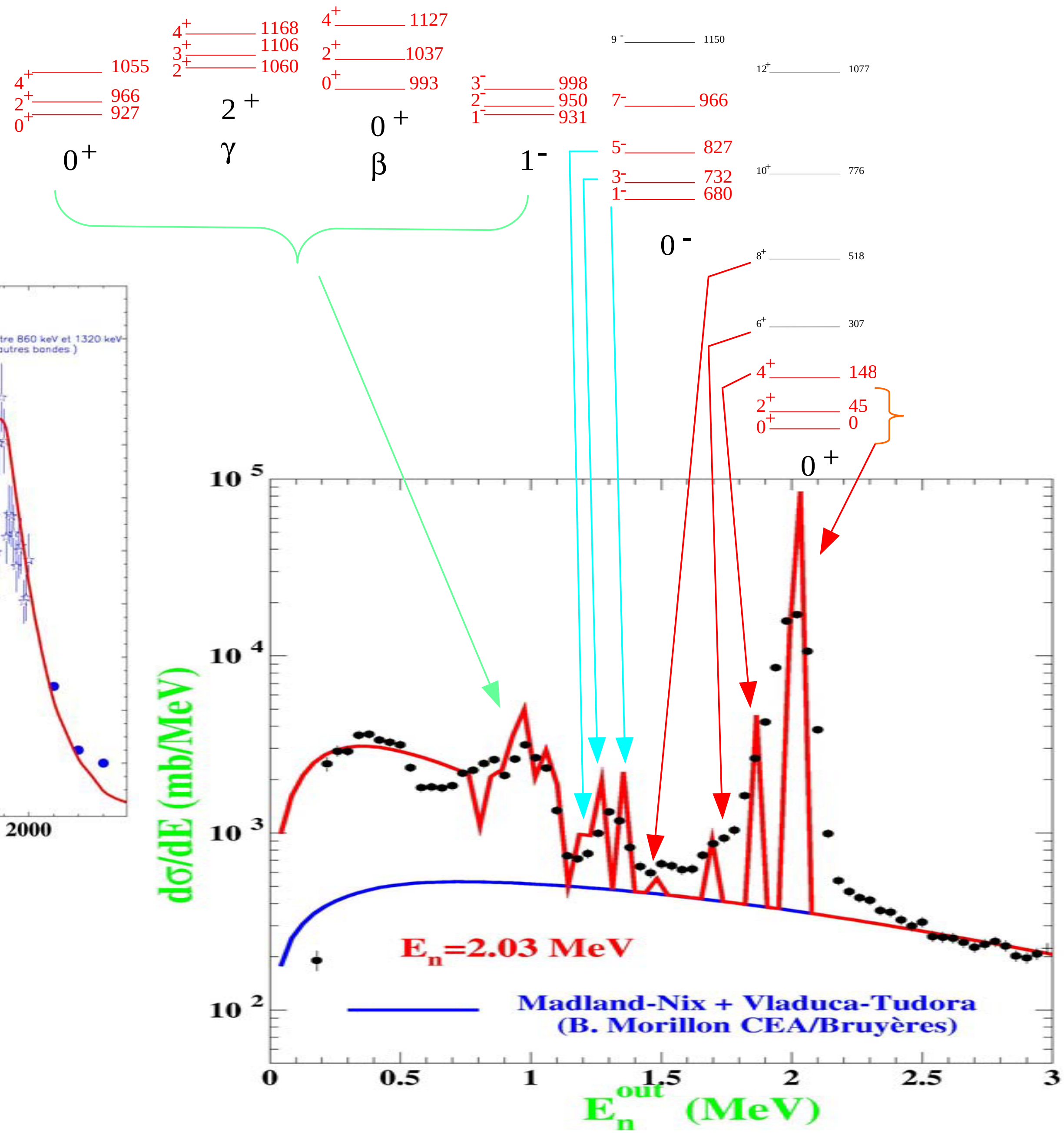
n + 238U
σn,f
Section efficace (barn)
Energie Neutron (MeV)
(n,pf)
Pa8
4nU5
(n,4nf)
p
U6
Th5
(n,αf)
3n
α
U7
(n,2nf)
2n
U8
(n,nf)
n
U9
(n,f)
6
12
24
32
MeV

What is a coherent treatment

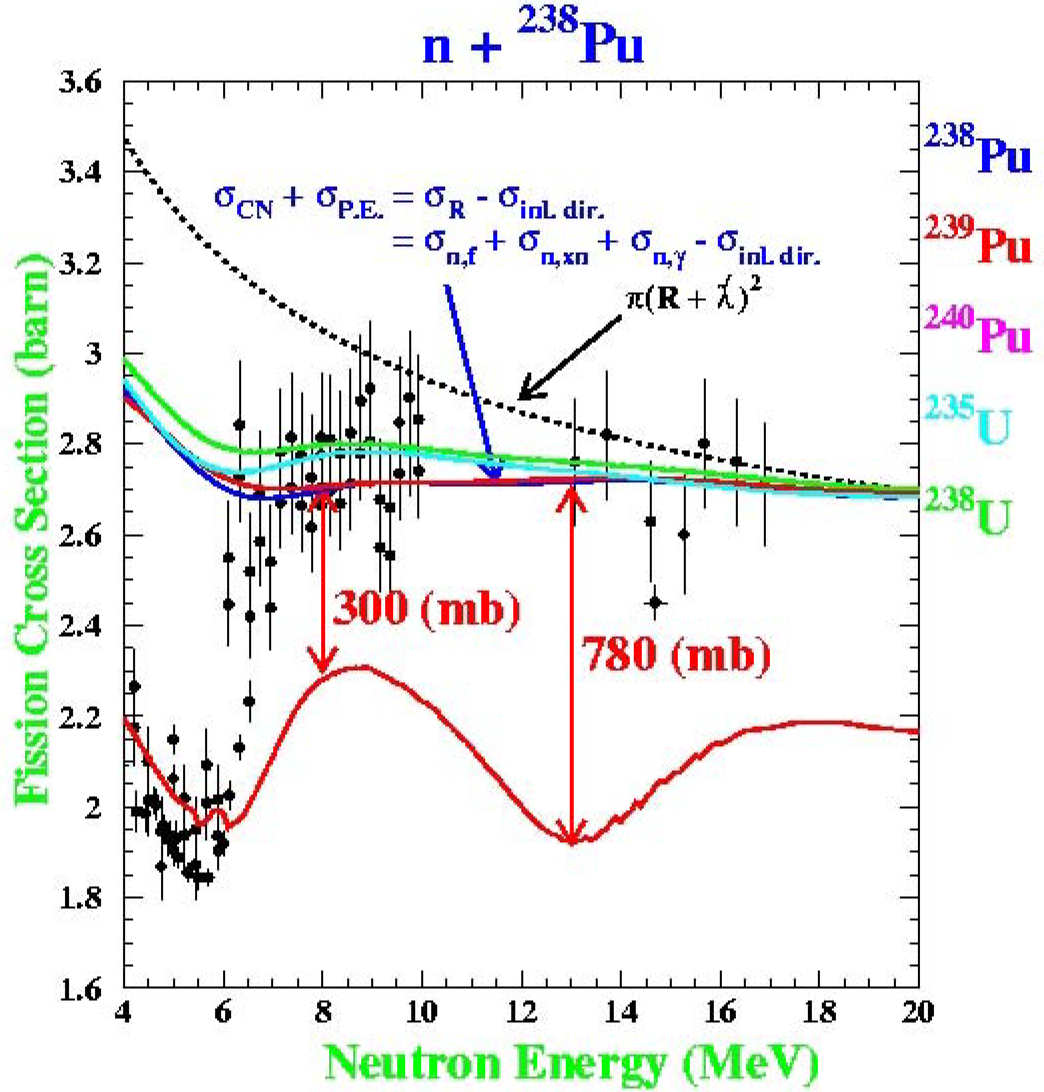


Coupled channel impact

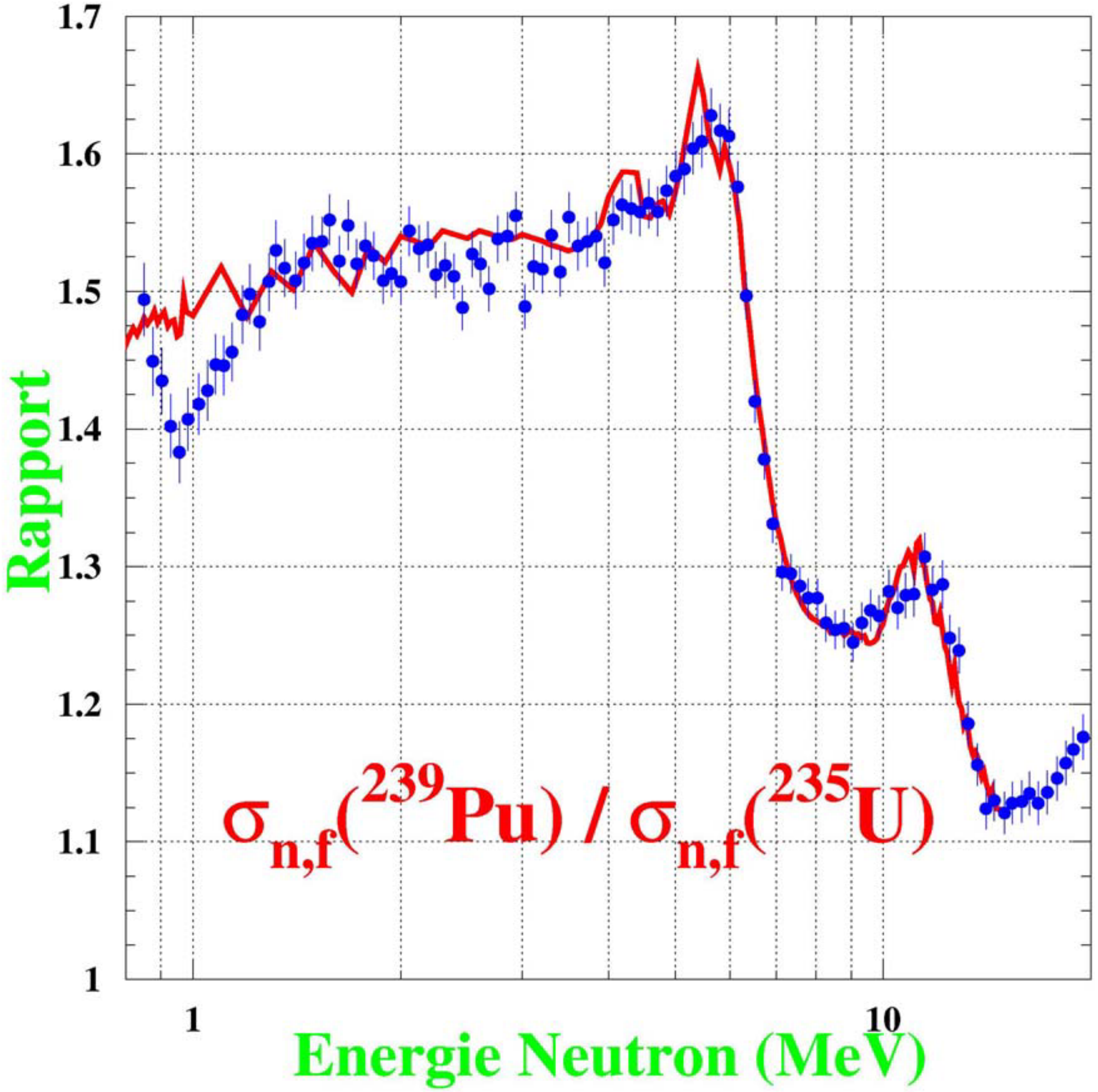




Strange experimental cross section for $^{238}Pu(n,f)$



Testing n+^{235}U vs n+^{239}Pu



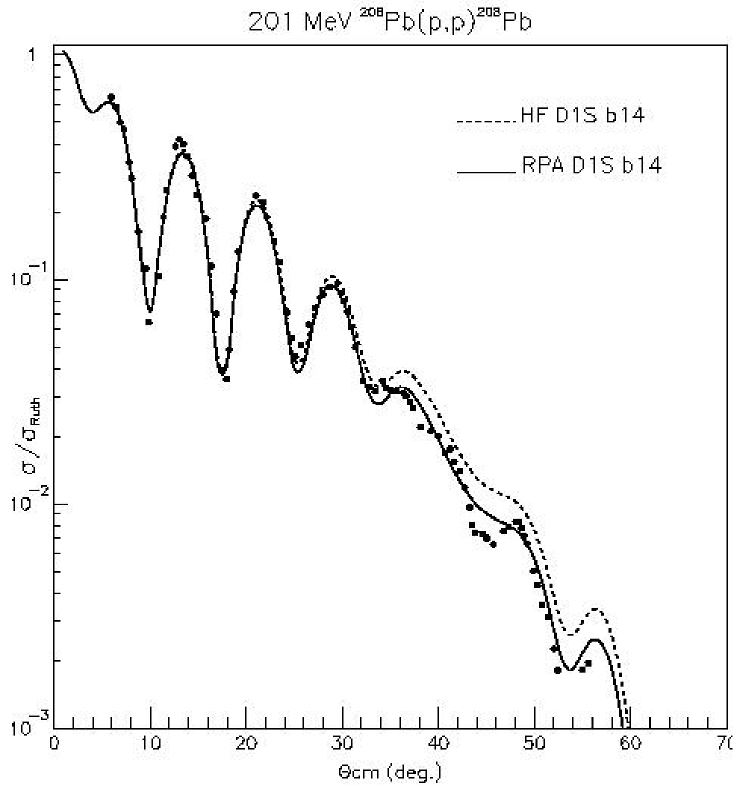
5th PART

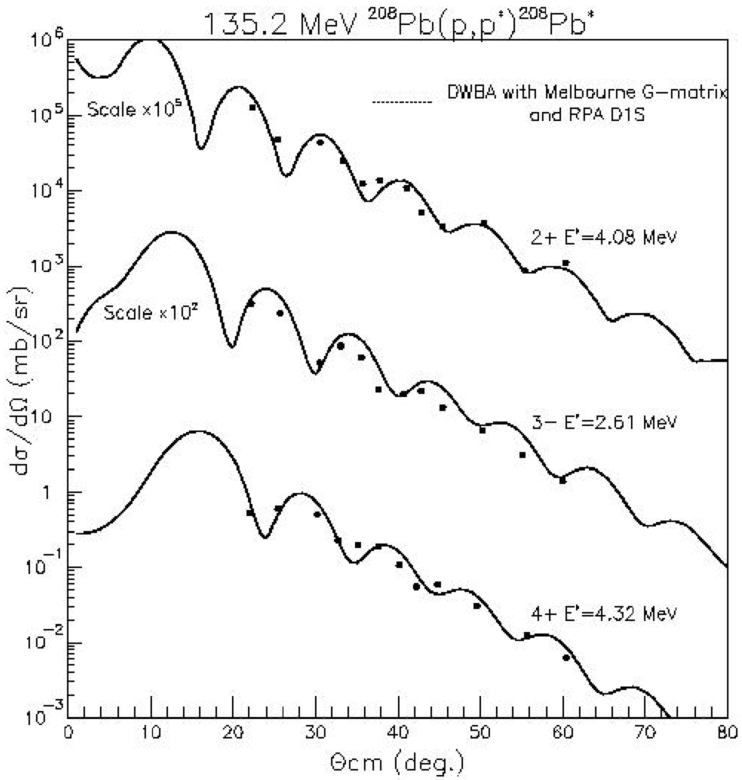
Prospects

Microscopic optical potential ?

Takes into account even more nuclear structure information than does the JLM model.

Under development but too much time consuming and not very good for low energy.





Microscopic pre-equilibrium ?

FKK : Quantum & realistic pre-equilibrium model in which particle-hole excitations are followed and calculated individually and precisely using microscopic ingredients.

Advantages :

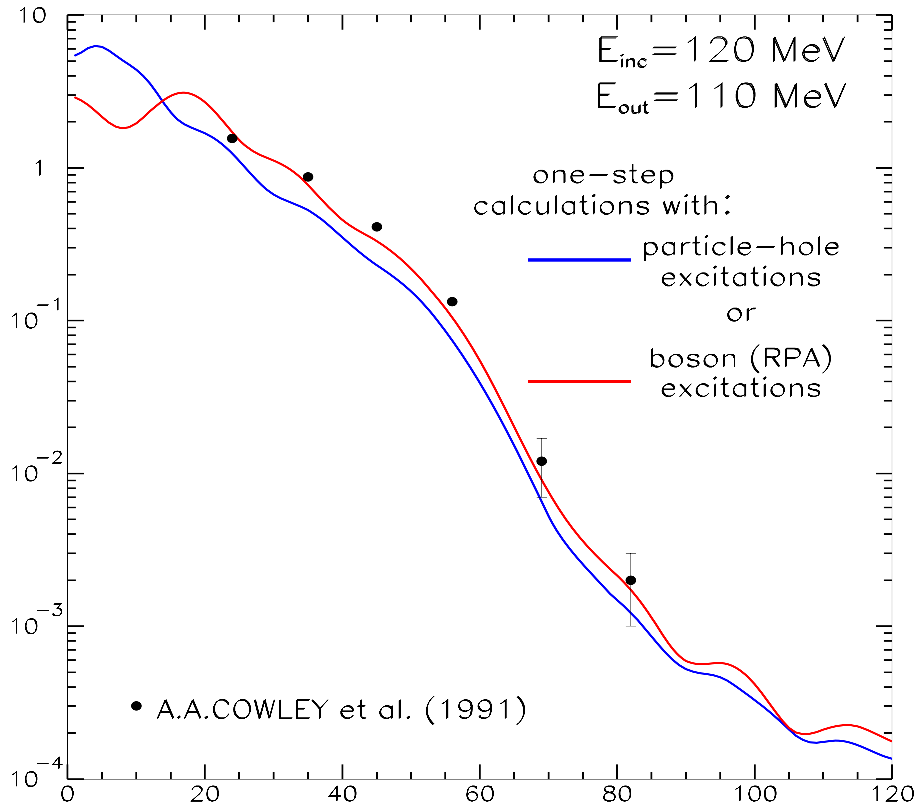
Transitions are calculated one by one and not on average as usually done.

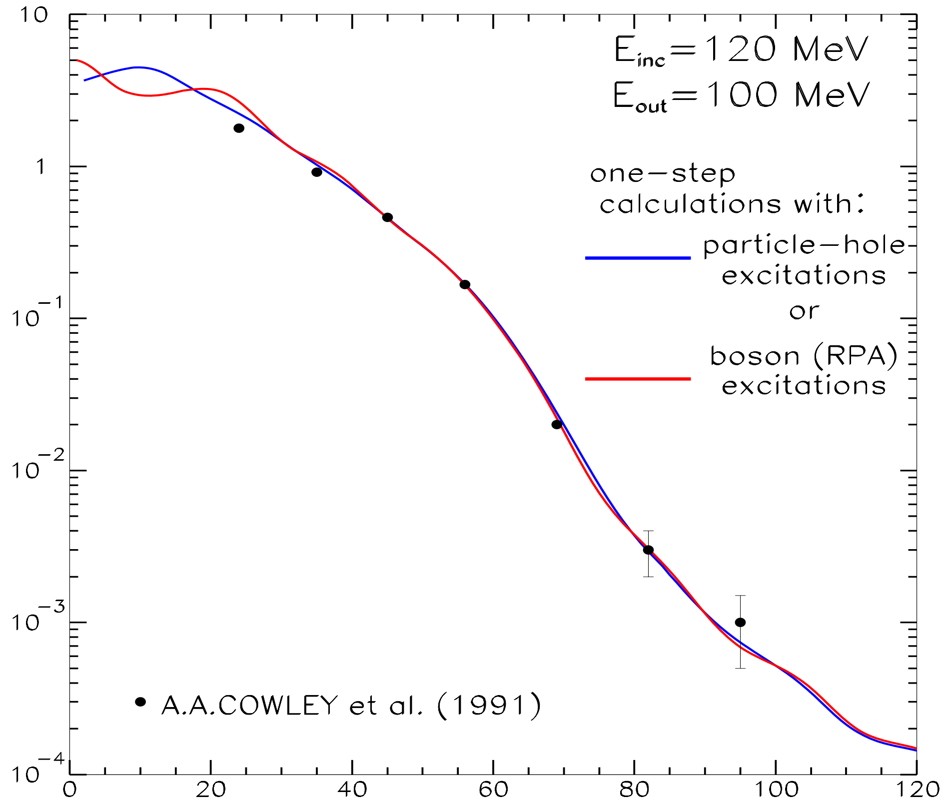
Drawbacks :

Requires time consuming calculation

No adjustement possible

Microscopic pre-equilibrium
First results





Microscopic level densities

Combinatorial approach

Advantages :

Methode usable for all nuclei (exotic)

for all deformations (fission)

Drawbacks

Not always good

Still uncertainties (collective effects, soft nuclei)

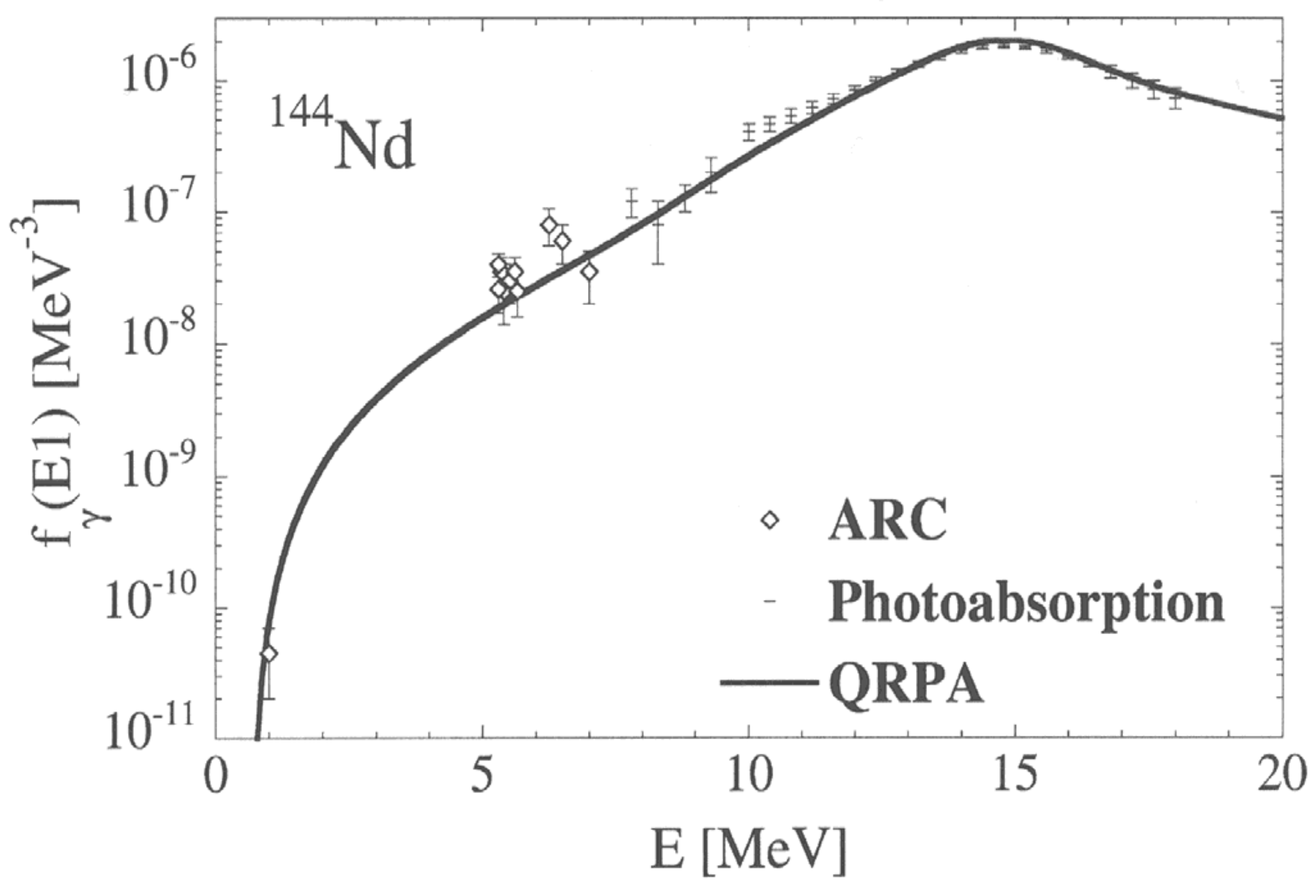
$\Rightarrow$ **Total level densities already used successfully in practical applications**

$\Rightarrow$ **p-h level densities to be tested in pre-equilibrium**

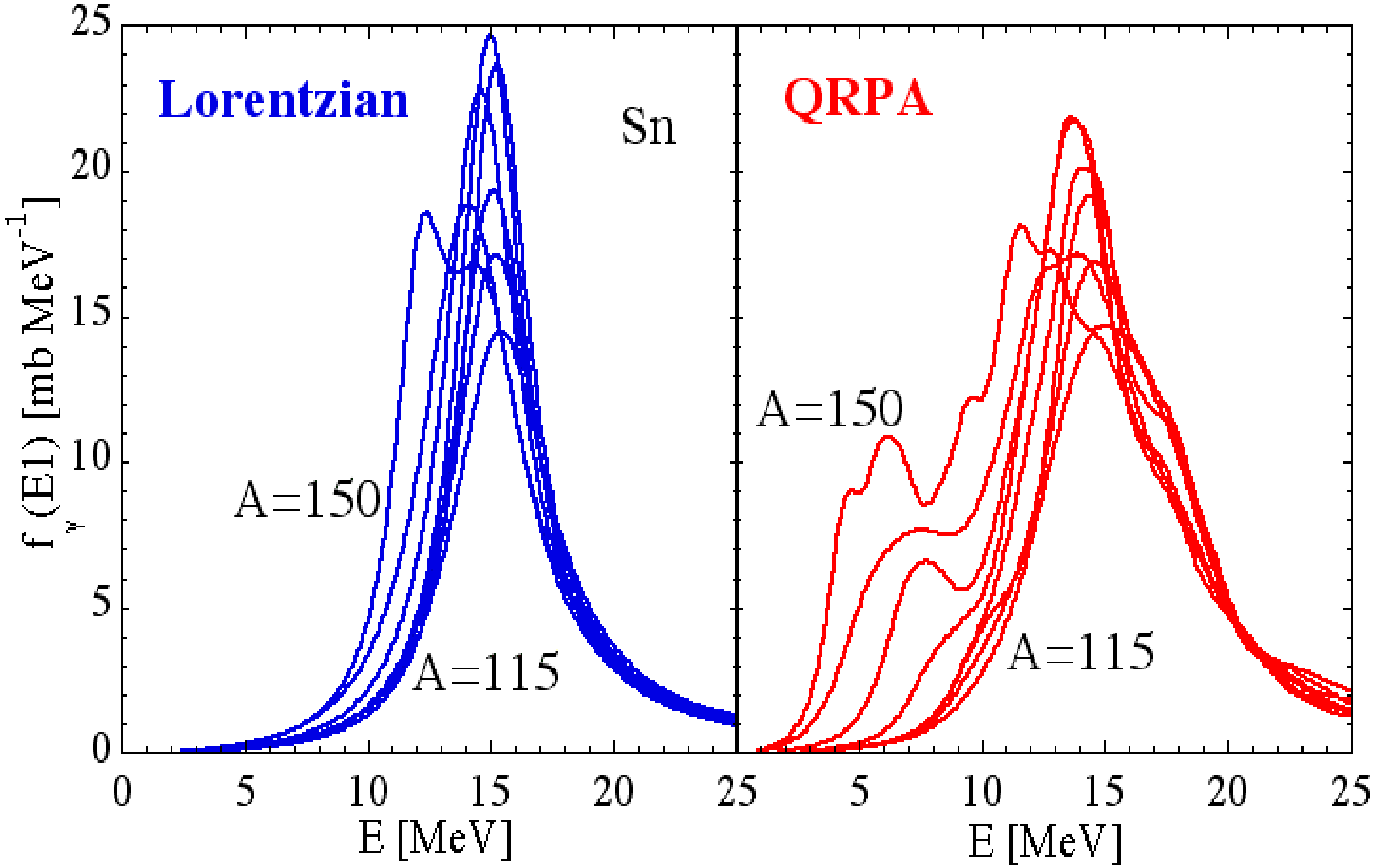
Microscopic γ-ray strength functions

First results quite good

S. Goriely, E. Khan / Nuclear Physics A 706 (2002) 217–232

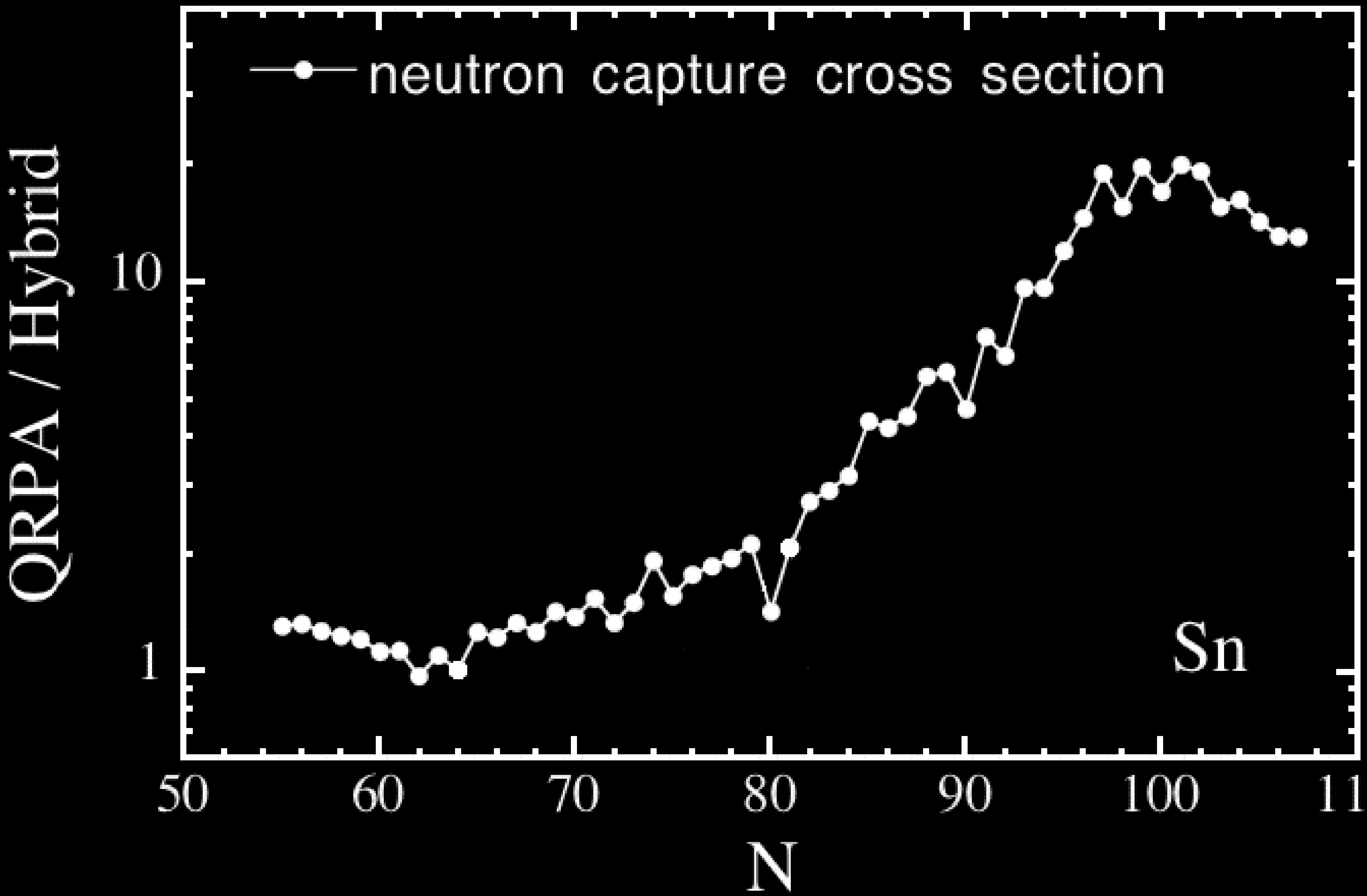


γ-ray strength functions models

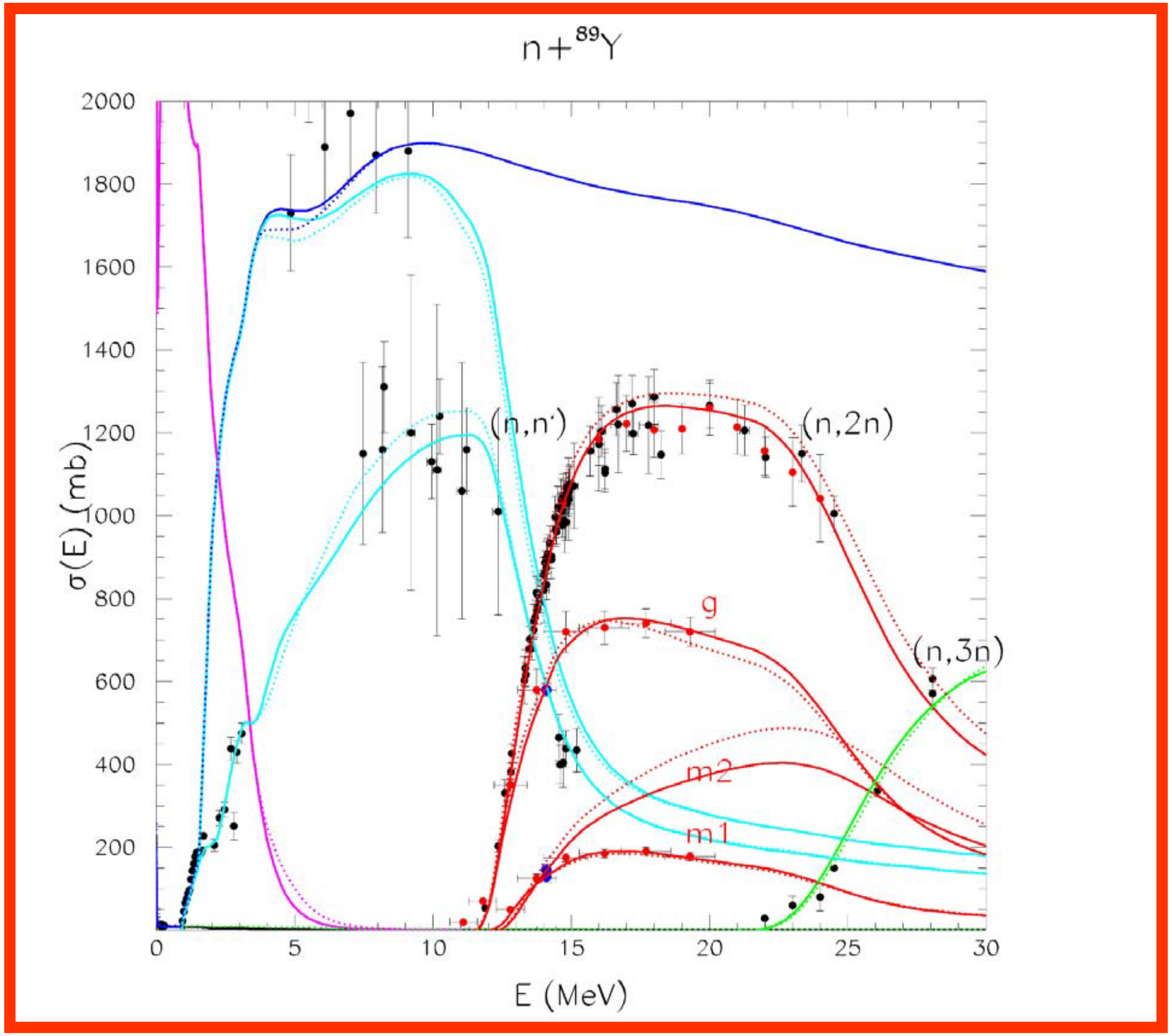


See S. Goriely & E. Khan, NPA 706 (2002) 217.
S. Goriely et al., NPA739 (2004) 331.

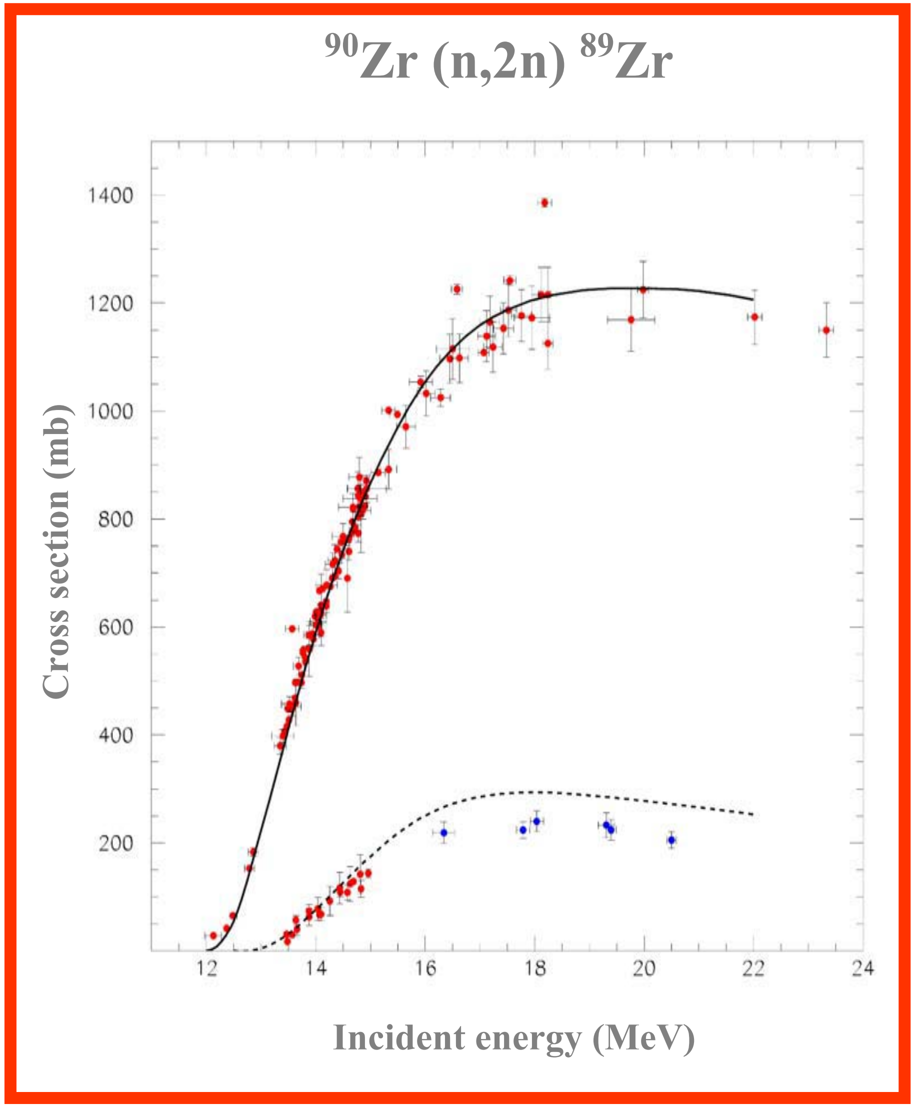
Microscopic γ-ray strength functions

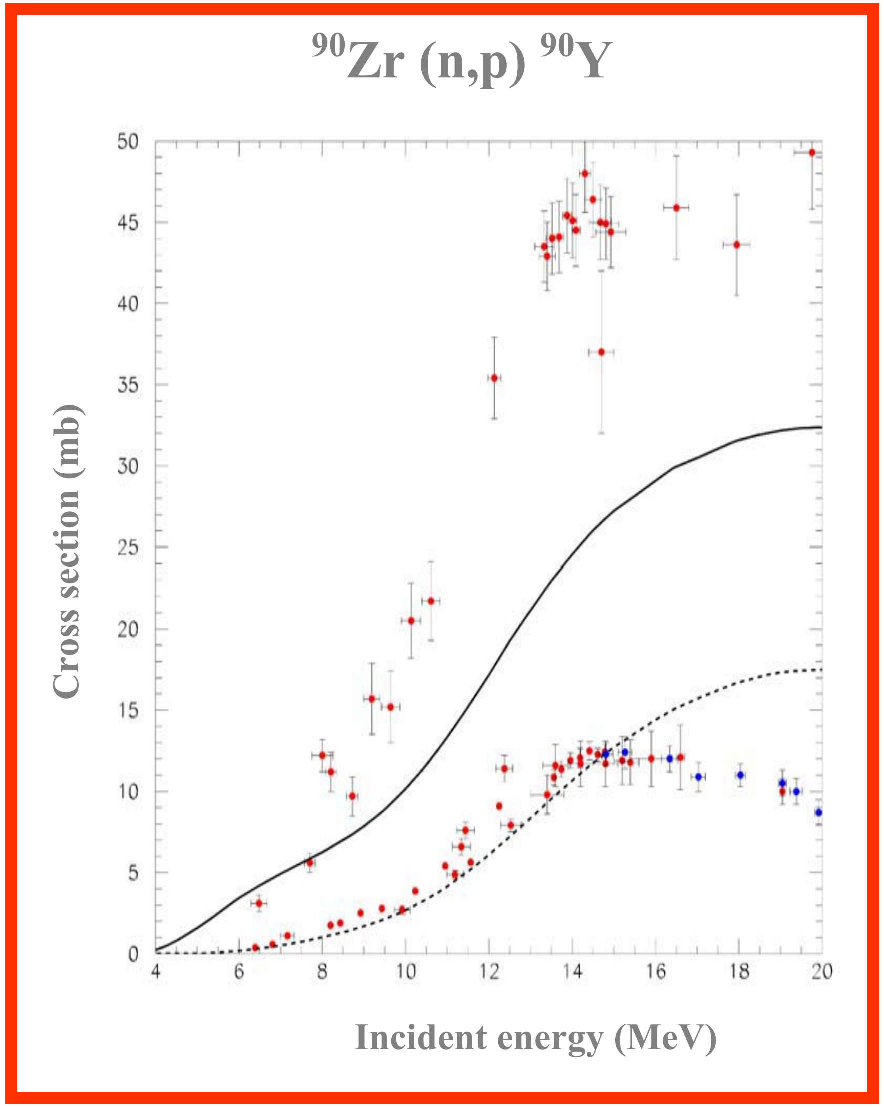


Microscopic vs Phenomenologic cross section



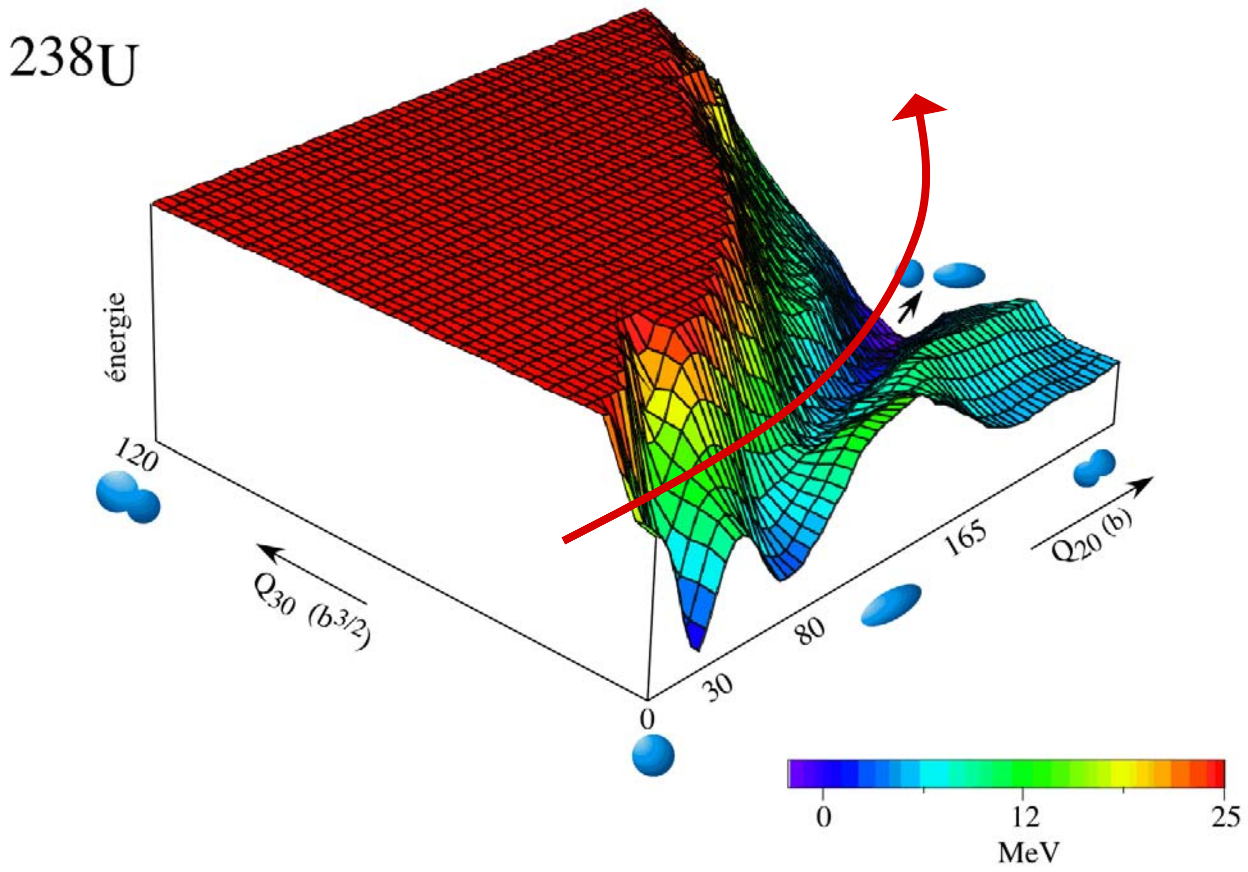
Fully microscopic cross section





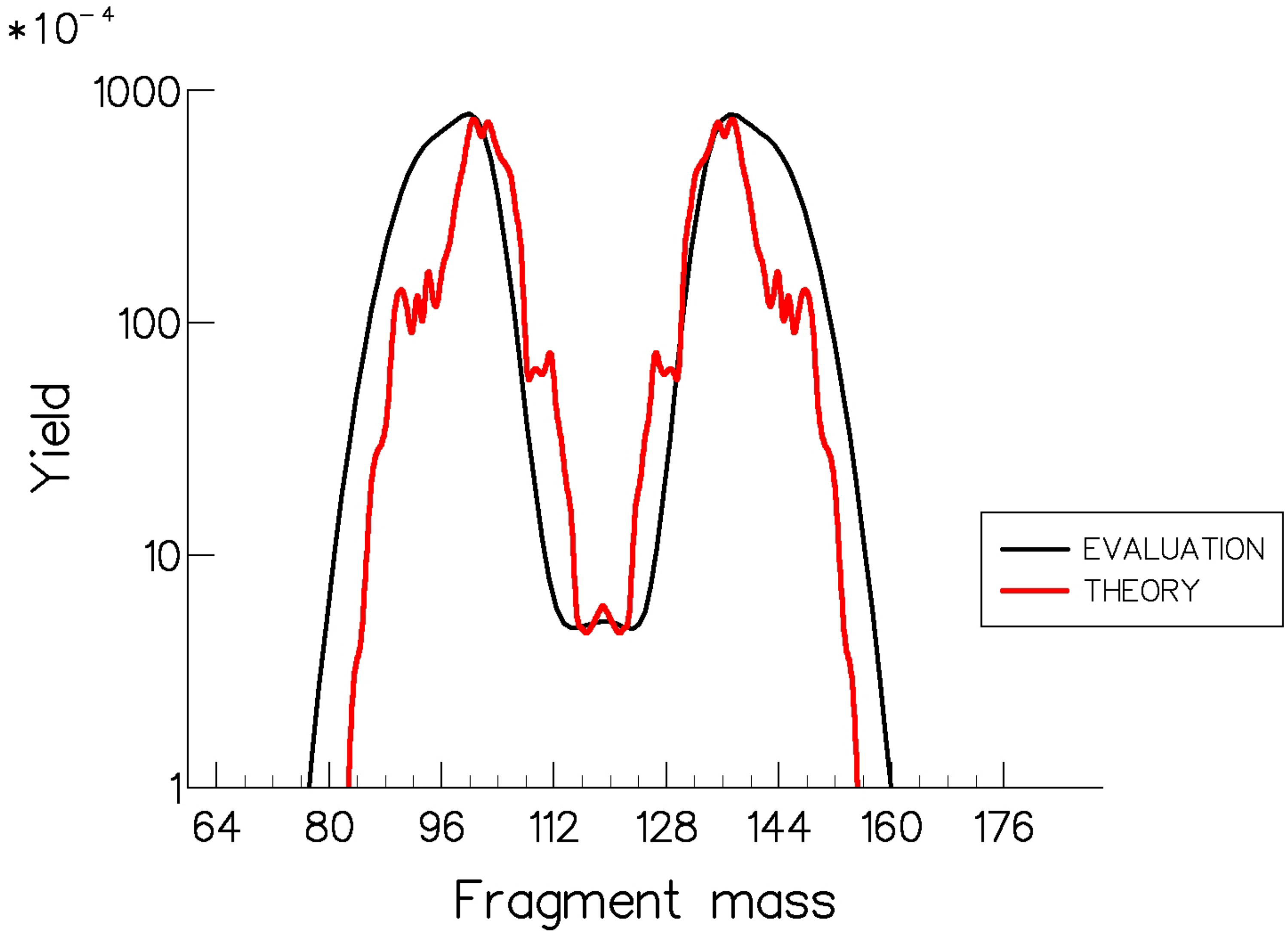
Microscopic fission ?

HFB+D1S potential energy surface followed by a dynamical propagation of a wave packet

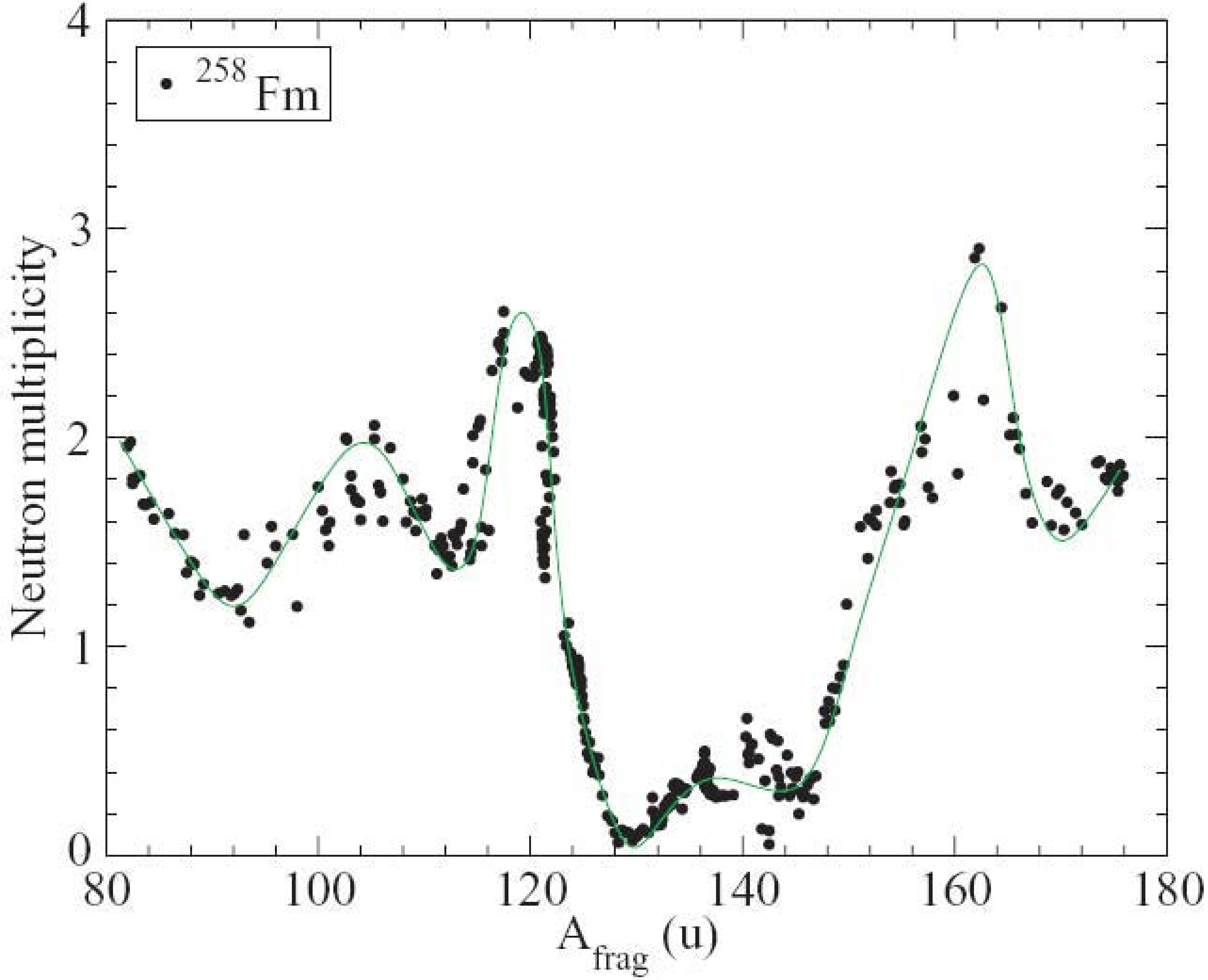


H. Goutte et al, PRC 71 (2005) 024316.

Fission fragments' yields



Fission fragments' neutron multiplicities



N. Dubray et al, PRC 77 (2008) 014310.

Neutron multiplicities via TALYS

- Total Energy = Fissioning nucleus energy – Fragments’ total energy

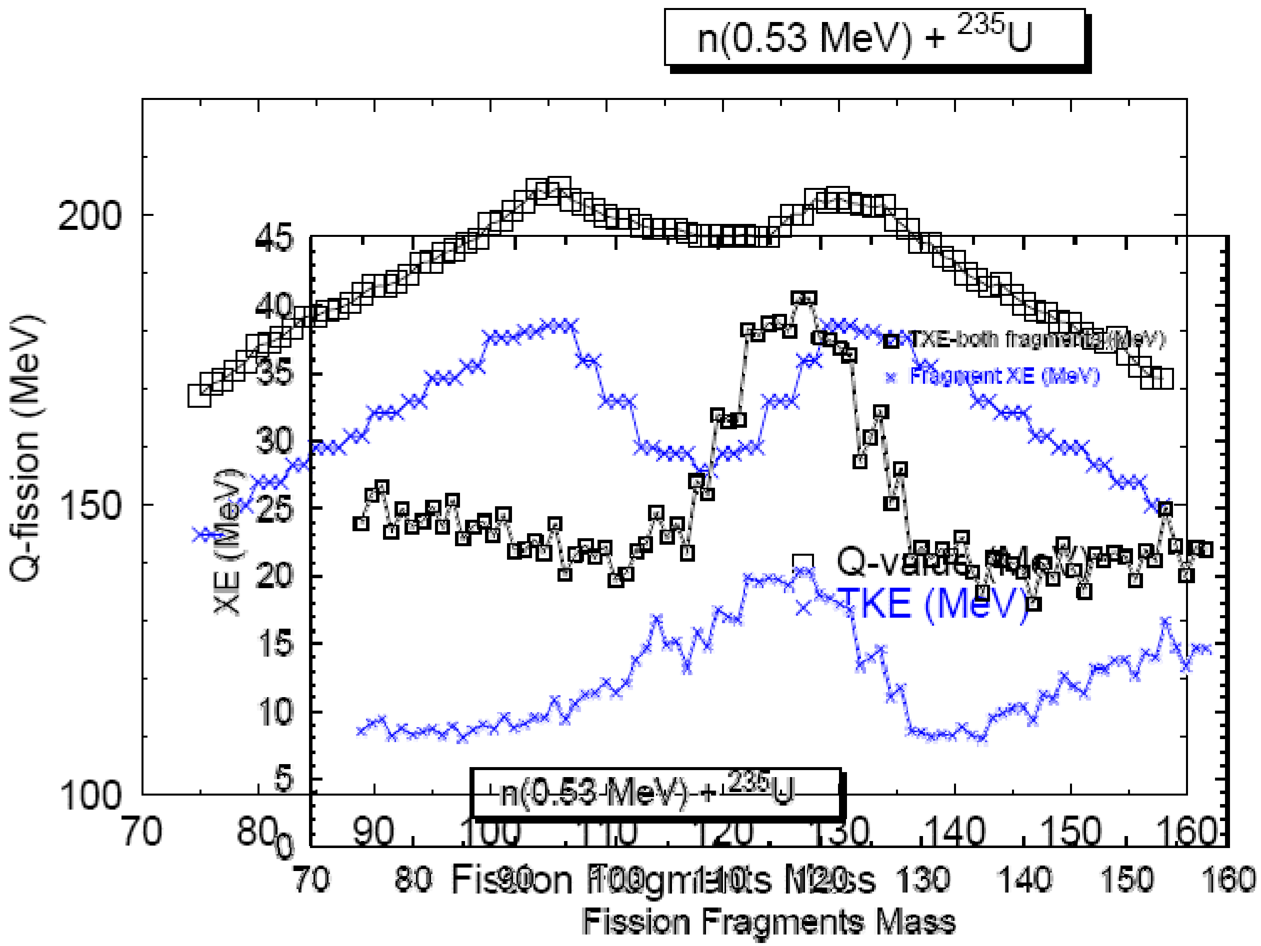
  ⇒ Fragments’ total excitation energy = Total Energy – Kinetic energy

- Partition of the Exci

  ⇒ Fragm

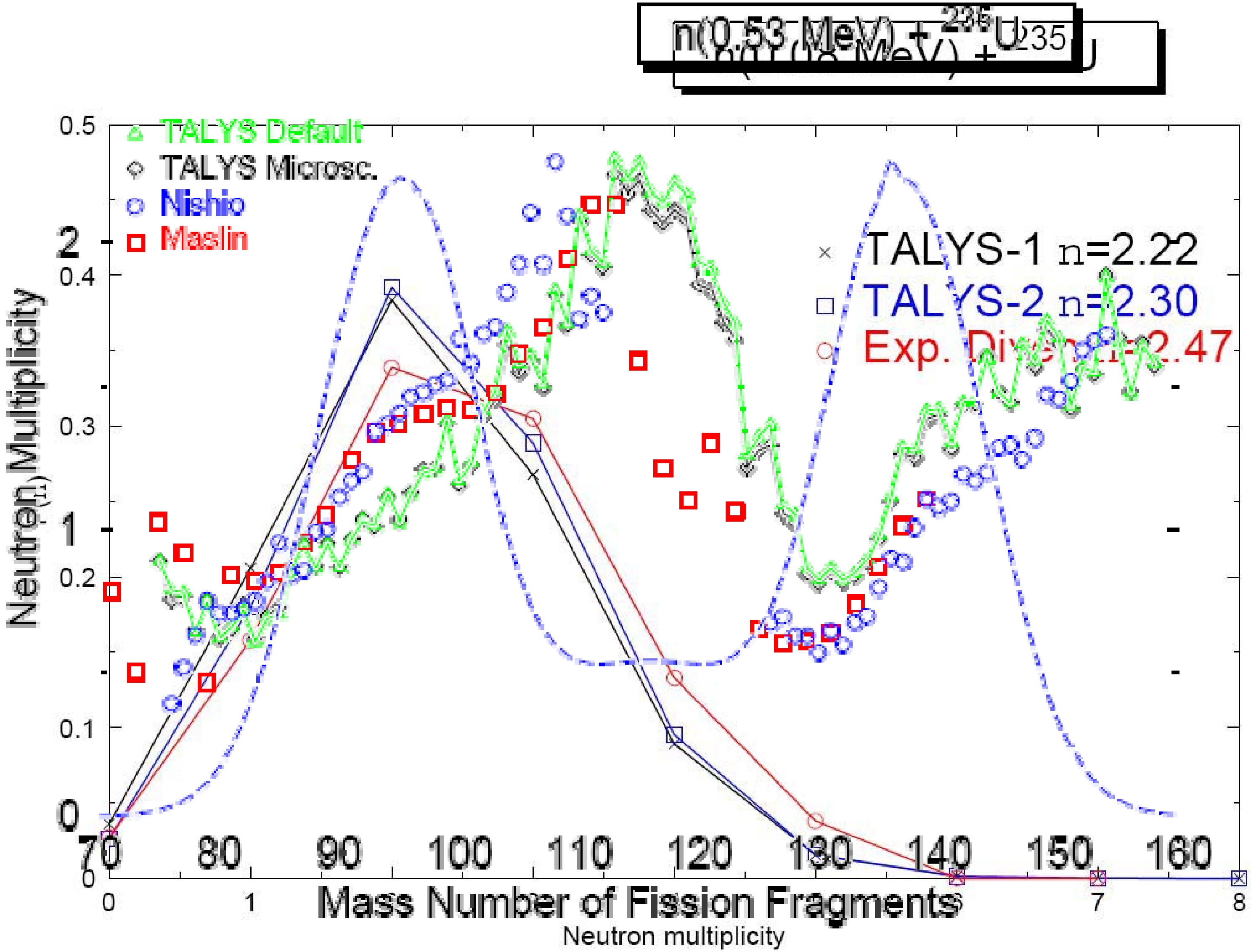
- Loop over / decay fi e)

  ⇒ neutro
  + other ir

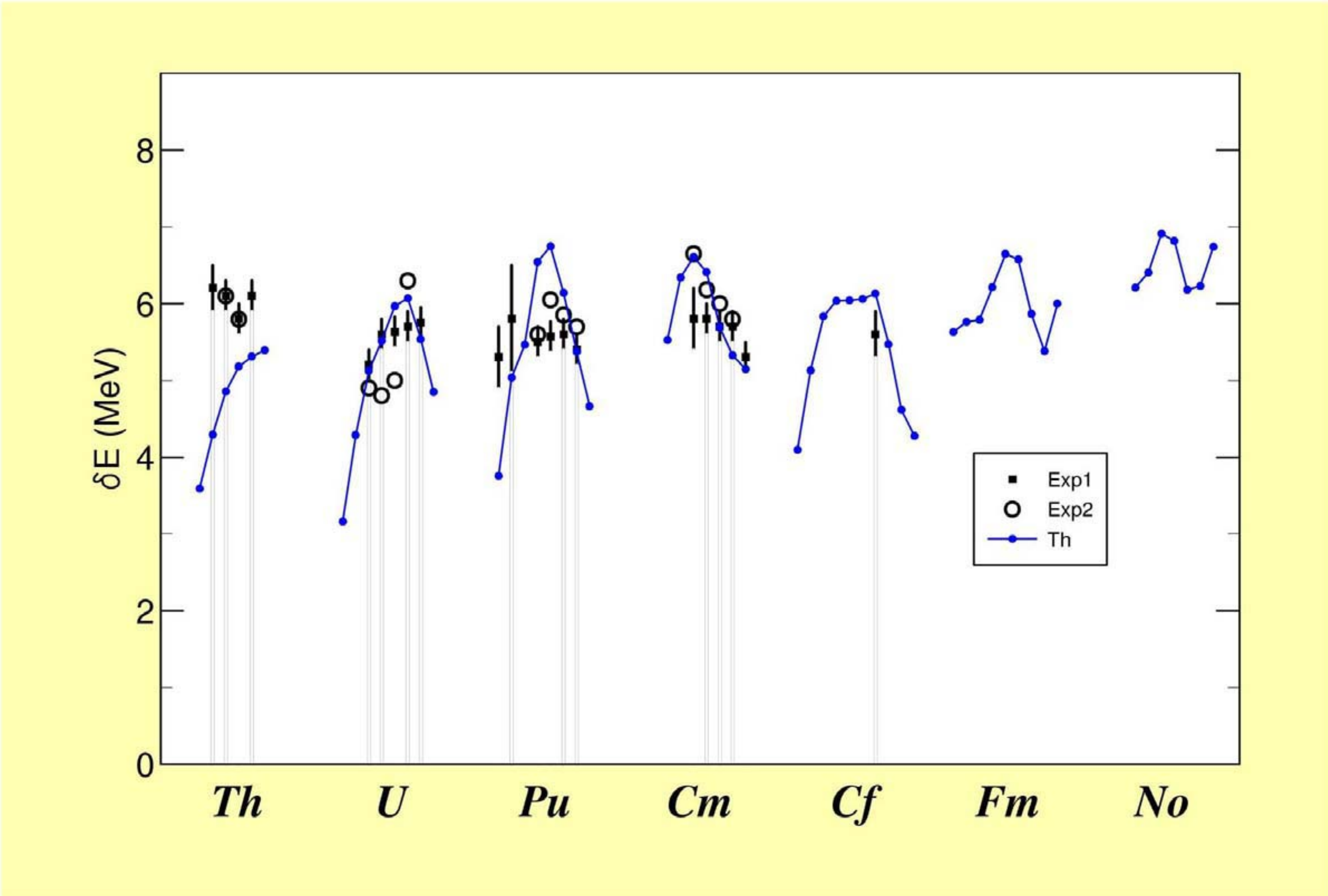


Neutron multiplicities via TALYS

Development by Sara Perez (now in CIEMAT)

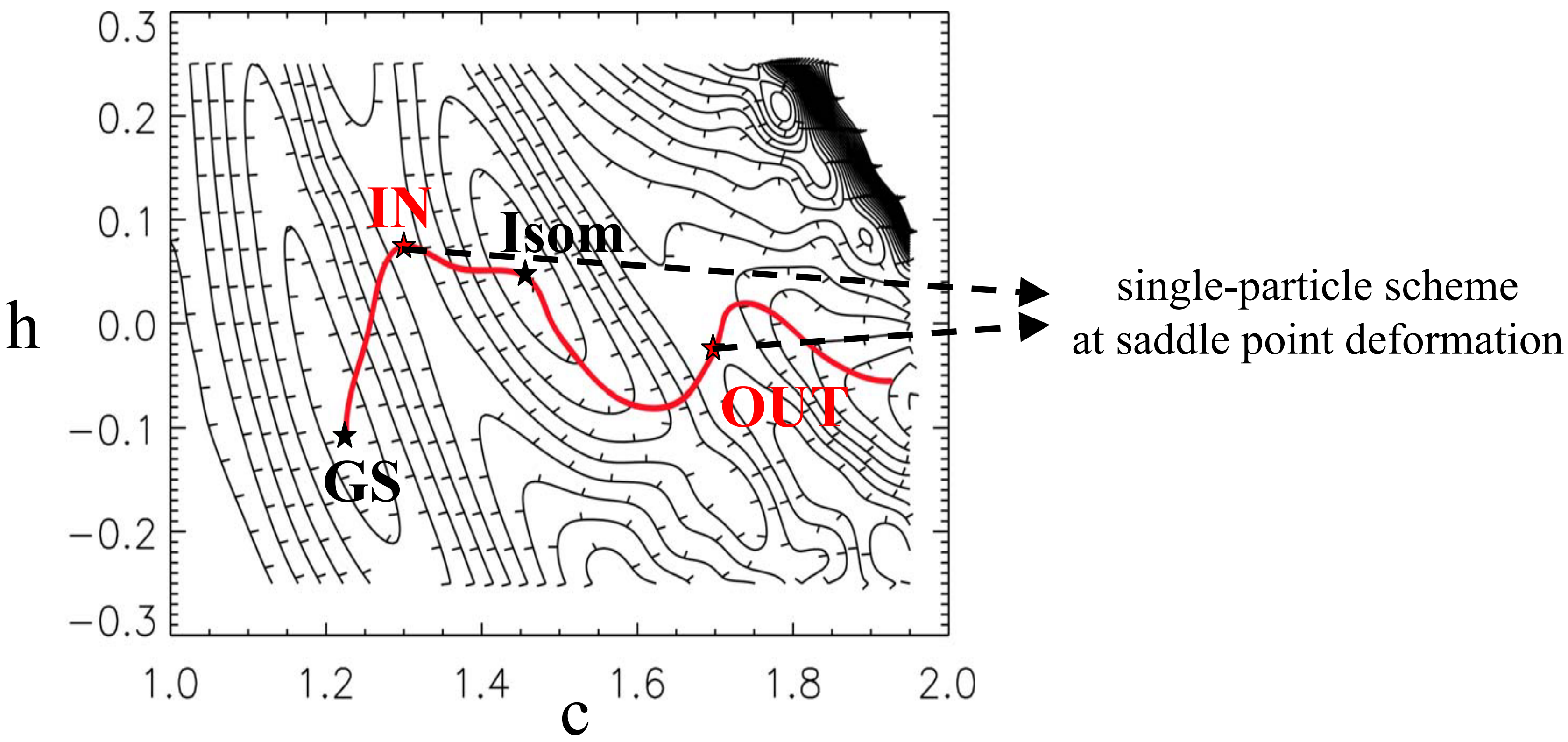


Fission barriers : Theory / Experiment



Nuclear level densities at the saddle points

HFB model constrained on Q,O,H moments provide at each deformation (and at saddle points) all nuclear properties needed to estimate the NLD



Possibility to estimate NLD at the saddle point within the HFB+Comb model

B_{in}(Exp) – B_{in}(HFB)

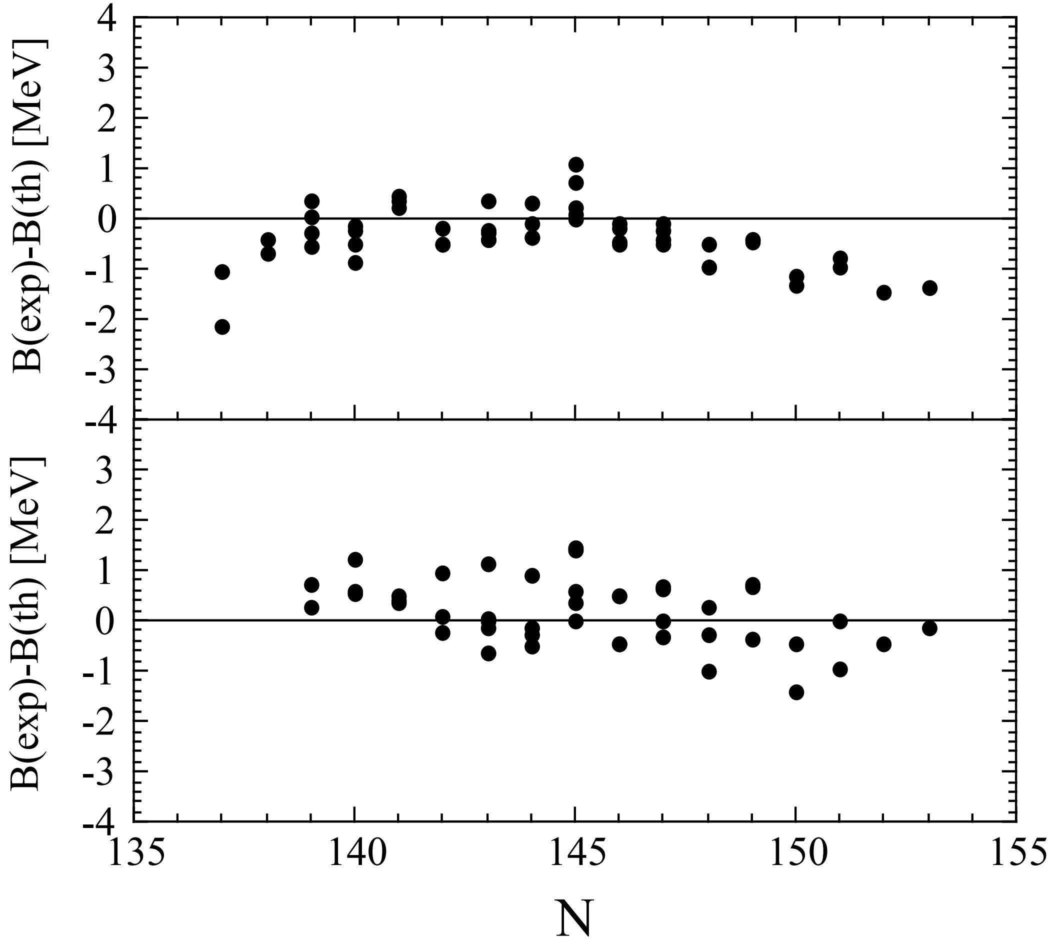
52 nuclei with Z ≥ 88

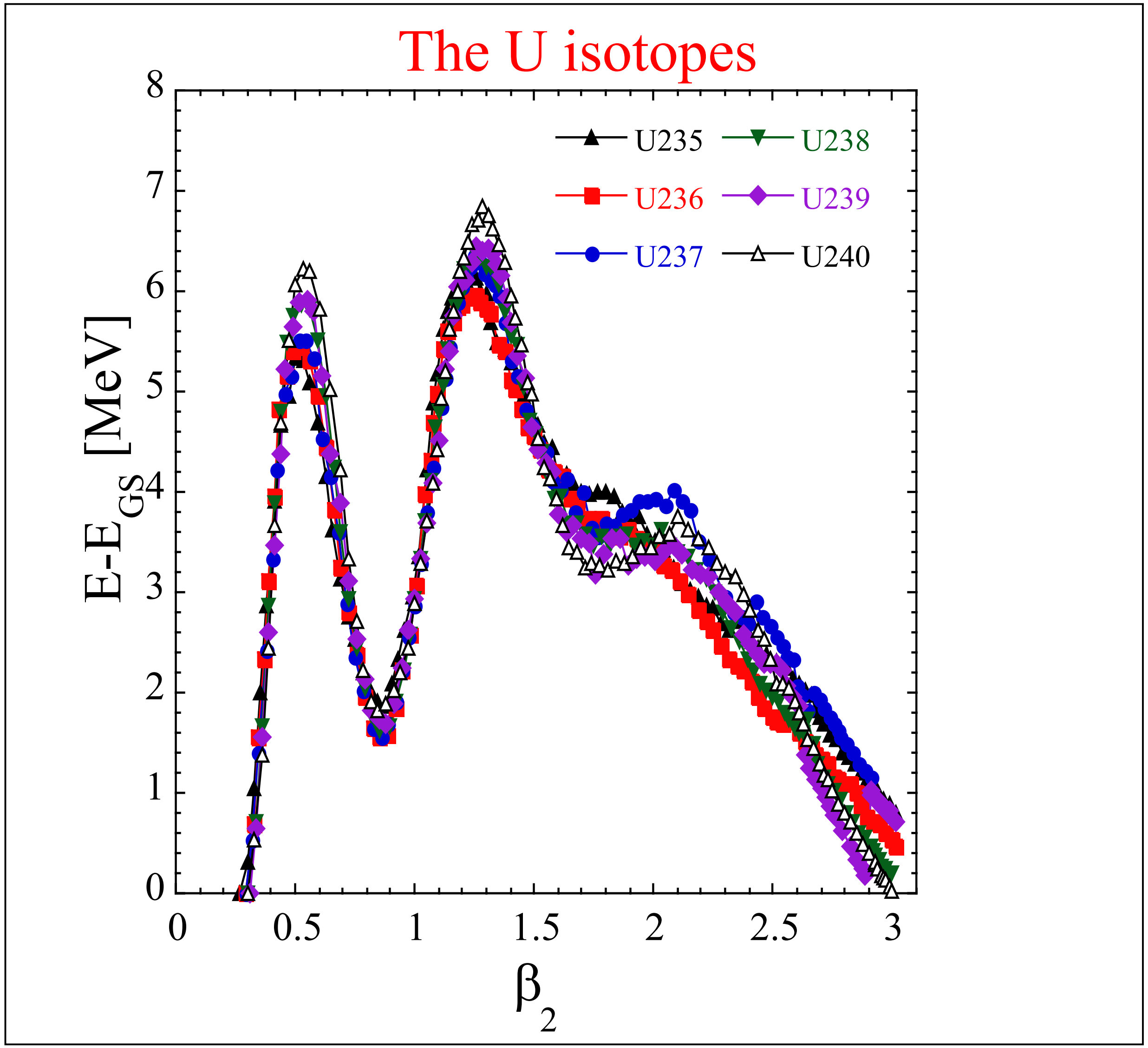
rms = 0.67 MeV

B_{out}(Exp) – B_{out}(HFB)

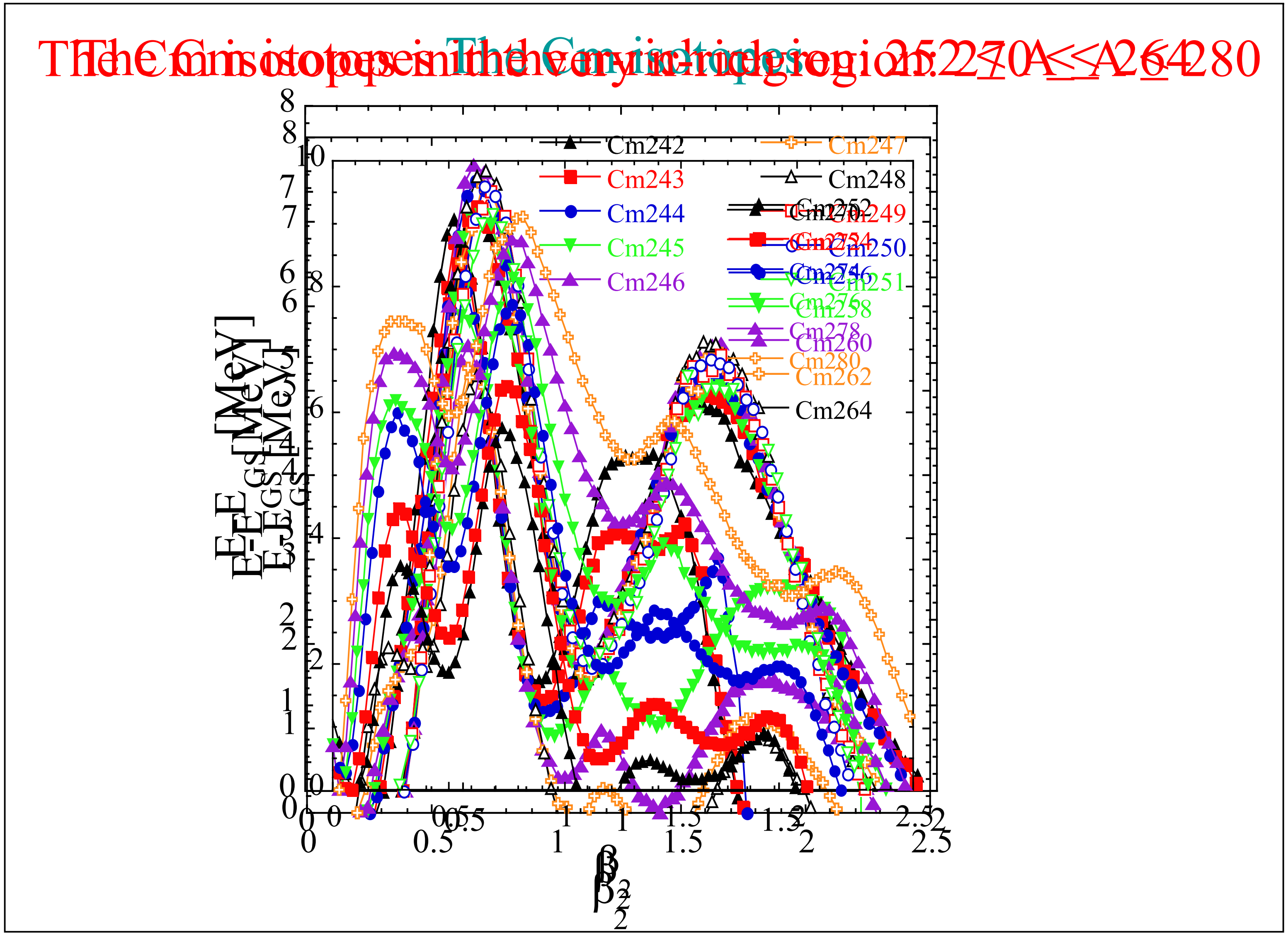
45 nuclei

rms = 0.65MeV



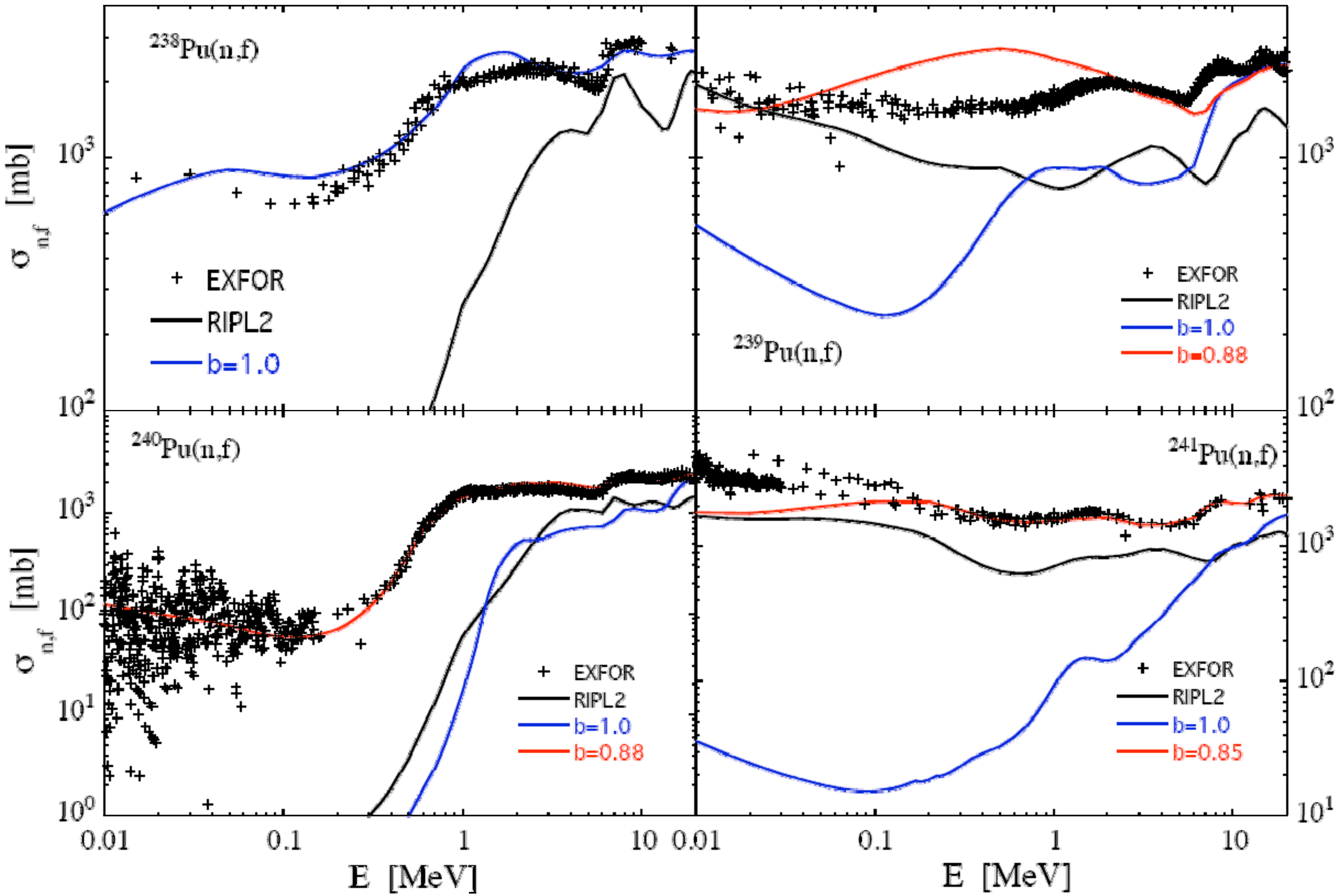


The U isotopes
U235
U238
U236
U239
U237
U240
E-E$_{GS}$ [MeV]
β_2



Cm242
Cm243
Cm244
Cm245
Cm246
Cm247
Cm248
Cm249
Cm250
Cm251
Cm258
Cm260
Cm262
Cm264
Cm280

Microscopic cross section calculation



Improve the link between ν-ν interaction and cross sections predictions

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R. Capote
M. Sin

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  M. Herman, R. Capote, B. Carlson, P. Oblozinsky, M. Sin, A. Trkov and V. Zerkin

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- *TALYS-1.0 : A Nuclear reaction code.*

  A.J. Koning, S.Hilaire, M.Duijvestijn.

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