

BRC
neutron evaluations
of
actinides
with the
TALYS
code

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What is a neutron evaluation ?

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A set of cross sections ... :

$\sigma_T(E)$, $\sigma_{n,n'}(E)$, $\sigma_{n,2n}(E)$, $d\sigma/d\Omega$, $d^2\sigma/dEd\Omega$, ... (also $\sigma_{n,f}(E)$ for actinides)

given : on an energy mesh

in a specific format (ENDF)

**In order to be used by computing codes
for different studies and nuclear applications**

how to get them ?



**In our approach
at
BRuyères-le-Châtel (BRC) :
we have chosen
the**

**FULL MODEL
approach**

using TALYS code



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TALYS

**adventures in wonderland
(of cross sections)**

**« railways » :
the new fission path**

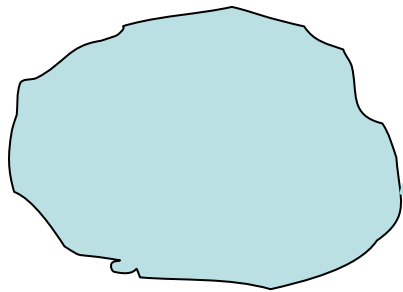


Optical Model

(able to describe : potential scattering)

or shape elastic

n



INTERACTING ZONE
(mean field)

=

potential created by
the A nucleons
of the target nucleus

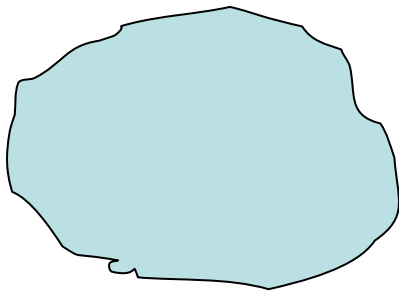
n

$$\begin{aligned} E |\Psi\rangle &= (T + V) |\Psi\rangle \\ &= H |\Psi\rangle \end{aligned}$$

BUT ...

(unable to describe :)

n
●



INTERACTING ZONE
(mean field)

=

potential created by
the A nucleons
of the target nucleus

n

n, 2n

n

$$\begin{aligned} \mathbf{E} |\Psi\rangle &= (\mathbf{T} + \mathbf{V}) |\Psi\rangle \\ &= \mathbf{H} |\Psi\rangle \end{aligned}$$

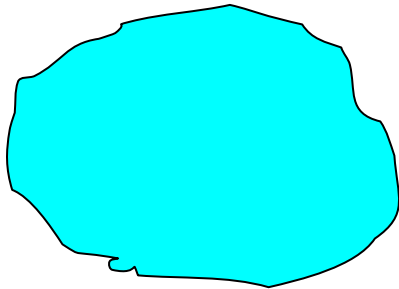


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BUT ...

(unable to describe :)

n



INTERACTING ZONE
(mean field)

=

potential created by
the A nucleons
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n



n, 2n



n

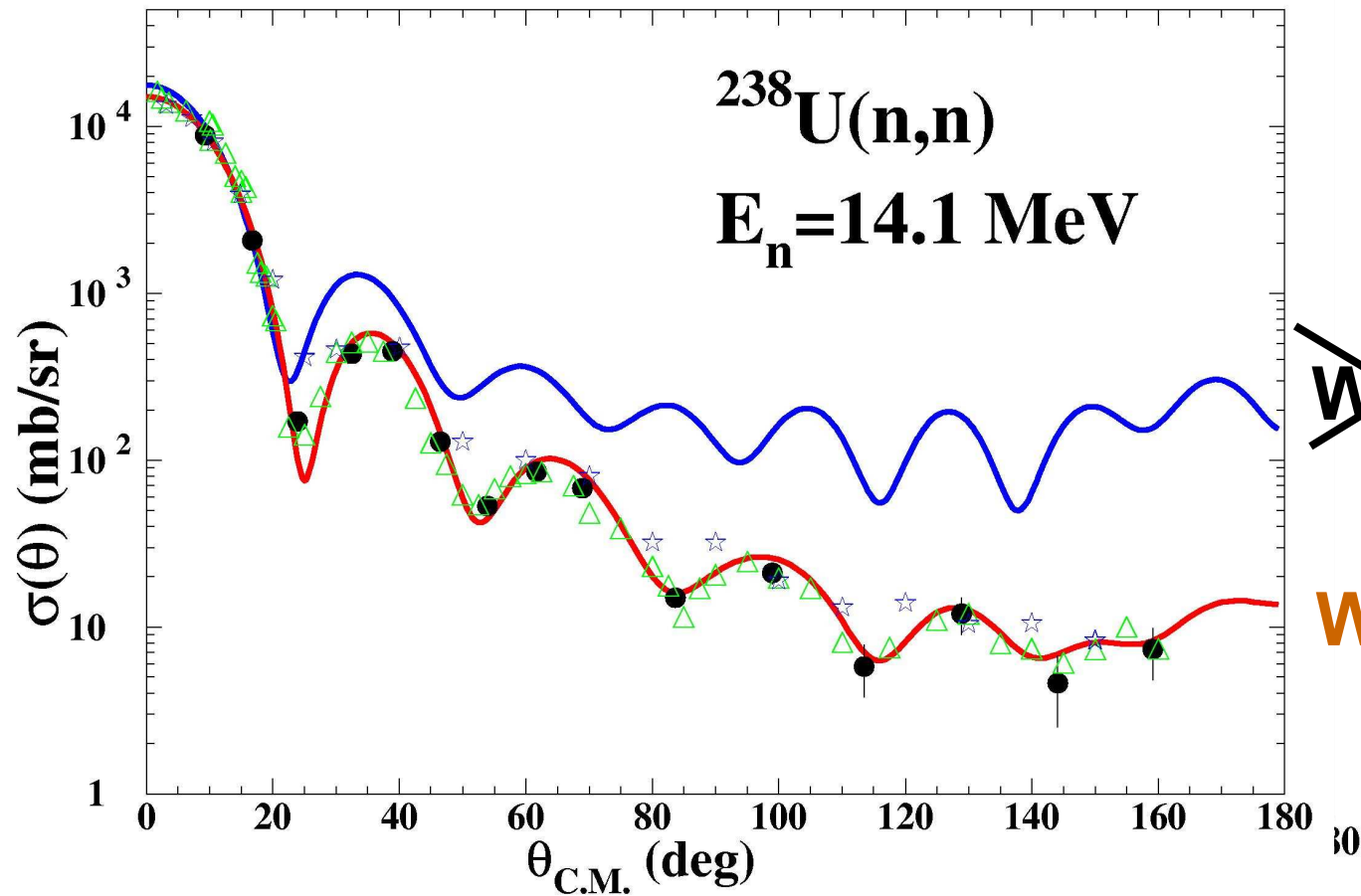
$$\begin{aligned}
 \mathbf{E} |\Psi\rangle &= (\mathbf{T} + \mathbf{U}) |\Psi\rangle \\
 &= \mathbf{H} |\Psi\rangle
 \end{aligned}$$

$$\mathbf{U} = \mathbf{V} + i \mathbf{W}$$

***U** : optical potential (depends of the target)*

$$U = V + i W \quad : \text{optical potential}$$

energie atomique



W : remove flux from elastic channel

$$U = V + iW \quad : \text{optical potential}$$



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W : to quantify the *absorption*

W : gives $\sigma_R \leftarrow T_\ell$

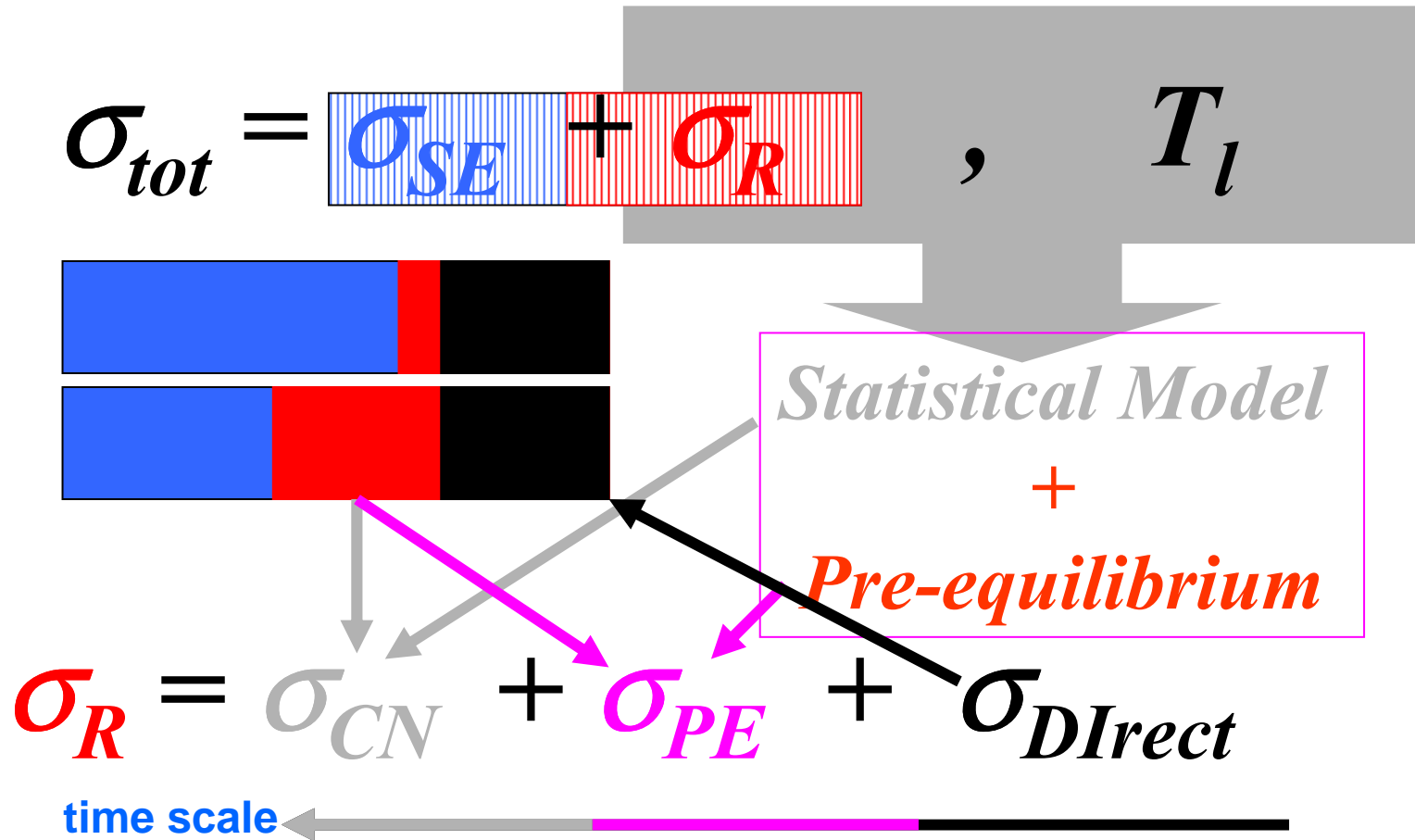
σ_{Tank}

It must have the « right dimension »

$$\sigma_R = \sum_\ell (2\ell + 1) T_\ell$$

Evaluation only from Models

Optical Model



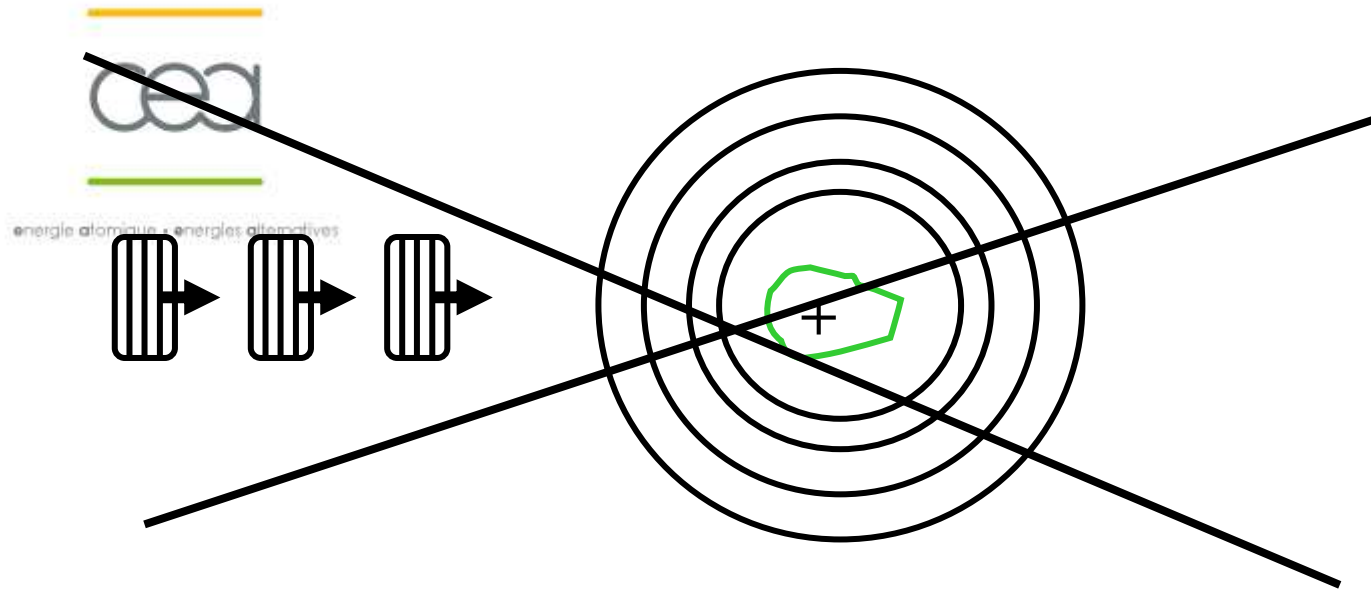


énergie atomique

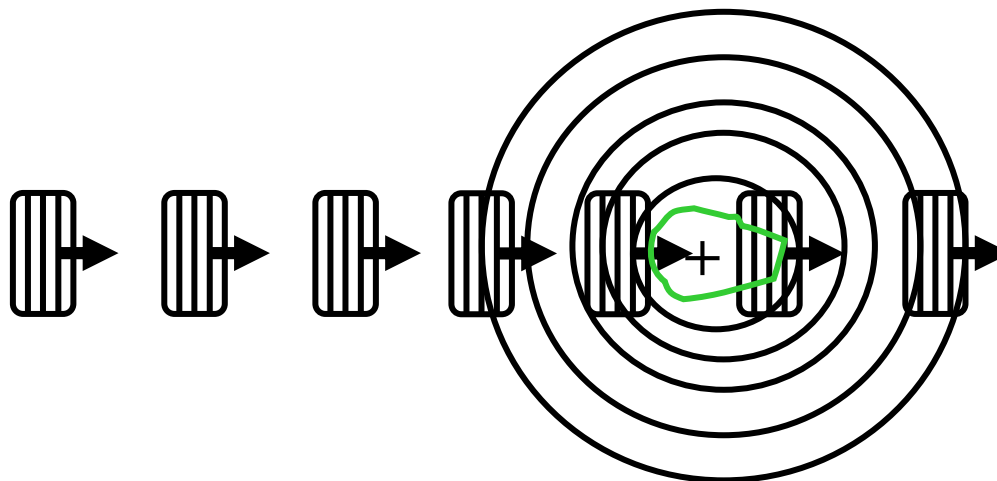
Optical Model

Dispersive Optical Model

(Dispersion relations \Leftrightarrow causality principle)



Causality principle: the scattered wave cannot be emitted before the incident wave has reached the target.





Pour notre problème de diffusion :

Causality principle : causes preceding effects

====> Dispersion Relations

$$\Delta V(E) = \text{Re}(U_{\text{dyn}}(E)) = \frac{1}{\pi} \text{P} \int \frac{\text{Im}(U_{\text{dyn}}(E'))}{E' - E} dE'$$

additional constraint when adjusting absorption

Coupled Channel Calculations *(ECIS)*

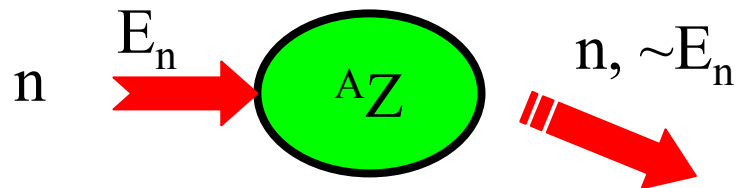
*(As everybody knows for
deformed nuclei in their g.s.)*



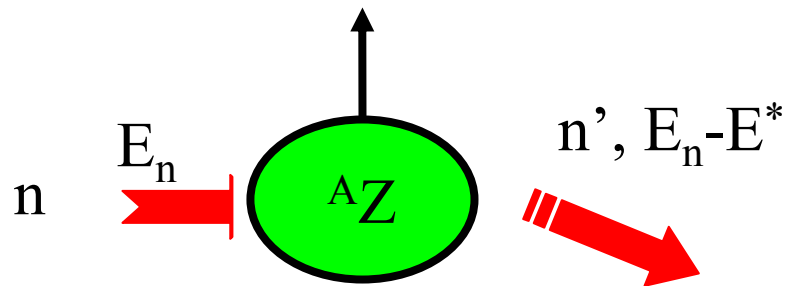
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Direct Interaction

rapid Process $t \sim 10^{-21}$ s



Elastic



Inelastic



Coupled Channel Calculations (ECIS)

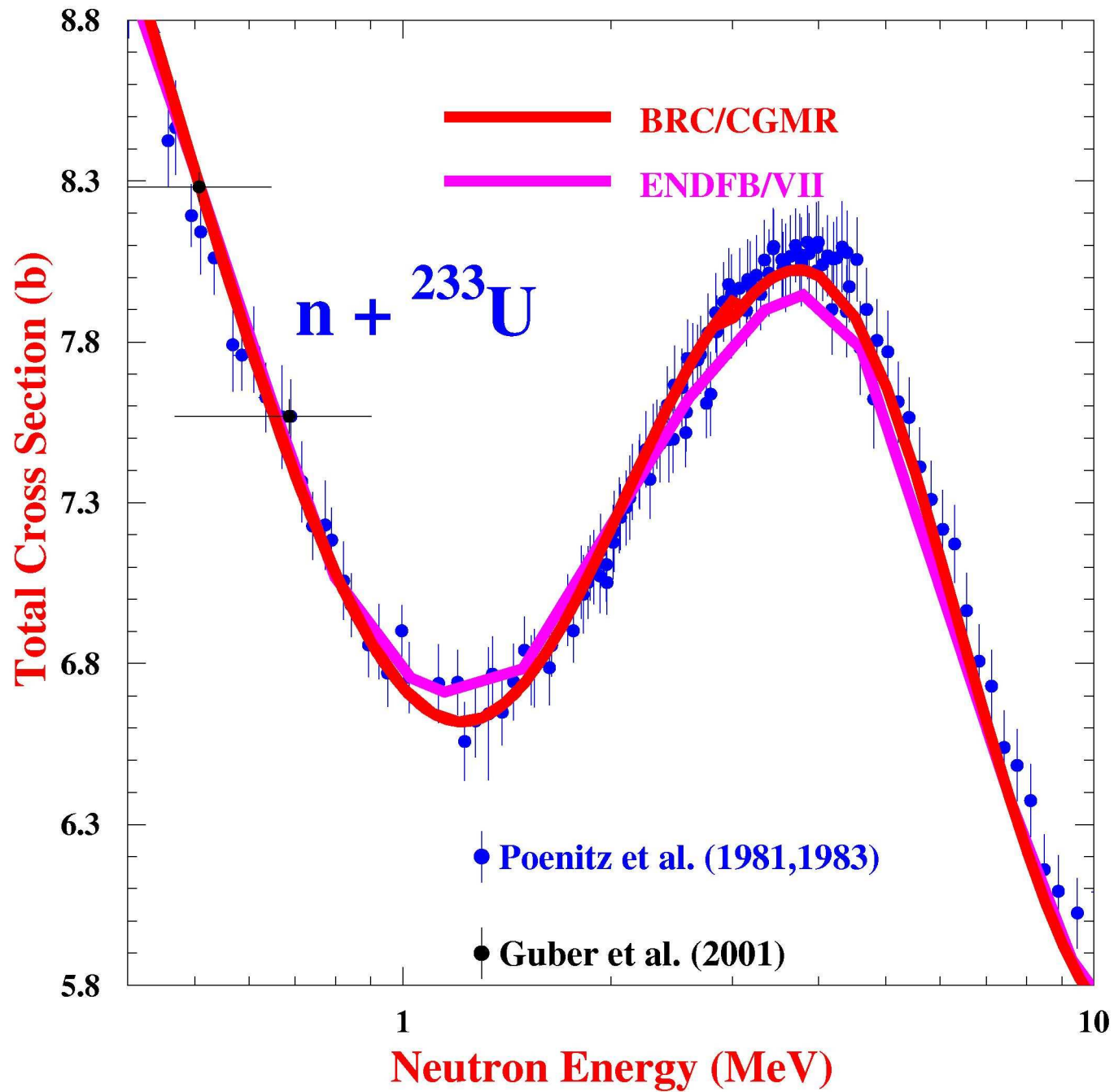
*(As everybody knows for
deformed nuclei in their g.s.)*

*Moreover for actinides a coupling† to
the lowest octupolar band is needed.*

*† (This idea originated from a previous work of V. Maslov
in 1998 on the system $n + {}^{238}\text{U}$)*

*(implies a new repartition between
DI  and CN  processes)*

energie



Evaluation only from Models



$$+ \sigma_R, T_l$$

Statistical Model

+

Pre-equilibrium

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

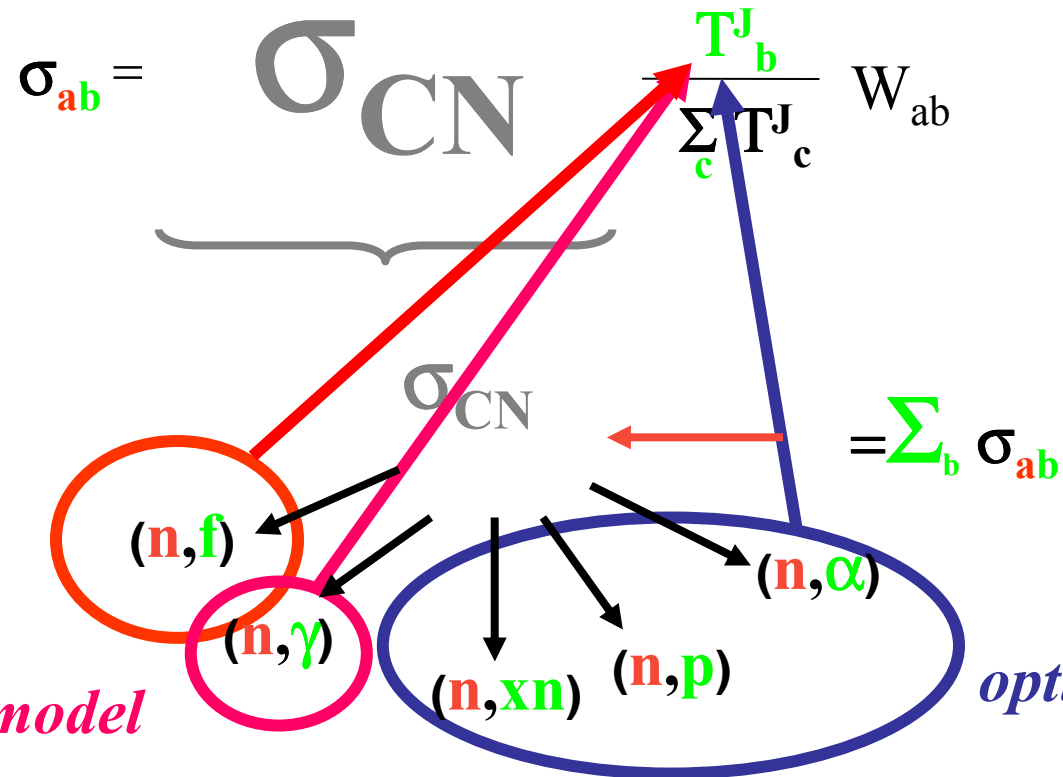
time scale ←



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Statistical Model (GNASH - TALYS - EMPIRE ...)

All open channel are simultaneously treated



GNASH - TALYS
EMPIRE
built around
this equation

*for fission the transmission coefficients
come from a penetration barrier model*



Transmission coefficients are the **keys** used to open
the compound nucleus cross section σ_{CN} **TANK**

*(we need one **key** per emitted type of particule)*

n,p,d,t, α \Leftrightarrow **keys** built at **optical potential machine**

related to σ_{CN} ($b+B$ où $b=n,p,d,t,\alpha$)

$$C^* \longleftarrow b + B$$

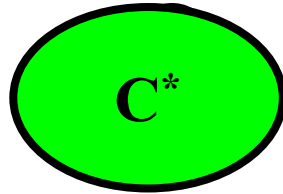
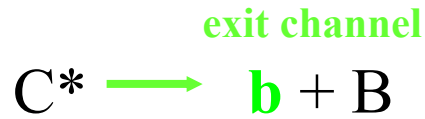
γ \Leftrightarrow **keys** bought at the **GDR supermarket**

fission \Leftrightarrow **keys** or **pass-keys** ???????



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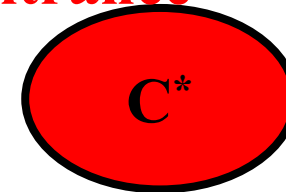
(**keys** built at **optical potential machine**)



key / exit



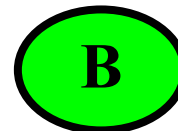
key / entrance



entrance channel



(**study inverse reaction**)





Transmission coefficients are the **keys** used to open
the compound nucleus cross section σ_{CN} **TANK**

*(we need one **key** per emitted type of particule)*

n,p,d,t, α \Leftrightarrow **keys** built at **optical potential machine**

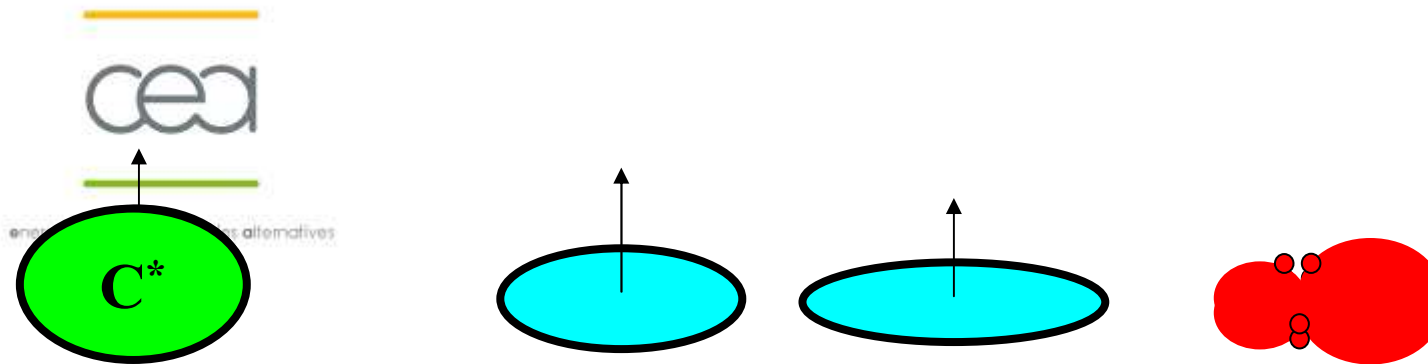
related to σ_{CN} ($b+B$ où $b=n,p,d,t,\alpha$)

$$C^* \longleftarrow b + B$$

γ \Leftrightarrow **keys** bought at the **GDR supermarket**
related to the **photo**-absorption cross section

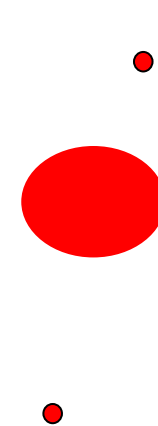
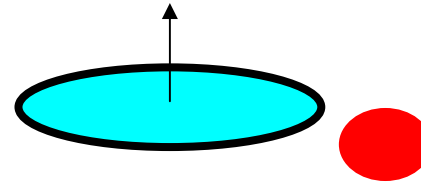
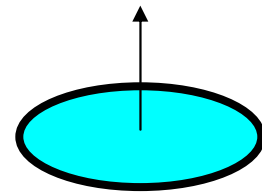
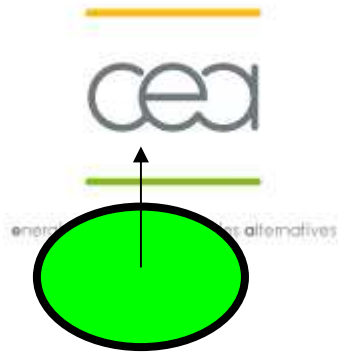
fission \Leftrightarrow **keys** or **pass-keys** ???????

not easily related to fusion cross section $b+B$,
especially too much couples $b+B$ fragments!!!!!!!



deformation

inverse mecanism ???



deformation



many sets of fragments

moreover

fragments more or less excited and deformed

AND

emitted neutrons with velocities distributions

AND

etc, etc ...



and then !!!



But we can drink it

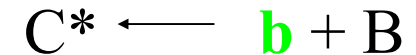


Transmission coefficients are the **keys** used to open
the compound nucleus cross section σ_{CN} **TANK**

*(we need one **key** per emitted type of particule)*

n,p,d,t, α \Leftrightarrow **keys** built at **optical potential machine**

reliées à σ_{CN} ($b+B$ où $b=n,p,d,t,\alpha$)



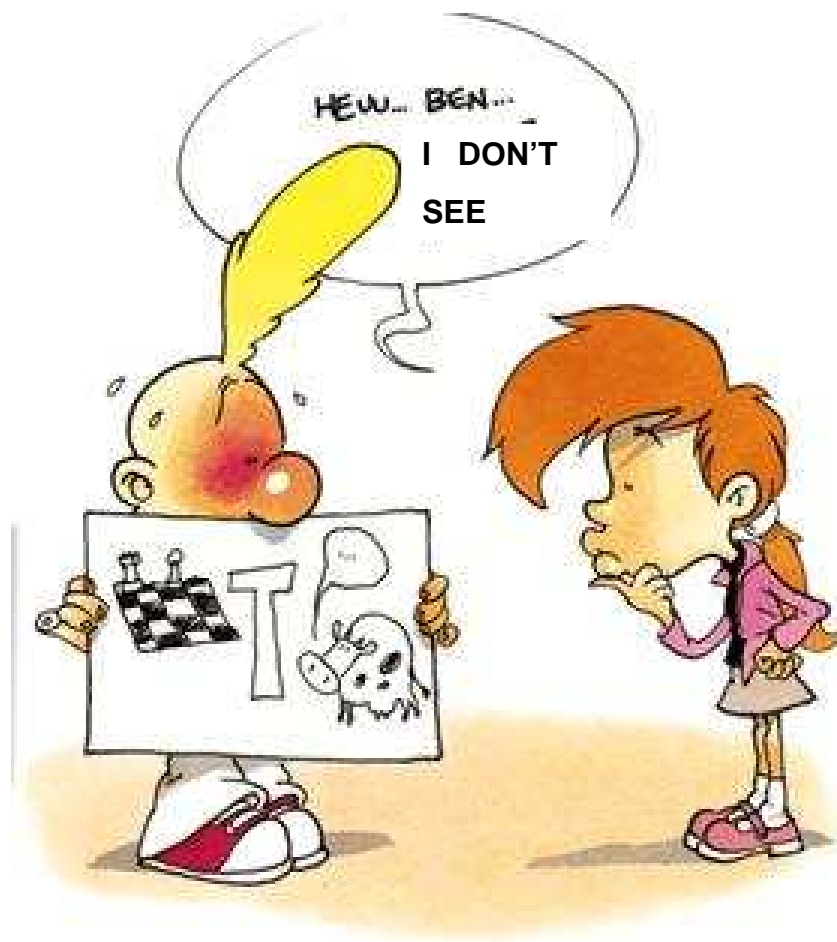
γ

\Leftrightarrow **keys** bought at the **GDR supermarket**
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fission \Leftrightarrow **keys** or **pass-keys** ???????

not related to fusion cross section $b+B$,
especially that many couples $b+B$ fragments!!!!!!

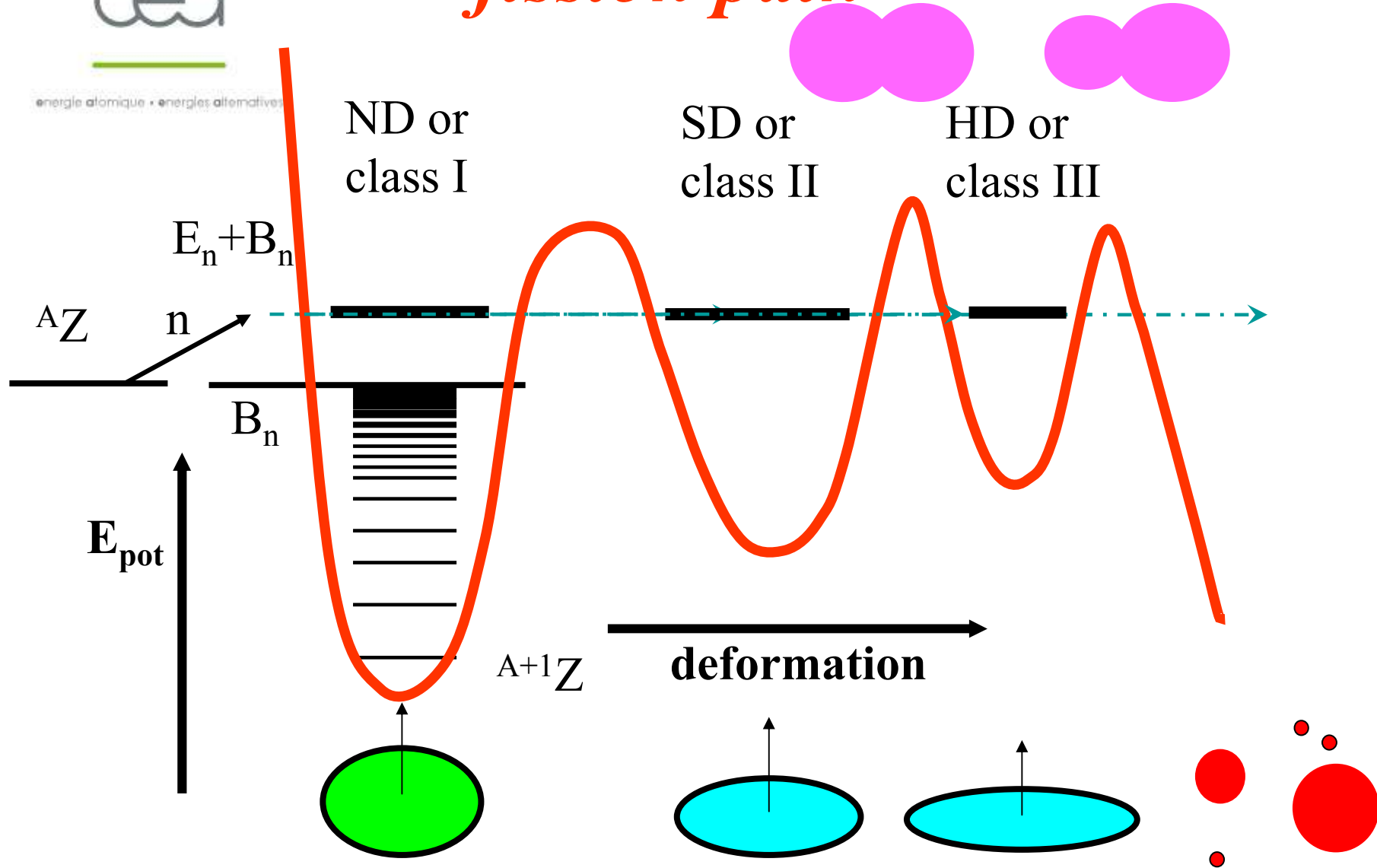
keys built on line
adjust with **S**tatistical **M**odel





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fission path



B. Morillo

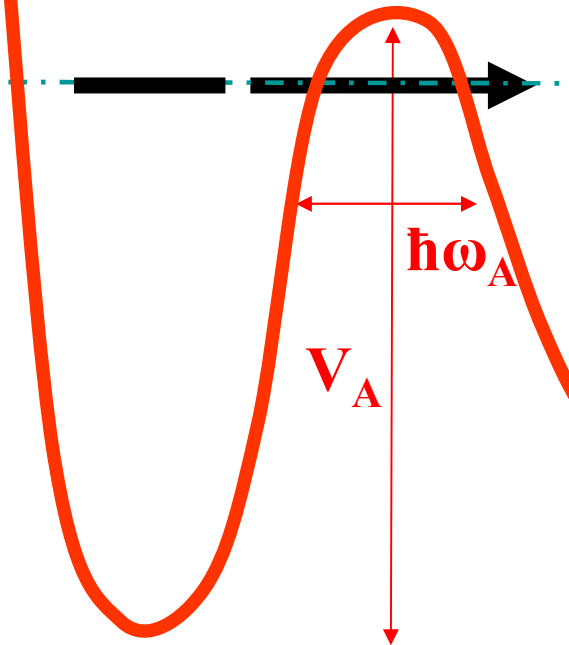
key or pass-key ??



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fission barrier with 1 hump

E **A**



$$T_f = T_A$$

$$T_i = 1/[1 + \exp(2\pi(V_i - E)/\hbar\omega_i)]$$

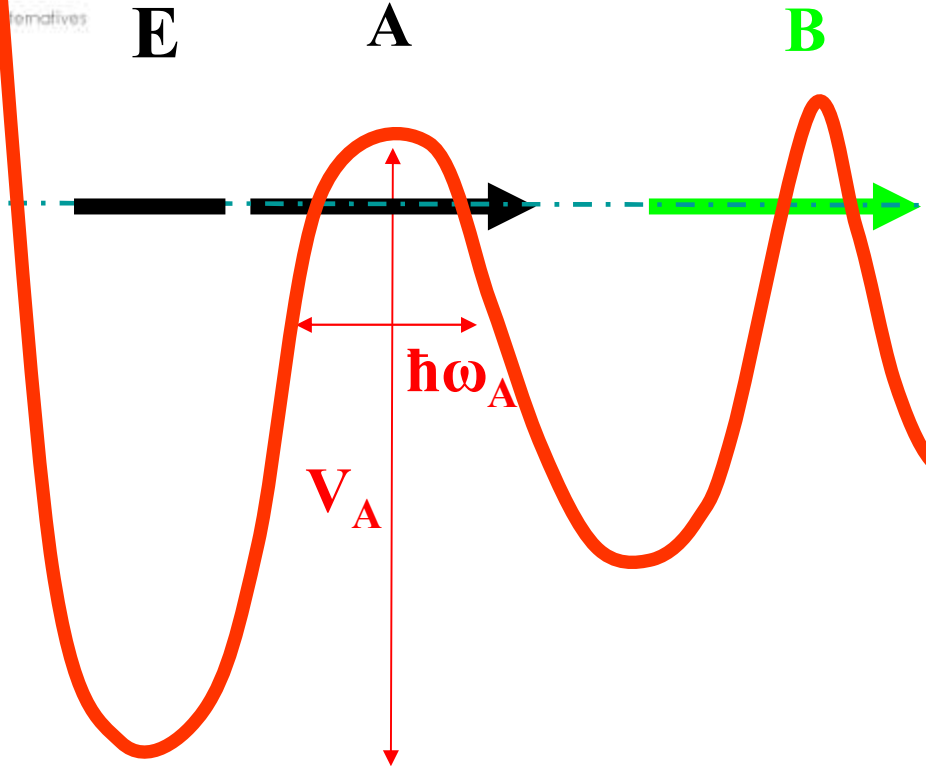
Hill-Wheeler

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deformation →



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fission barrier with 2 humps



$$T_i = 1/[1 + \exp(2\pi(V_i - E)/\hbar\omega_i)]$$

Hill-Wheeler

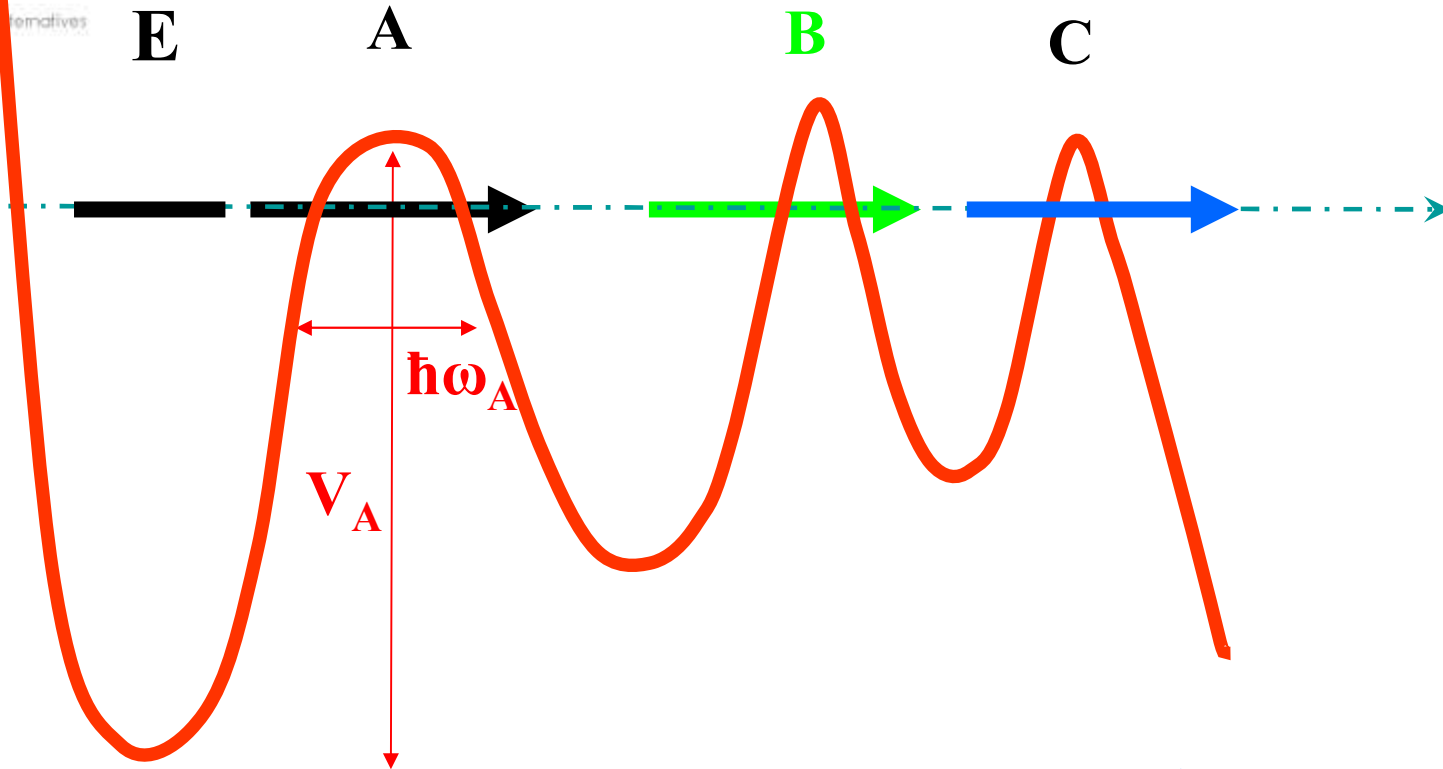
$$T_f = T_A \frac{T_B}{T_A + T_B}$$

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deformation



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fission barrier with 3 humps



$$\frac{1}{T_f} = \frac{1}{T_A} + \frac{1}{T_B} + \frac{1}{T_C}$$

$$T_i = 1/[1 + \exp(2\pi(V_i - E)/\hbar\omega_i)]$$

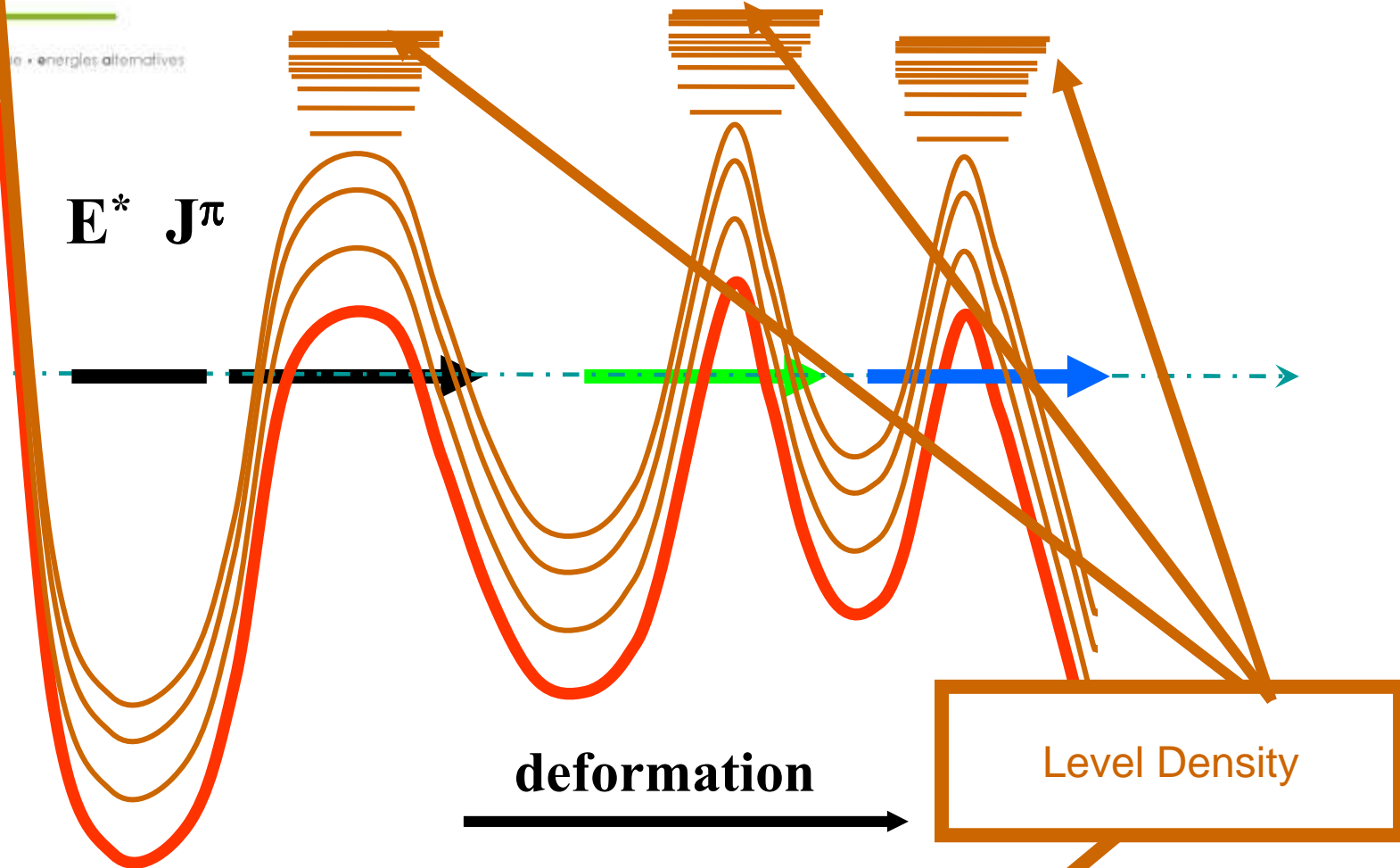
Hill-Wheeler

B. Morillon, H. Duarte, P. Romain
deformation



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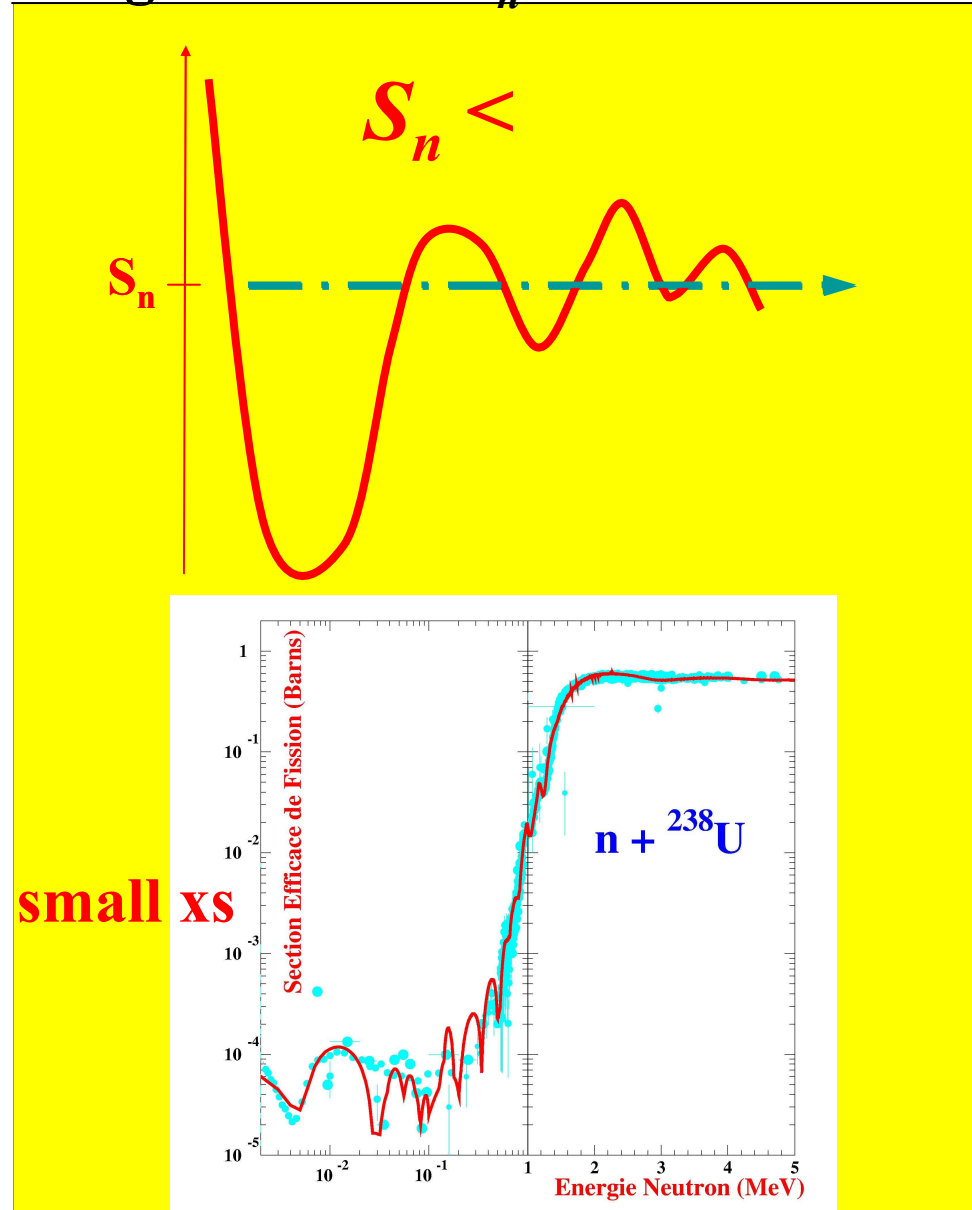
Transition States



$$T_i^{J^\pi}(E^*) = \sum_k T_i^k(E^*, \varepsilon_i^k) + \int \rho_i(\varepsilon_i^x, J^\pi) T_i^x(E^*, \varepsilon_i^x) d\varepsilon_i^x.$$



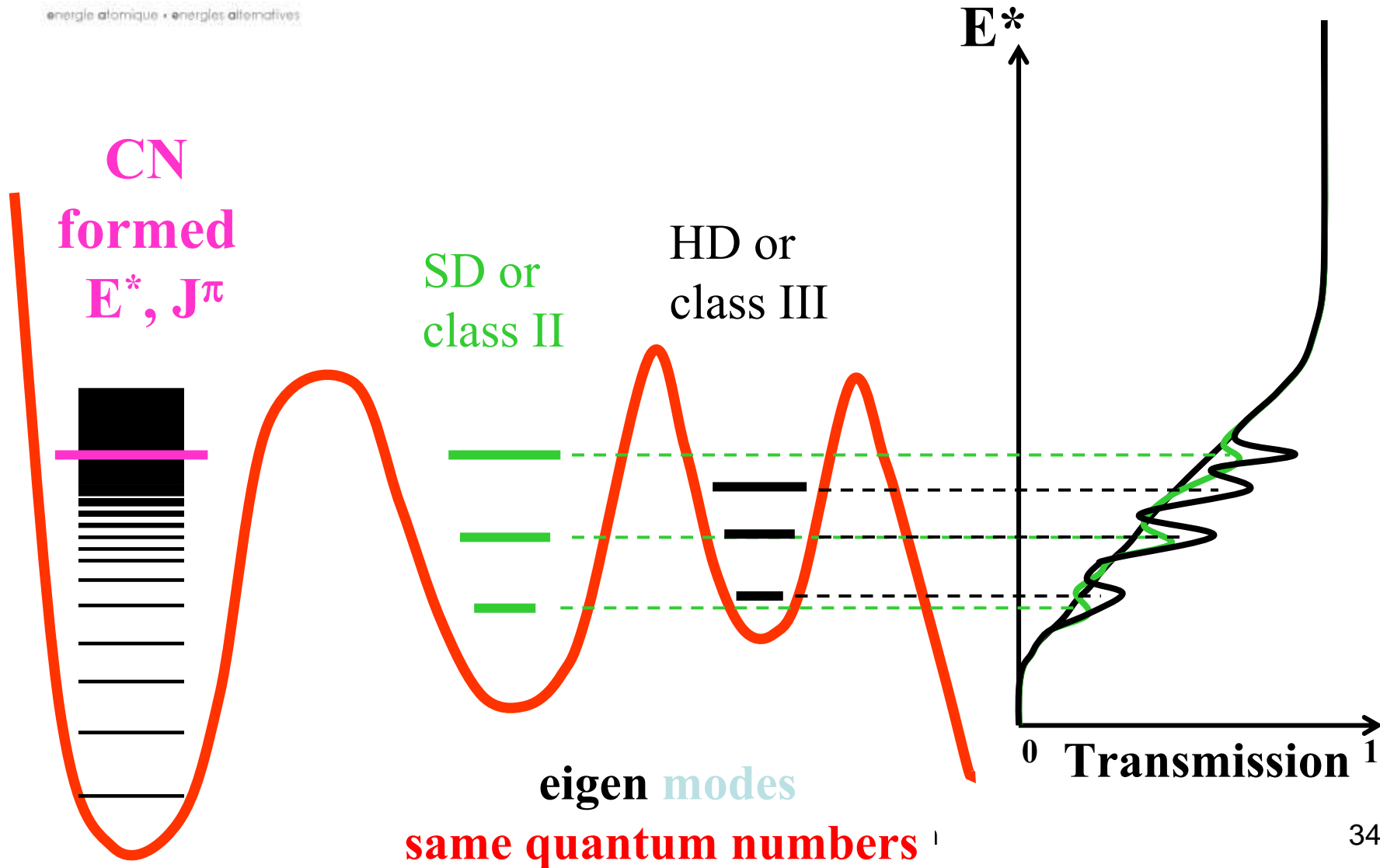
At low neutron incident energies, CN is formed at excitation energies close to S_n .



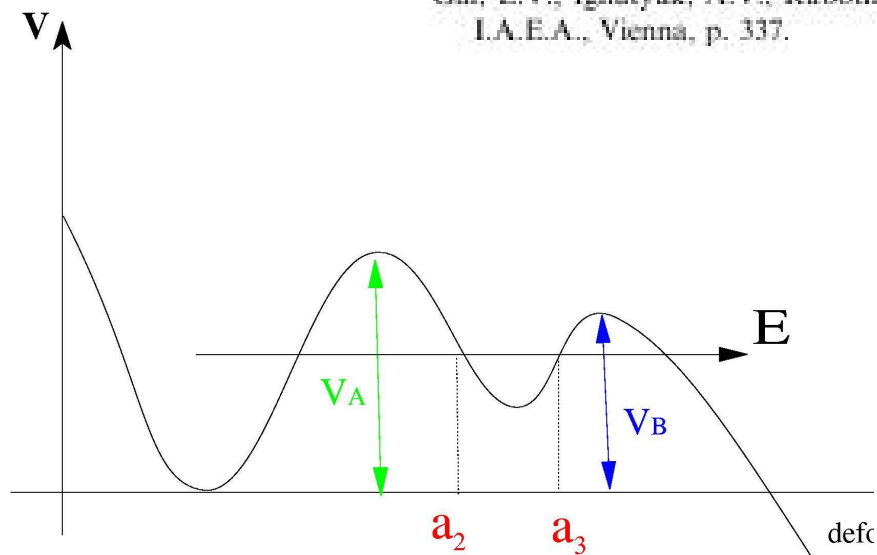


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Resonant Transmission



Gai, E.V., Ignatyuk, A.V., Rabortnov, N.S., Smirenkin, G.N., 1969. Physics and Chemistry of Fission. I.A.E.A., Vienna, p. 337.



$$T_{moy}(E) = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} \frac{\frac{T_A T_B}{4}}{\cos^2 \phi + \left(\frac{T_A + T_B}{4}\right)^2 \sin^2 \phi} d\phi$$

average

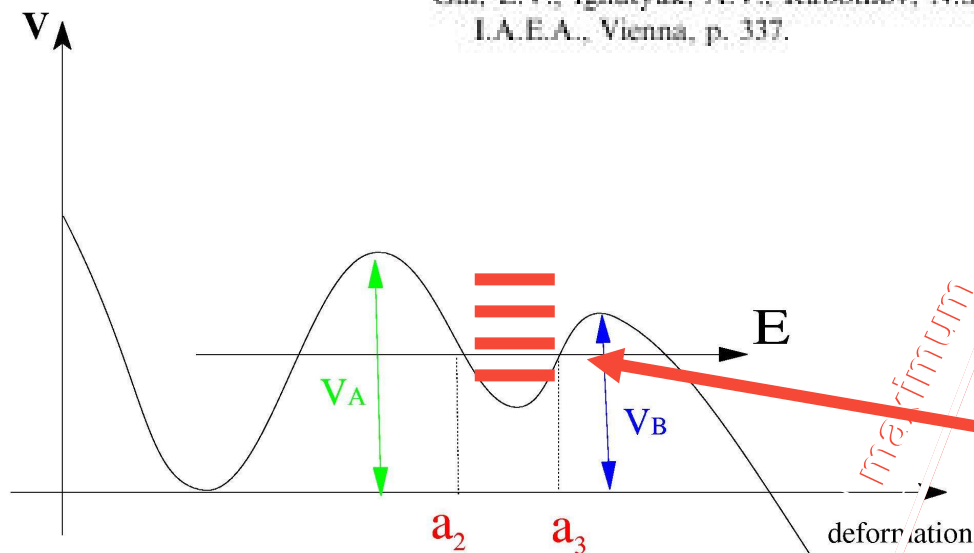
this leads to

$$T_{moy}(E) = \frac{T_A T_B}{T_A + T_B}$$

Academic model

$$T(E) \approx \frac{\frac{T_A T_B}{4}}{\cos^2 \phi + \left(\frac{T_A + T_B}{4}\right)^2 \sin^2 \phi}$$

Gai, E.V., Ignatyuk, A.V., Rabotnov, N.S., Smirenkin, G.N., 1969. Physics and Chemistry of Fission. I.A.E.A., Vienna, p. 337.



$$T_{max}(E) = \frac{4T_A T_B}{(T_A + T_B)^2}$$

when :

$$\phi(E) = \int_{a_2}^{a_3} K(x) dx = \pi(E - E_{II}) / \hbar\omega_{II} = (2n+1) \frac{\pi}{2}$$

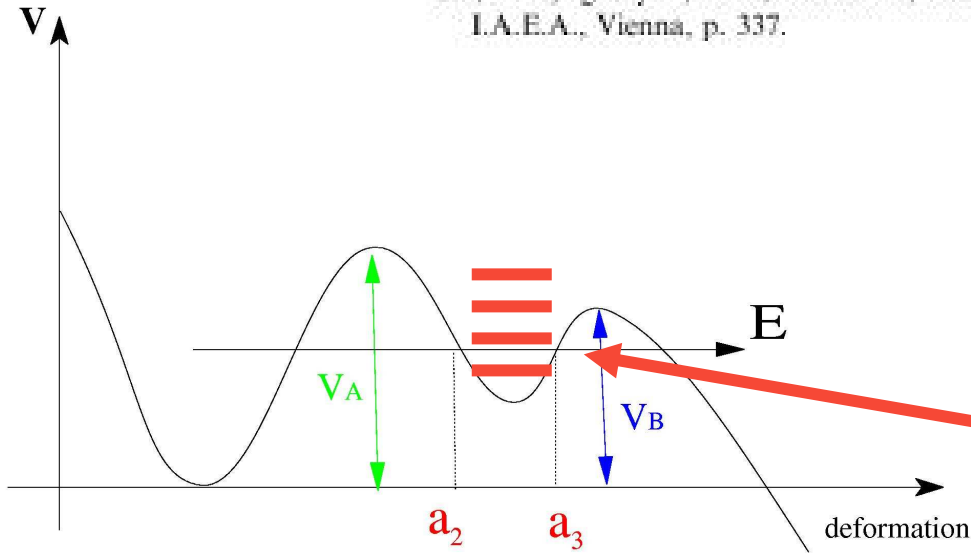
assuming $V(x)$ well oscillator

$$E - E_{II} = (n + \frac{1}{2}) \hbar\omega_{II}$$

Academic model

$$T(E) \approx \frac{\frac{T_A T_B}{4}}{\cos^2 \phi + \left(\frac{T_A + T_B}{4}\right)^2 \sin^2 \phi}$$

Gai, E.V., Ignatyuk, A.V., Rrobotnov, N.S., Smirenkin, G.N., 1969. Physics and Chemistry of Fission. I.A.E.A., Vienna, p. 337.



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assuming $V(x)$ well oscillator

$$E - E_{II} = (n + \frac{1}{2}) \hbar \omega_{II}$$

Resonant transmission

Academic model

$$RT_2 = \frac{T_A \times T_B}{T_A + T_B} \times \frac{4}{T_A + T_B} = \frac{4T_A^{j^*} T_B^{j^*}}{(T_A^{j^*} + T_B^{j^*})^2}$$

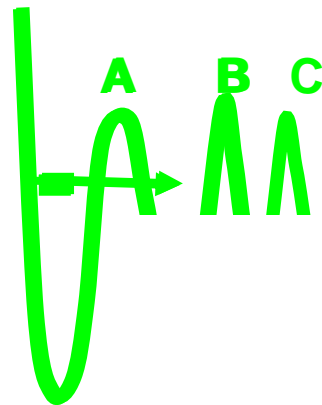
Enhancement factor for transmission that we will now apply to our simplified model for fission channel



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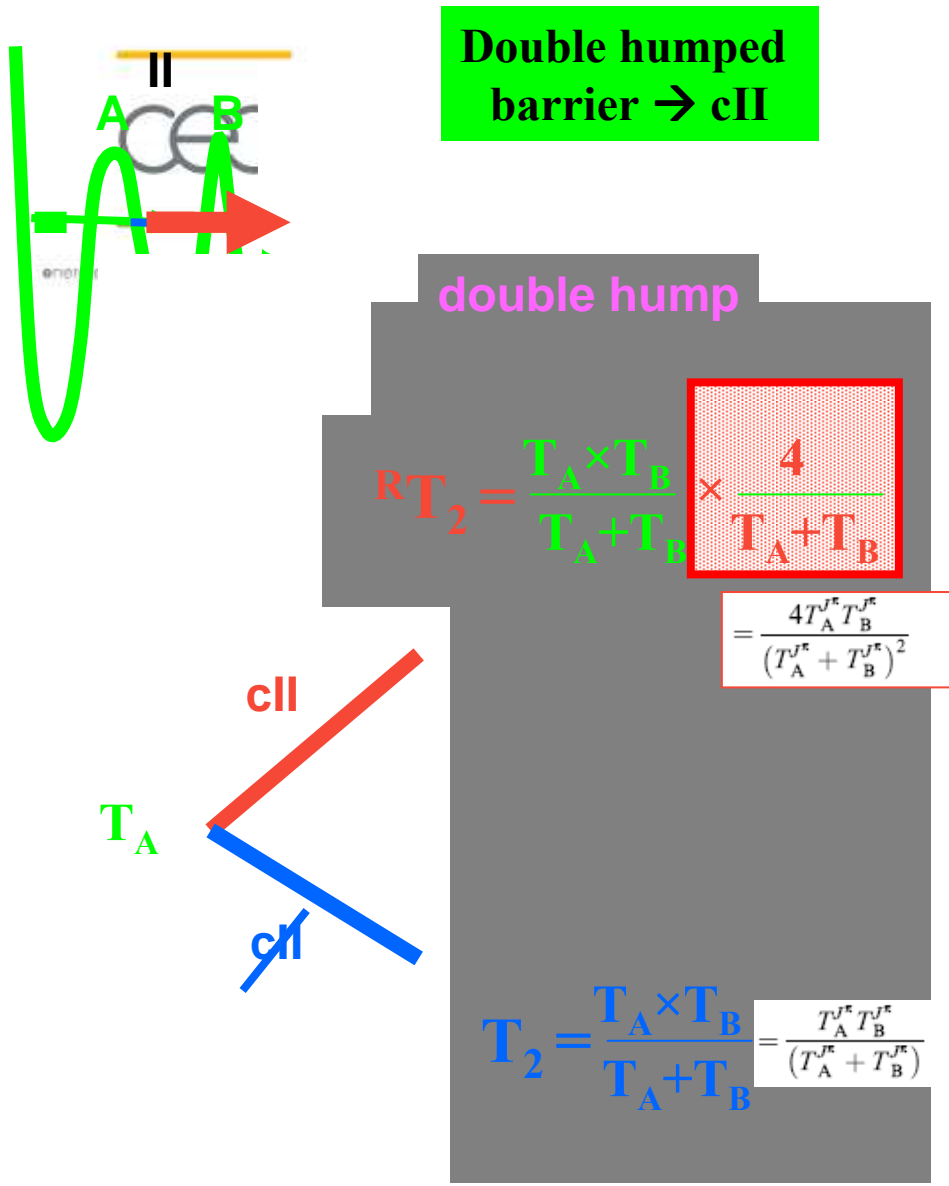
Extension to a Simplified model and generalization

{ like in previous
GNASH code
(1996) }



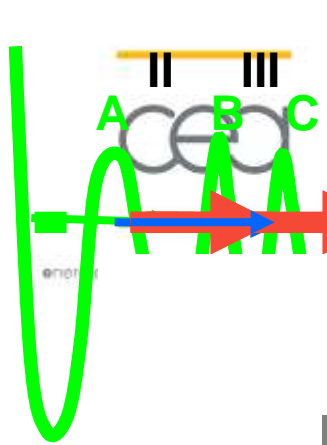
Inverse parabola

$$\text{Hill – Wheeler formula : } T_A(E) = \frac{1}{1 + \exp\left[\frac{-2\pi}{\hbar\omega}(E - V_A)\right]}$$



Ann. Nucl. Energy **32**, 195 (2005)

B. Morillon H. Duarte P. Romain



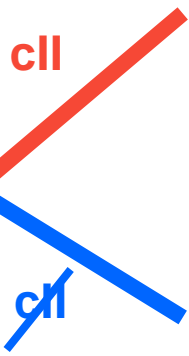
Triple humped barrier → cII and cIII

double hump

$$RT_2 = \frac{T_A \times T_B}{T_A + T_B} \times \frac{4}{T_A + T_B}$$

$$= \frac{4T_A^{J^k} T_B^{J^k}}{(T_A^{J^k} + T_B^{J^k})^2}$$

T_A



$$T_2 = \frac{T_A \times T_B}{T_A + T_B} = \frac{T_A^{J^k} T_B^{J^k}}{(T_A^{J^k} + T_B^{J^k})}$$

cIII

~~cII~~

cIII

~~cII~~

triple hump

$$\frac{RT_2 \times T_C}{RT_2 + T_C} \times \frac{4}{RT_2 + T_C}$$

$$= \frac{16T_A^{J^k} T_B^{J^k} T_C^{J^k} (T_A^{J^k} + T_B^{J^k})^2}{(4T_A^{J^k} T_B^{J^k} + T_C^{J^k} (T_A^{J^k} + T_B^{J^k})^2)^2}$$

$$\frac{RT_2 \times T_C}{RT_2 + T_C} = \frac{4T_A^{J^k} T_B^{J^k} T_C^{J^k}}{4T_A^{J^k} T_B^{J^k} + T_C^{J^k} (T_A^{J^k} + T_B^{J^k})^2}$$

$$\frac{T_2 \times T_C}{T_2 + T_C} \times \frac{4}{T_2 + T_C}$$

$$= \frac{4T_A^{J^k} T_B^{J^k} T_C^{J^k} (T_A^{J^k} + T_B^{J^k})}{(T_A^{J^k} T_B^{J^k} + T_A^{J^k} T_C^{J^k} + T_B^{J^k} T_C^{J^k})^2}$$

$$\frac{T_2 \times T_C}{T_2 + T_C} = \frac{T_A^{J^k} T_B^{J^k} T_C^{J^k}}{T_A^{J^k} T_B^{J^k} + T_A^{J^k} T_C^{J^k} + T_B^{J^k} T_C^{J^k}}$$

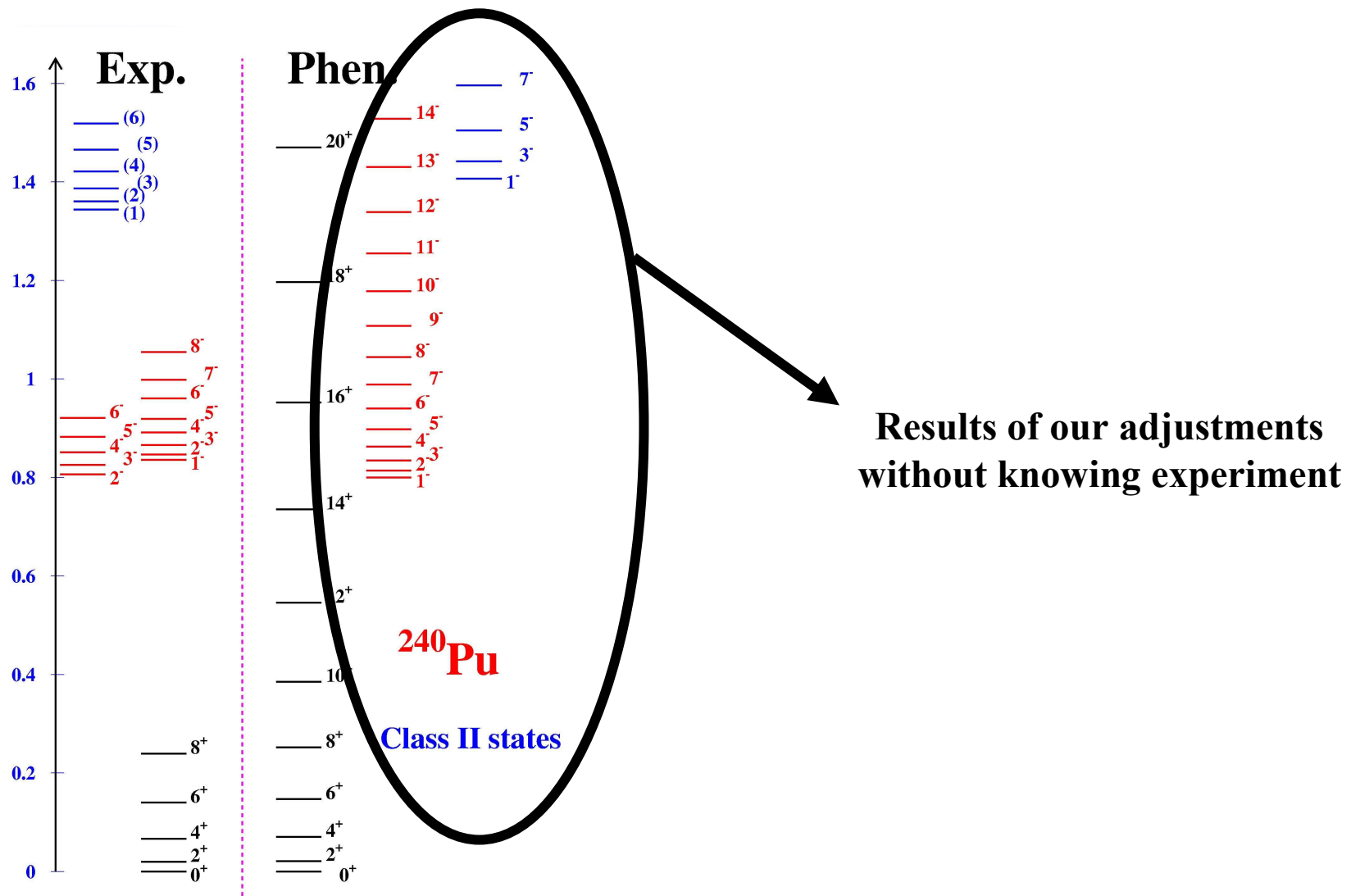
Ann. Nucl. Energy 32, 195 (2005)

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*In this **simplified model** we have only **to adjust** (to find E_i and J^π) **cII** and **cIII** quantum number in order **to reproduce** (**fit**) the first chance fission cross sections*



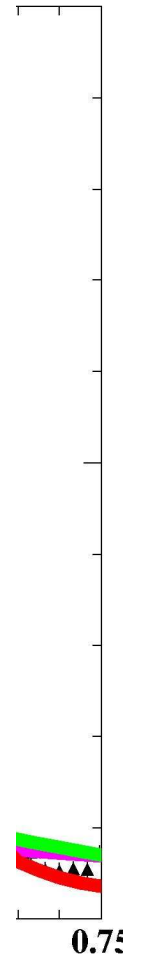
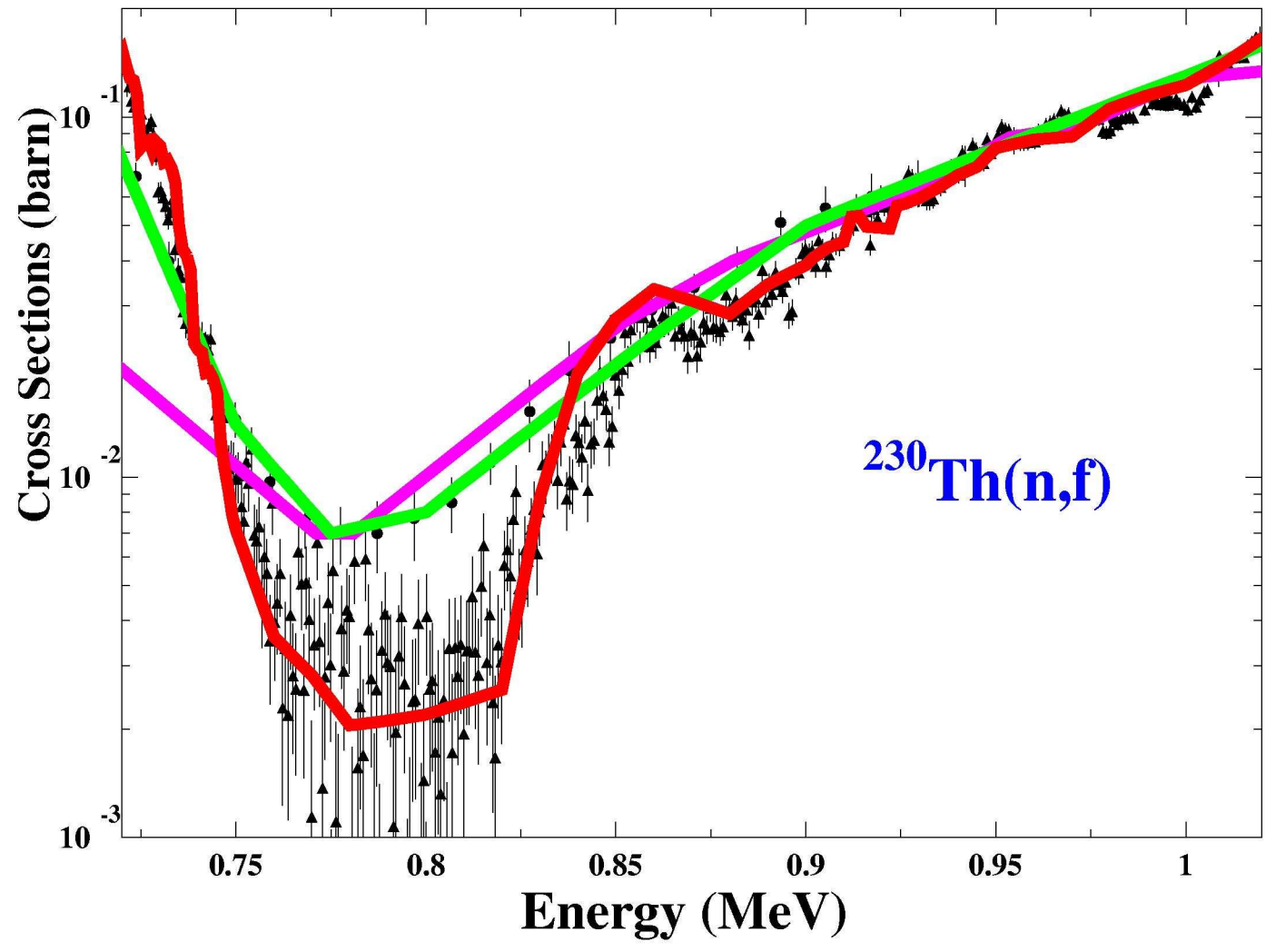


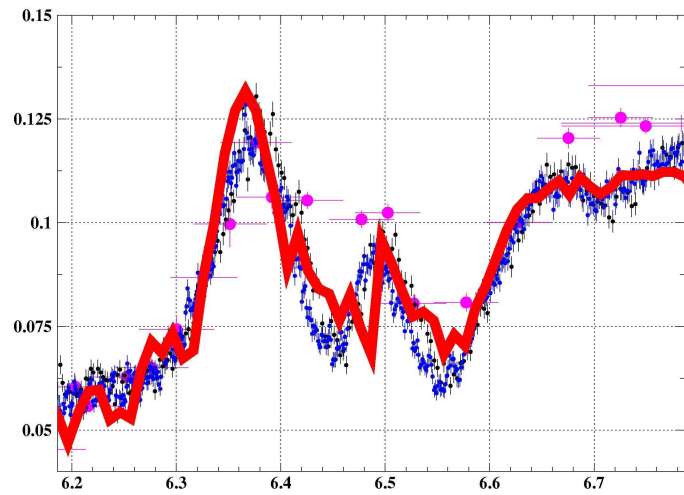
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TEST of our model on ^{230}Th

$$Z = 90$$

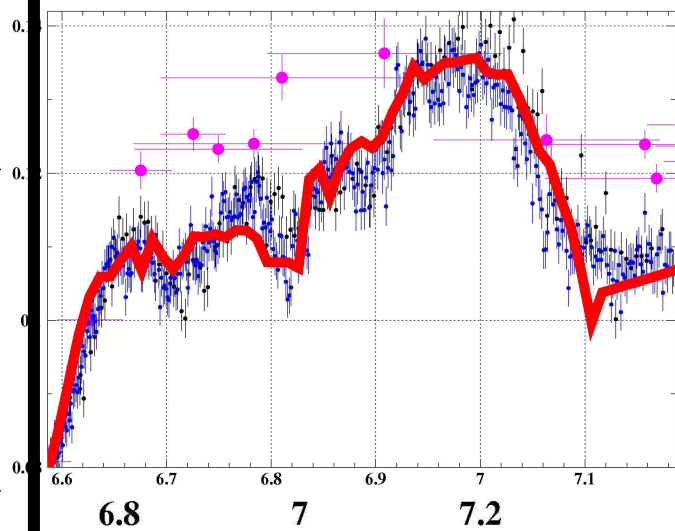
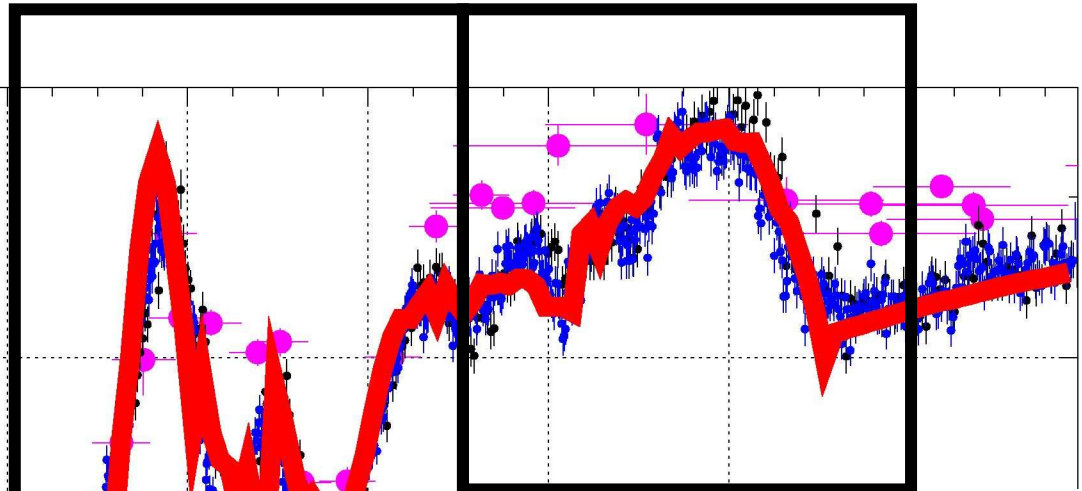
ener





$n + {}^{232}\text{Th}$

Fission cross section



Excitation Energy (MeV)



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TEST of our model on

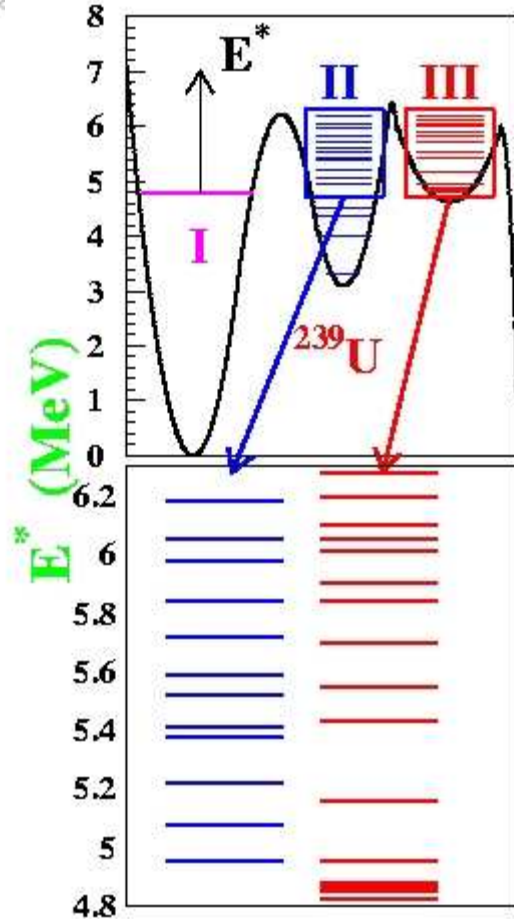
Z = 92

^{239}U : Triple-humped fission barrier

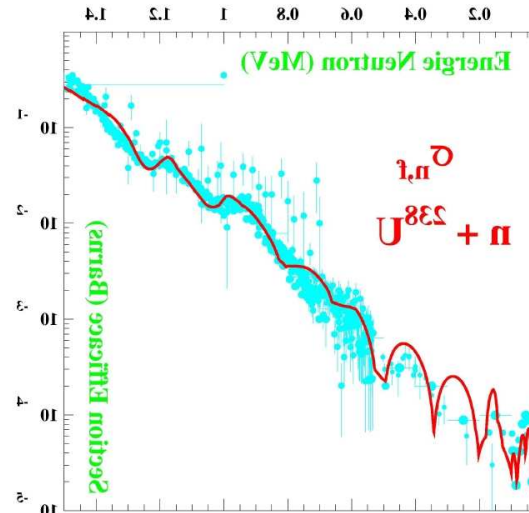
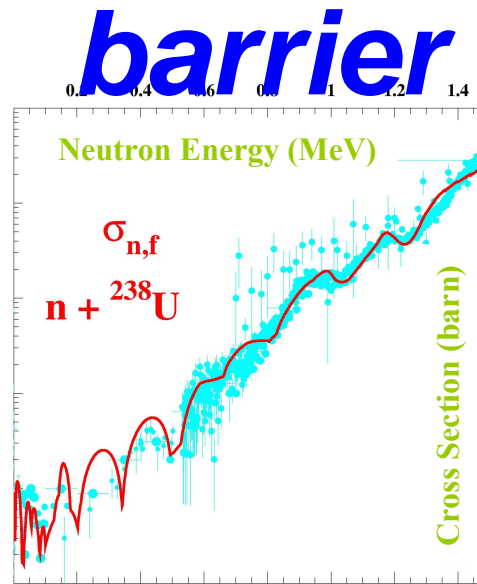


Resonant transmission

energies at:



Bandhead states

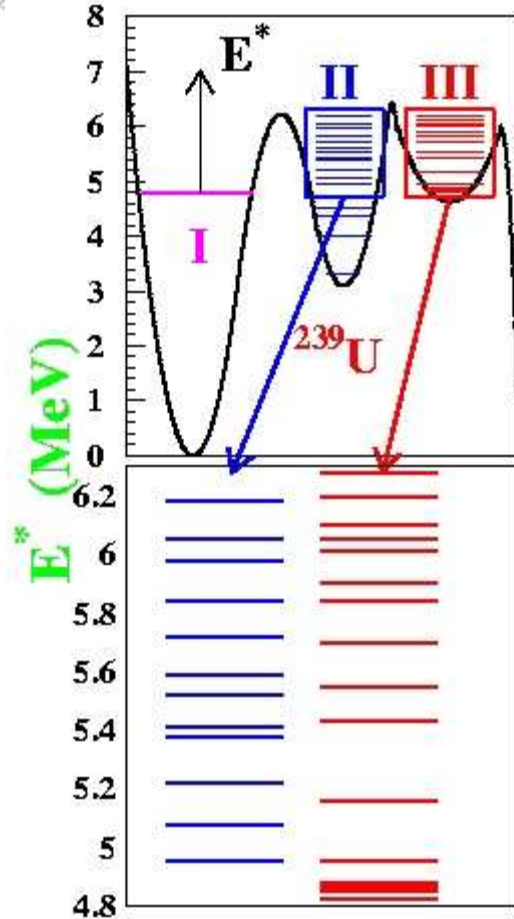


^{239}U : Triple-humped fission barrier

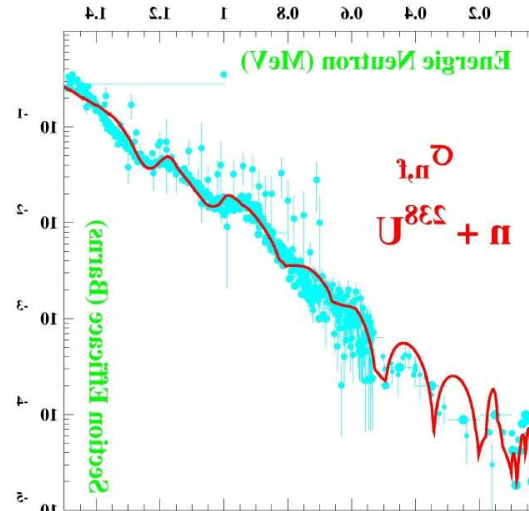
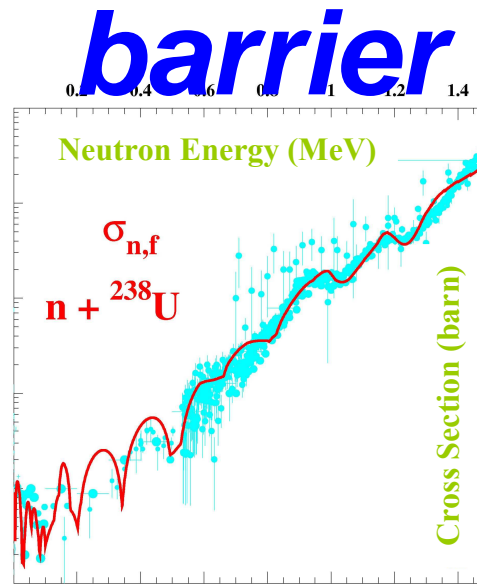


Resonant transmission

energies at:



Bandhead states

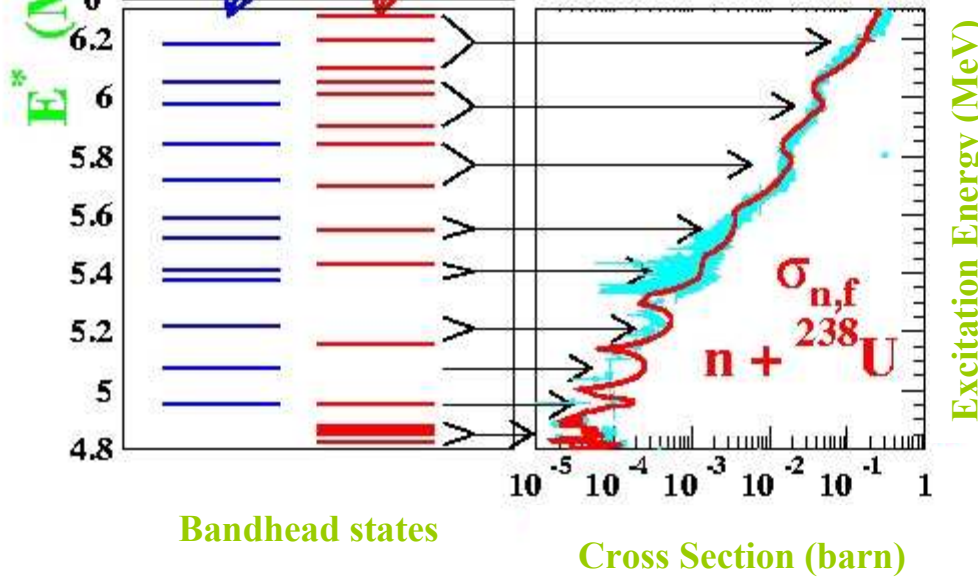
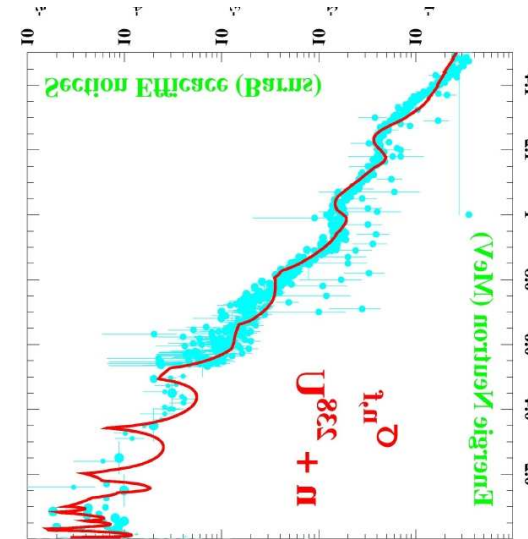
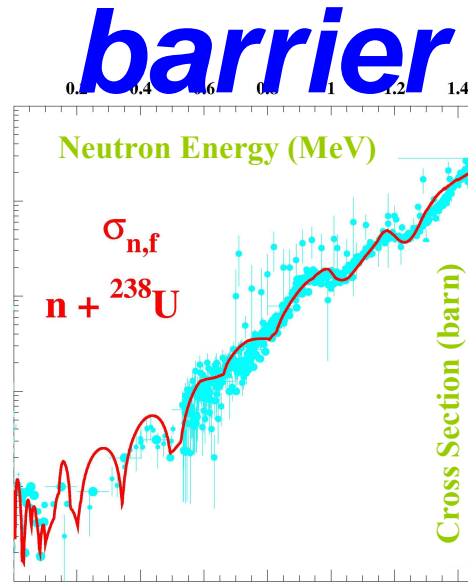
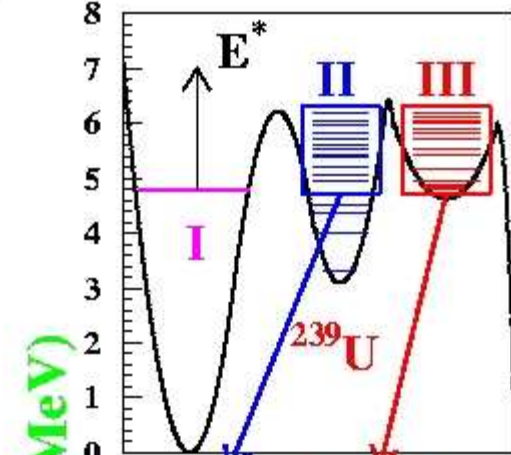


^{239}U : Triple-humped fission barrier



Resonant transmission

energie at:



Bandhead states

Cross Section (barn)

**Influence
of
Class II and Class III states
on
fission cross section**

^{238}U FISSION CROSS SECTION

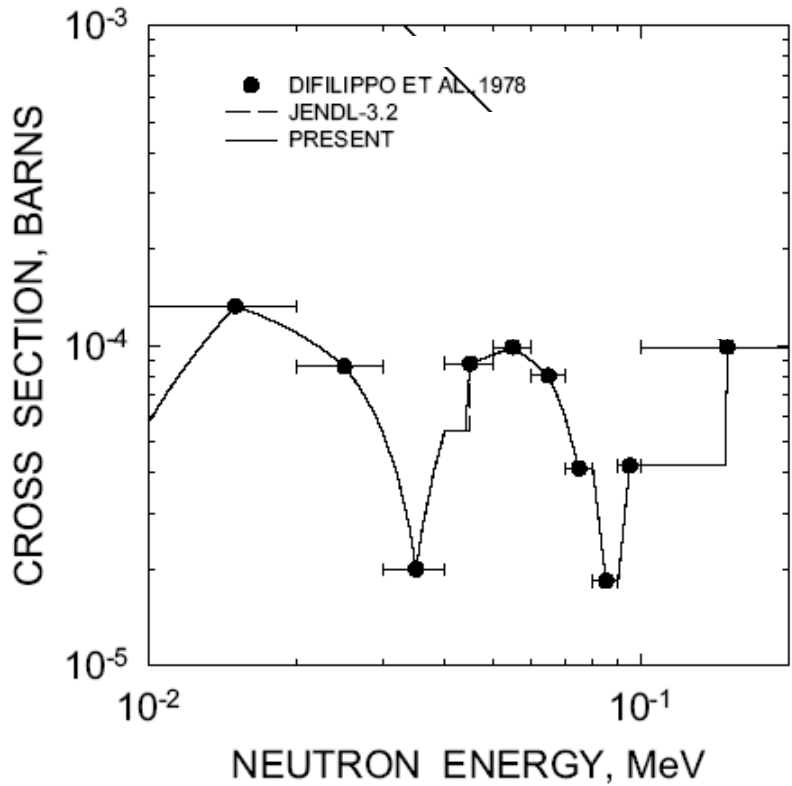
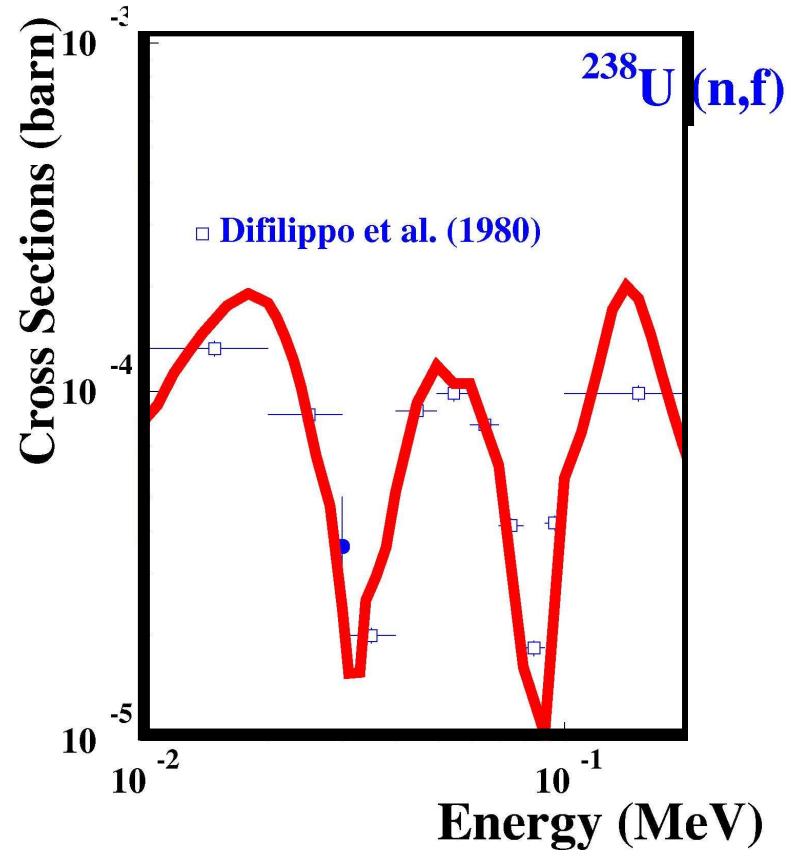


FIG. 10



V. MASLOV INDC(BLR)-014



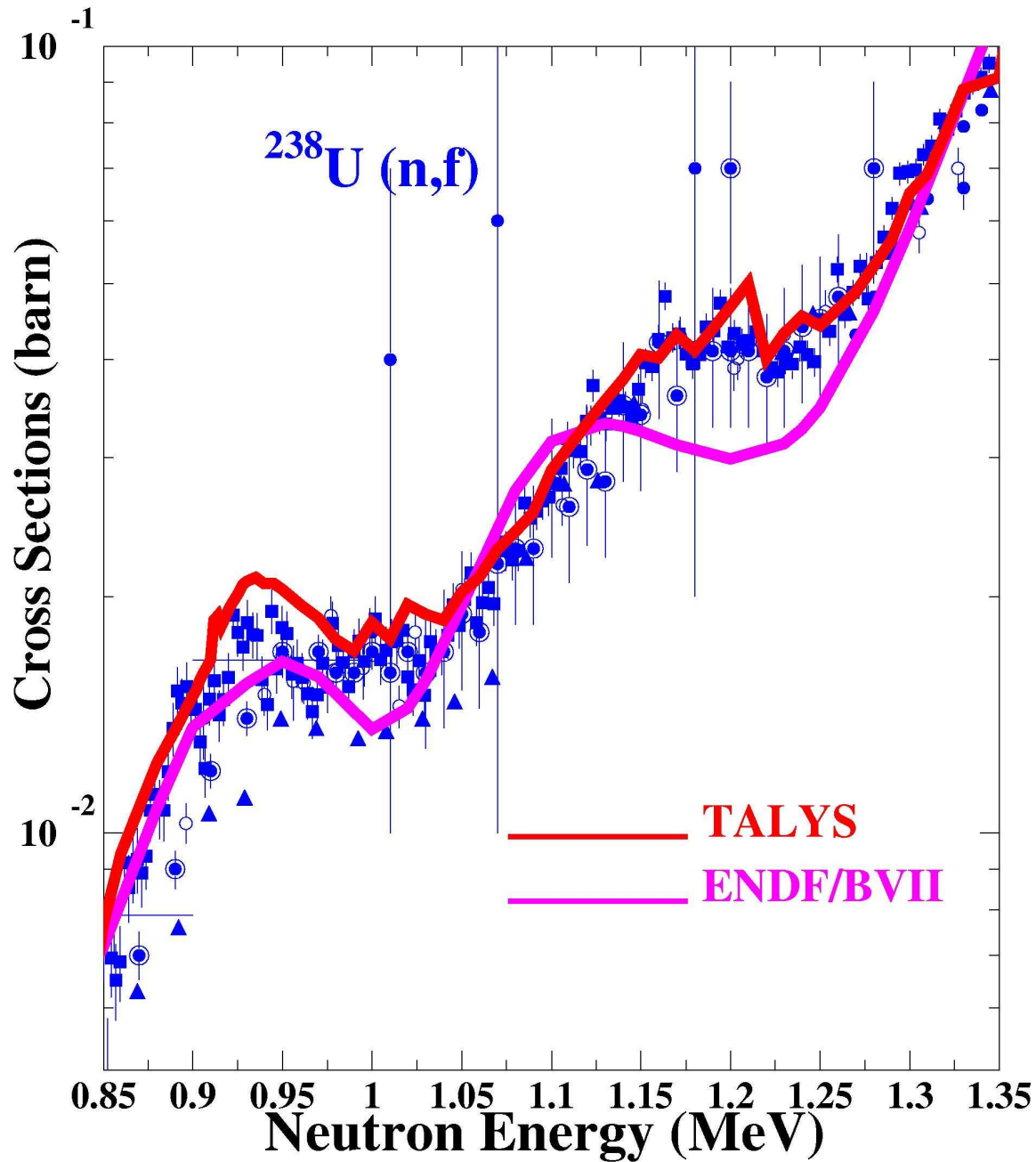
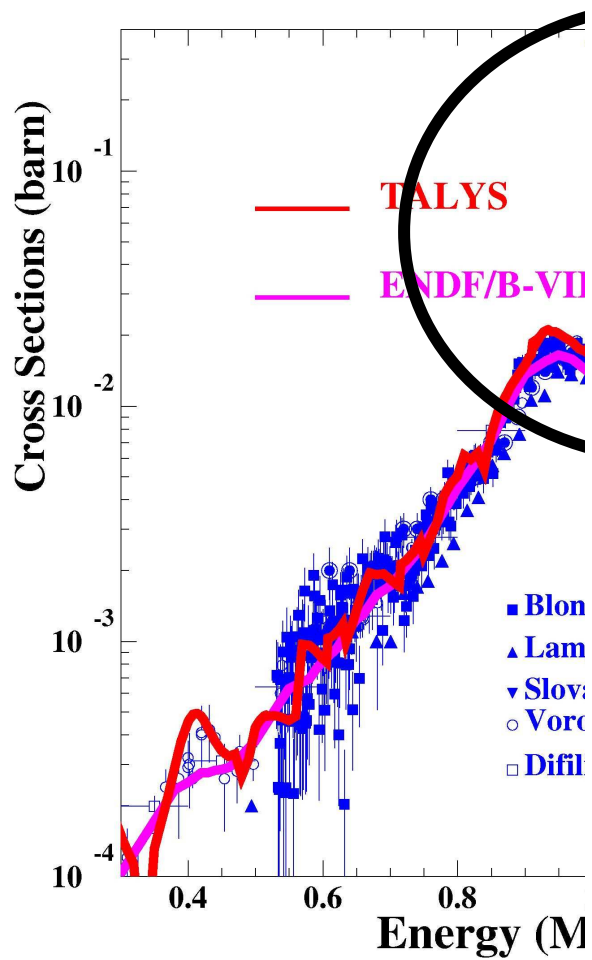
INTERNATIONAL ATOMIC ENERGY AGENCY
INDC(BLR)-014
Distr. J+TU/EL

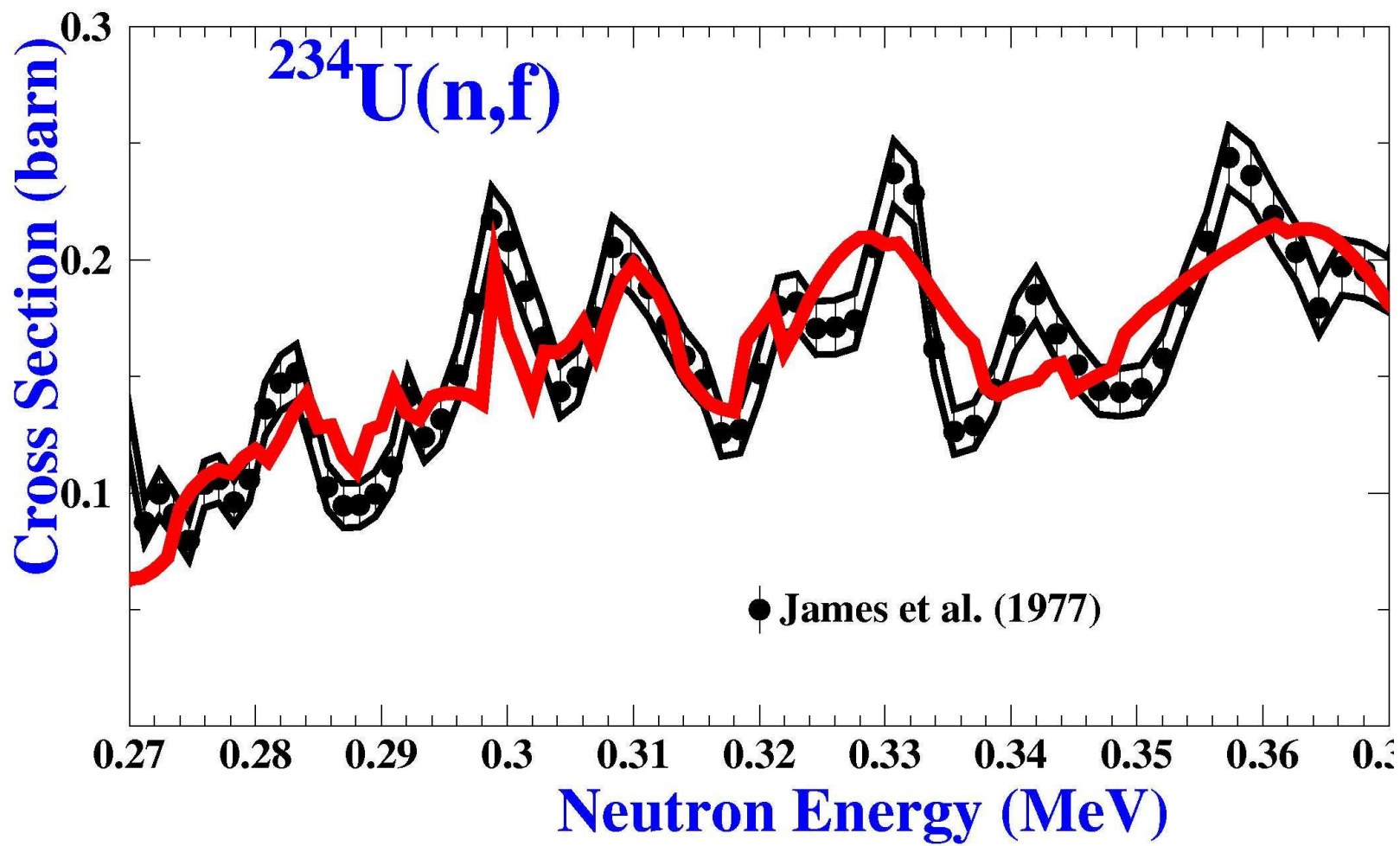
INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

H. Duarte P. Romain

TALYS

TALYS = BRC2008





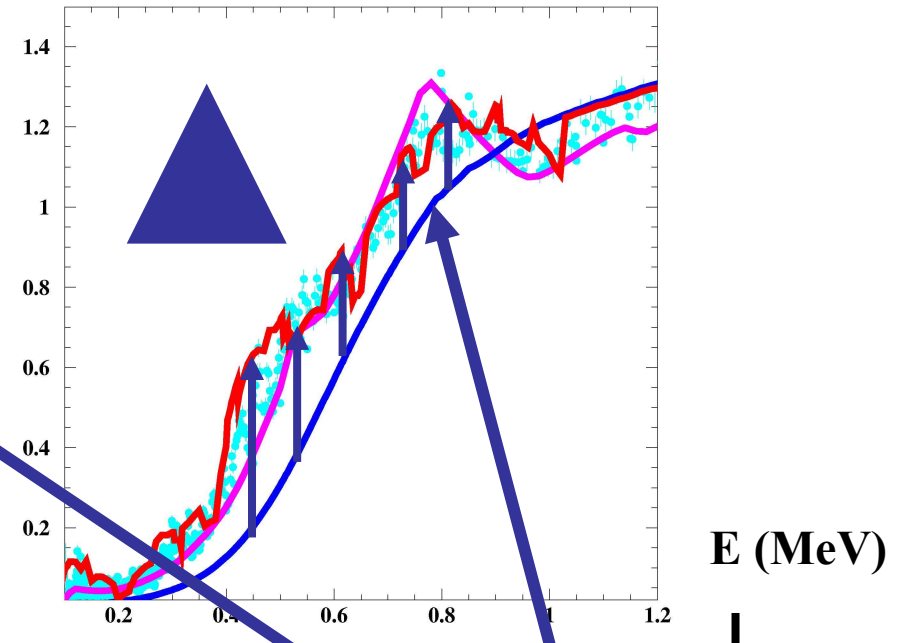
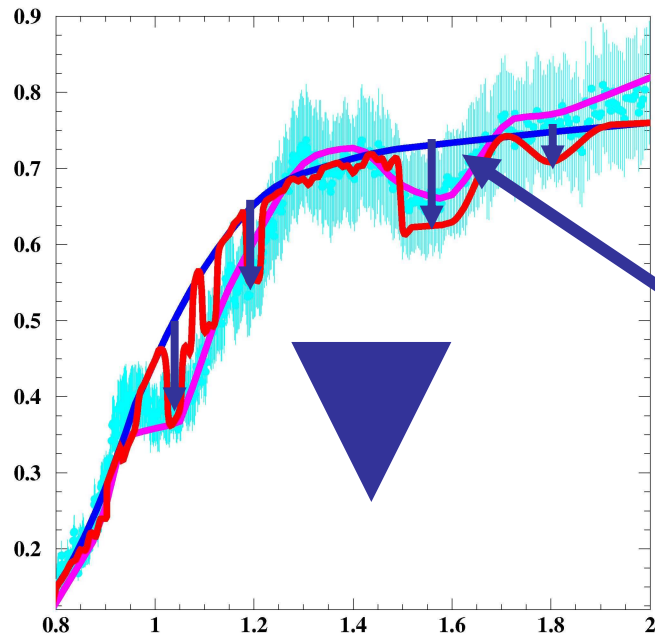
TALYS

$\sigma_f(b)$ $n + {}^{236}\text{U}$

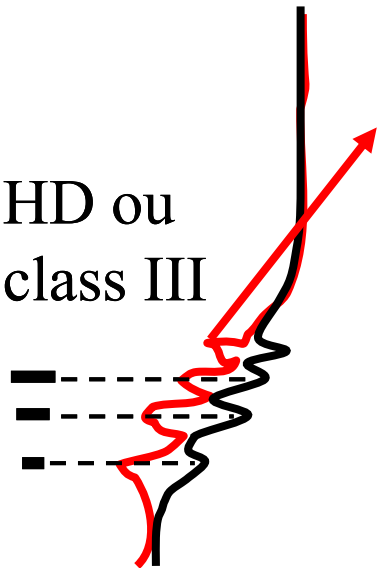
crazy effect

$\sigma_f(b)$ $n + {}^{234}\text{U}$

ENDF/B-VII
BRC/TALYS



HD ou
class III



antiresonance

**antiresonant circuit
= circuit bouchon**

(frenchy speaking)

« **bouchonance** »

B. Morillon H. Duarte P. Ro

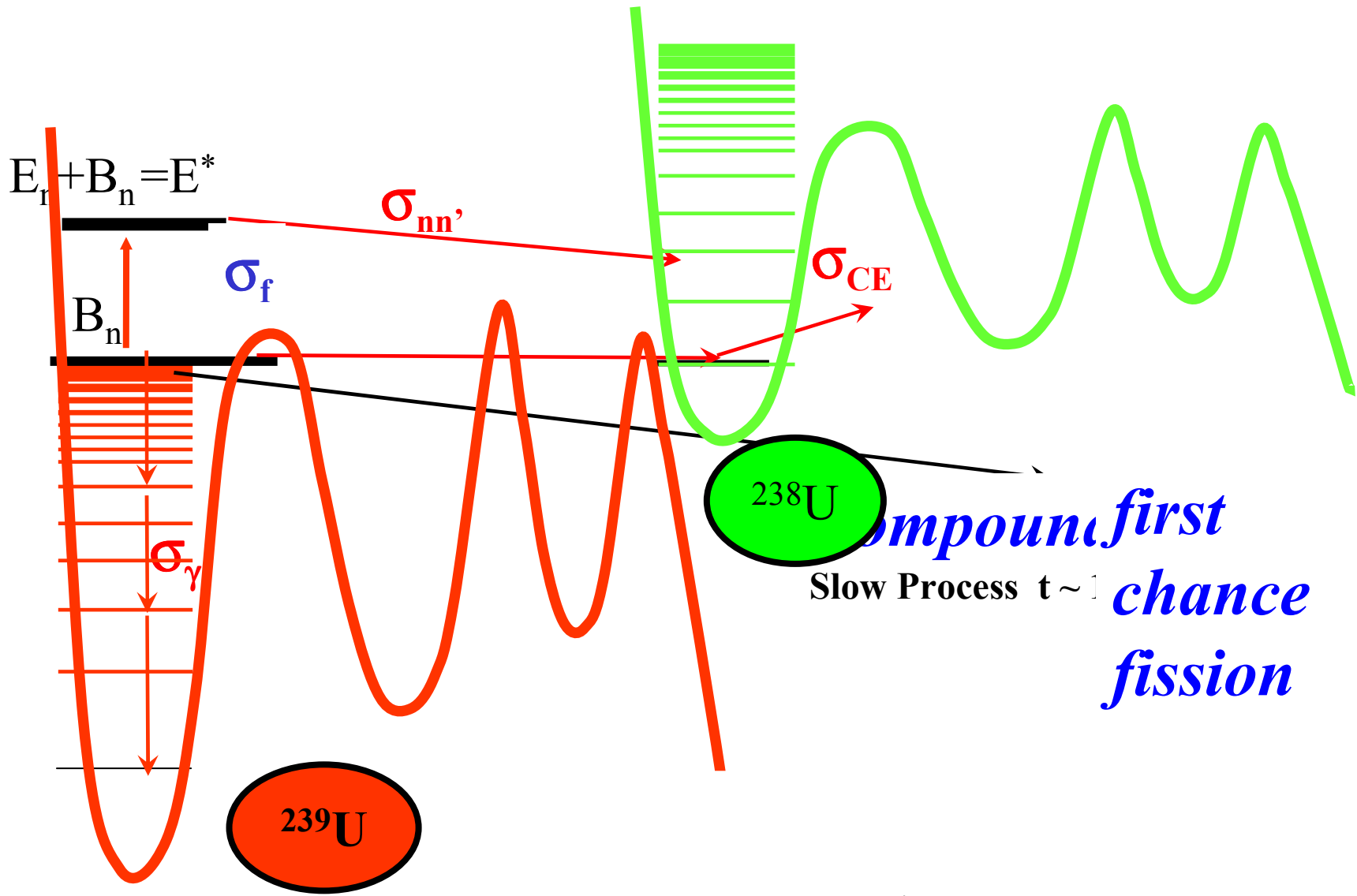
M.J. López-Jiménez

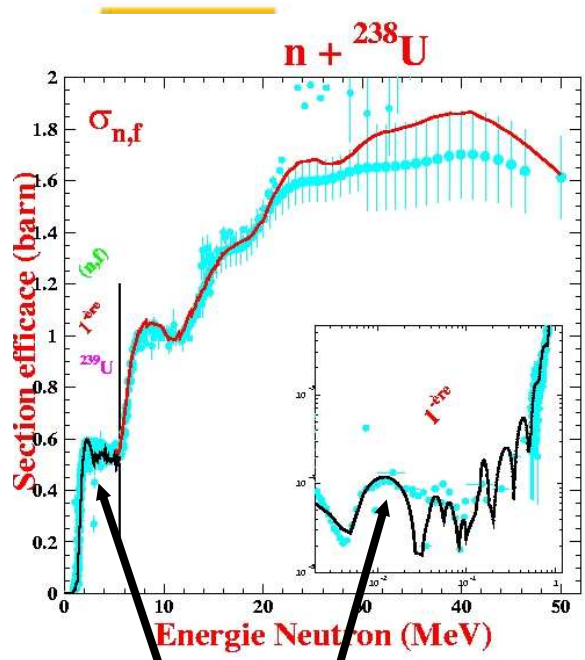
Post doc 2001-2003

at SPN

And now when neutron incident energy increases

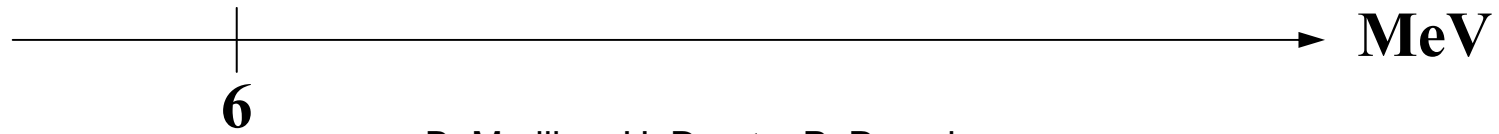
methodology

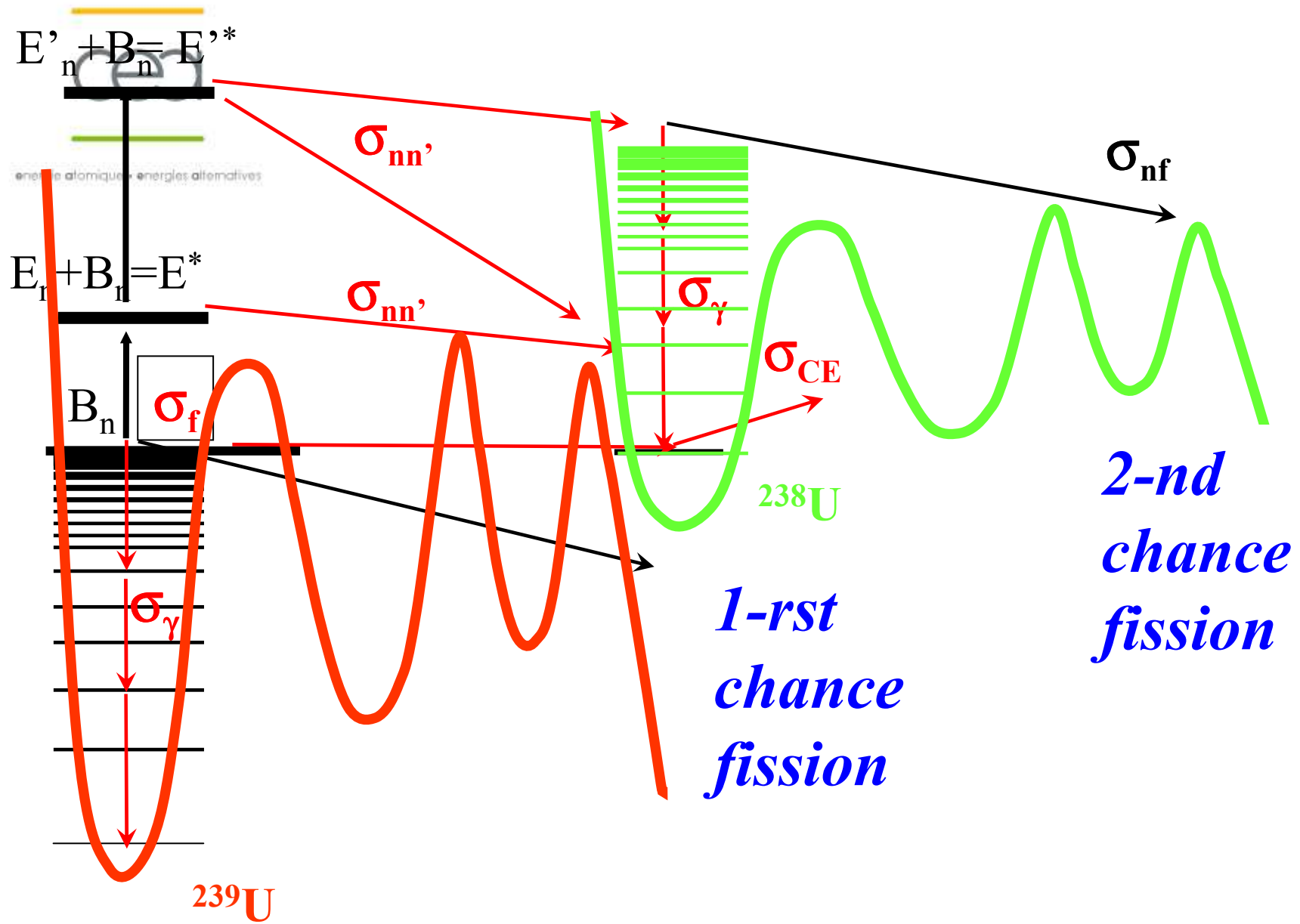


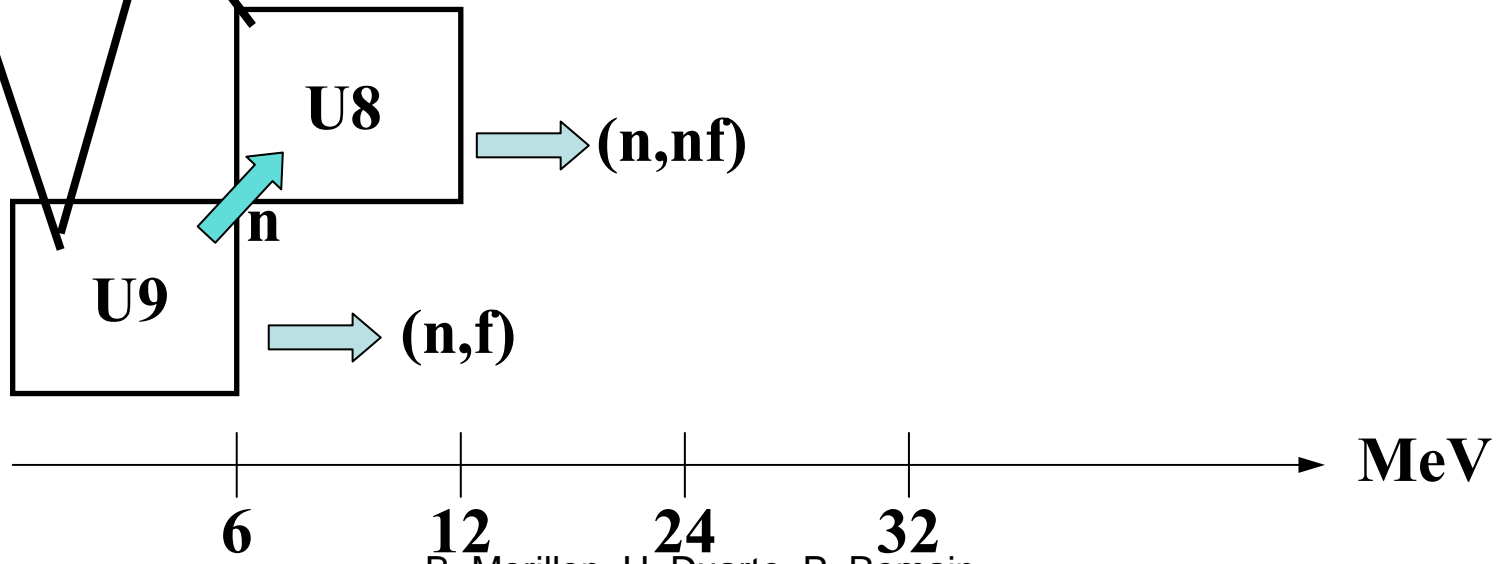
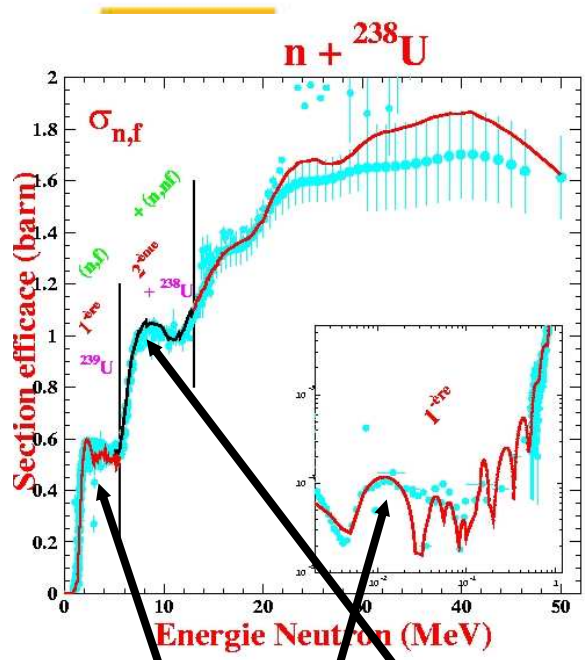


U9

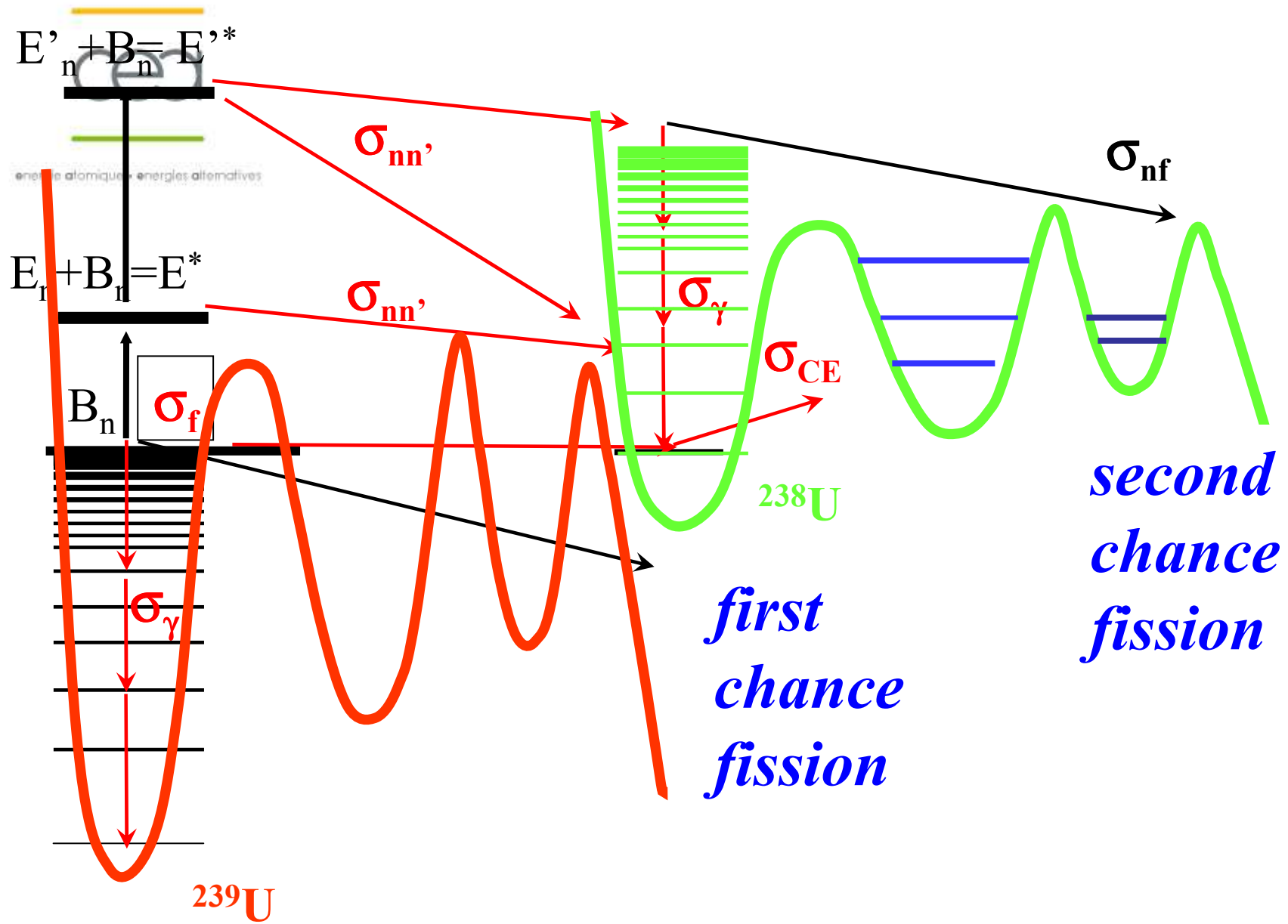
→ (n,f)



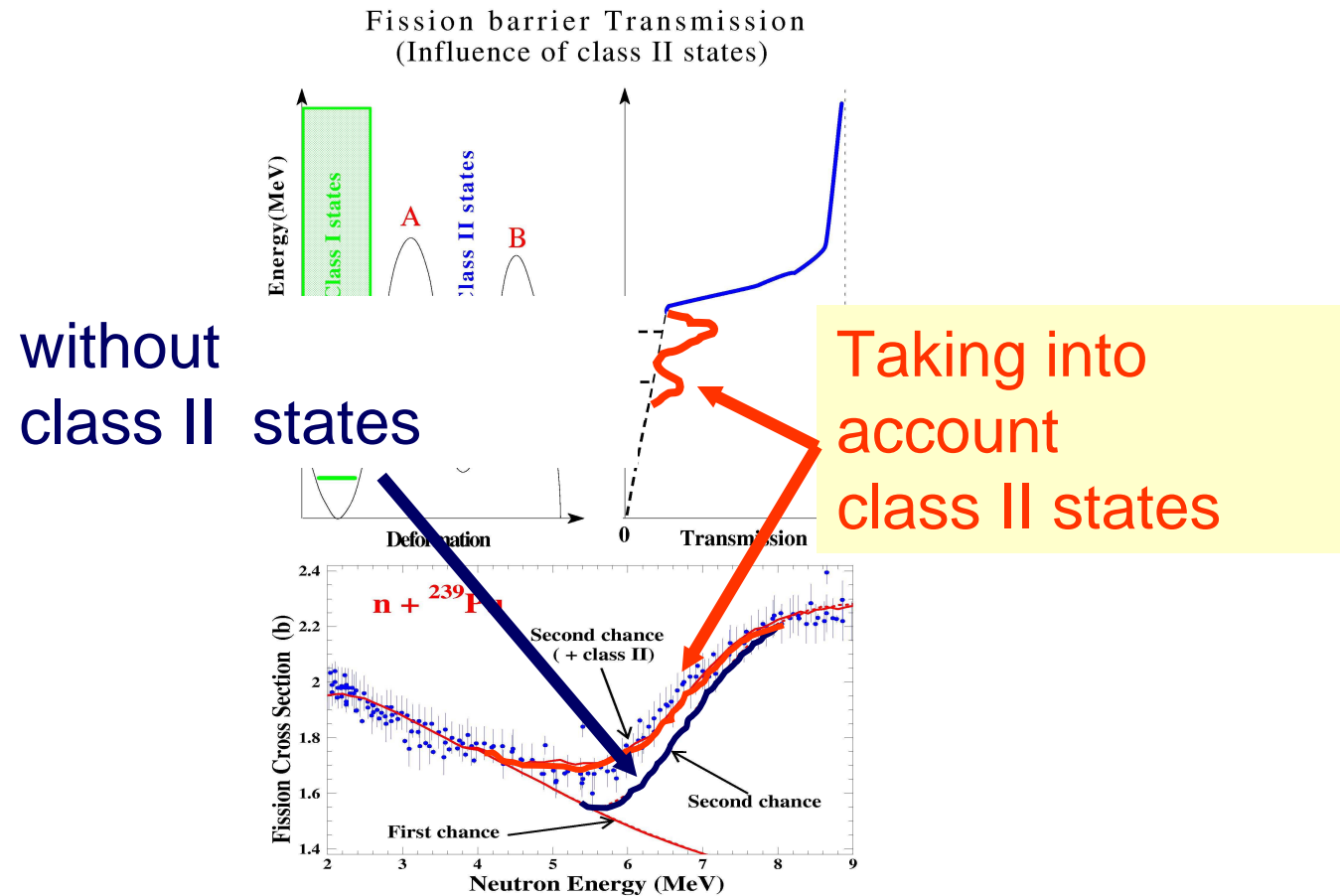


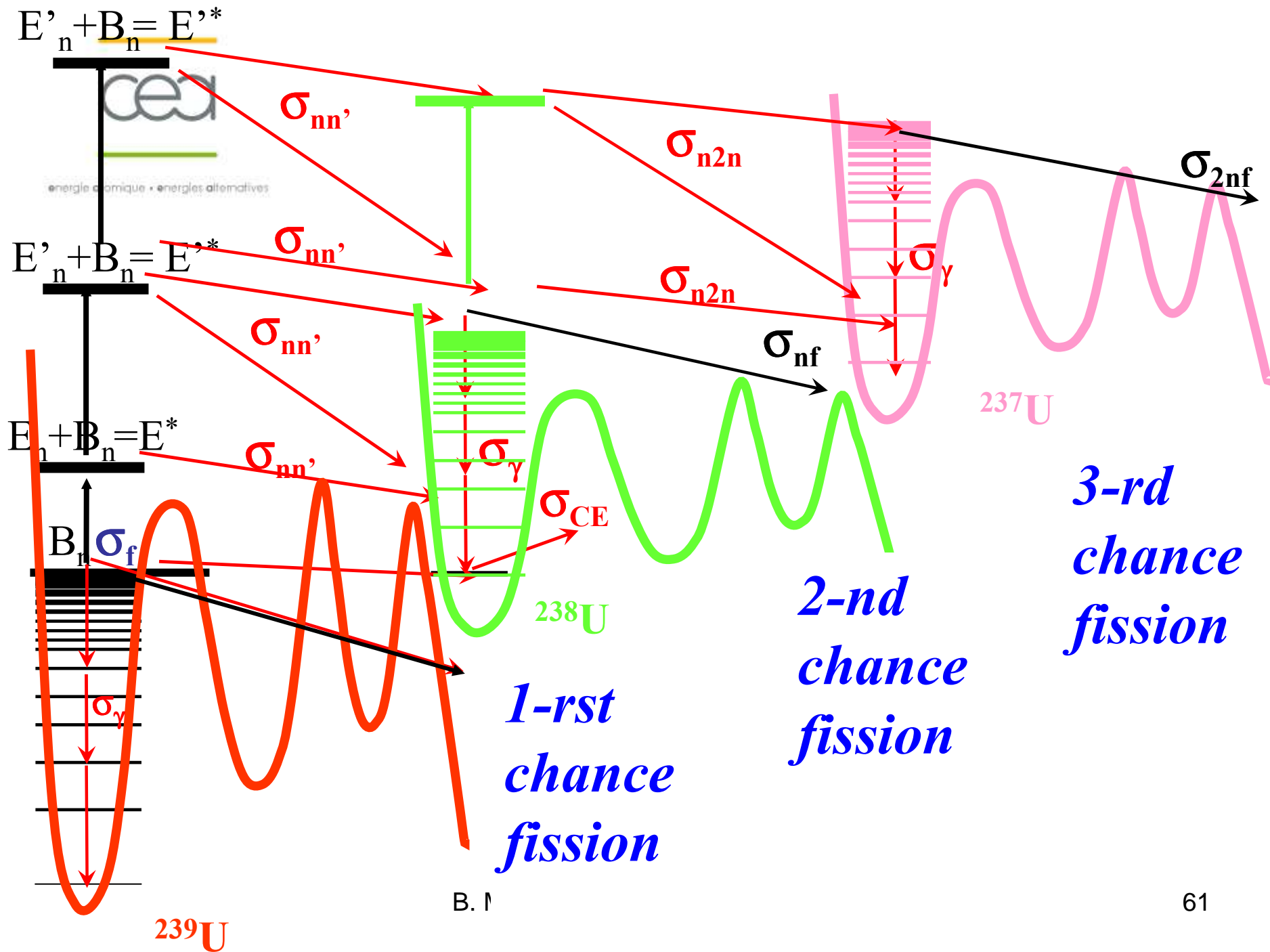


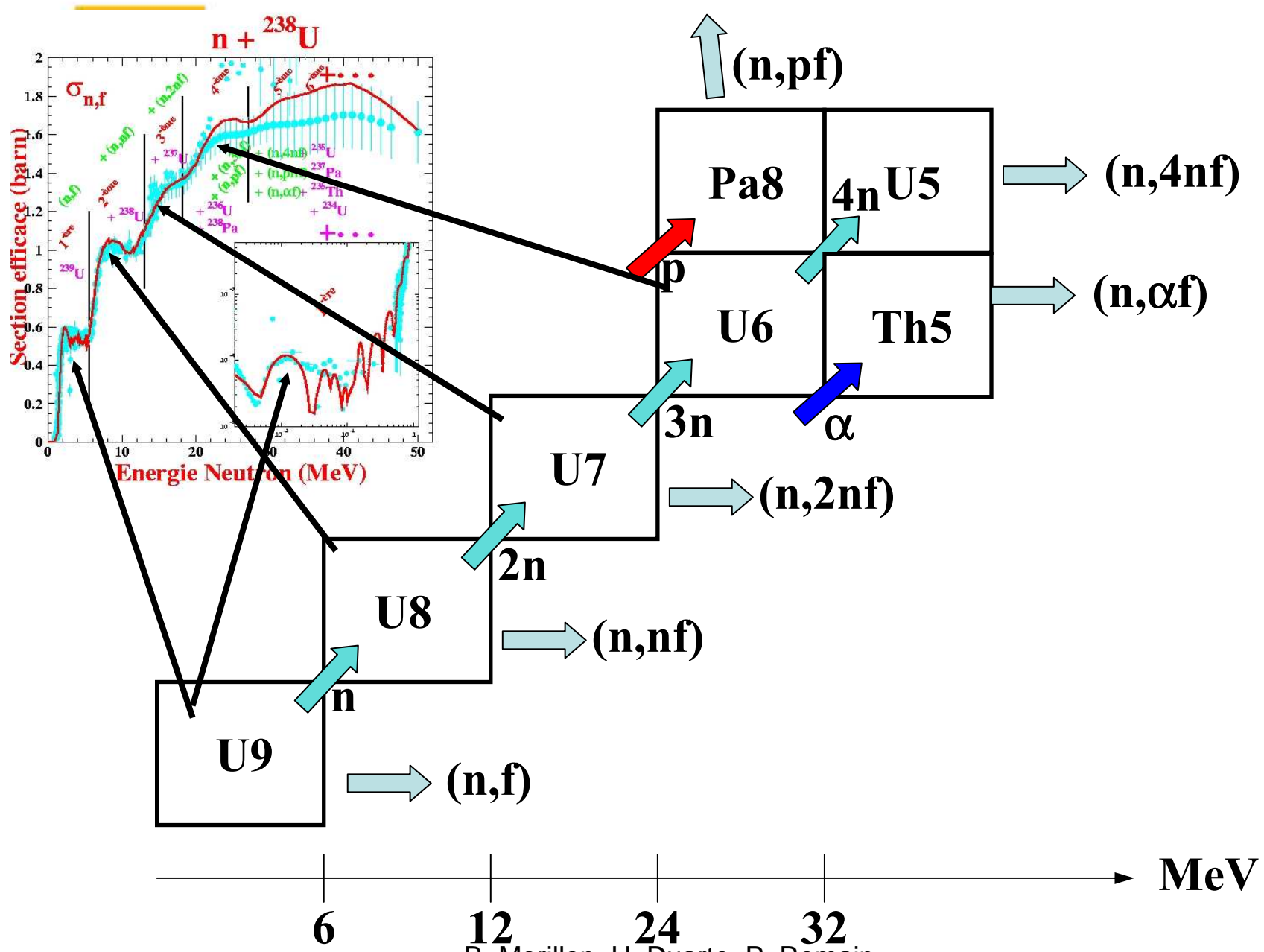
B. Morillon H. Duarte P. Romain

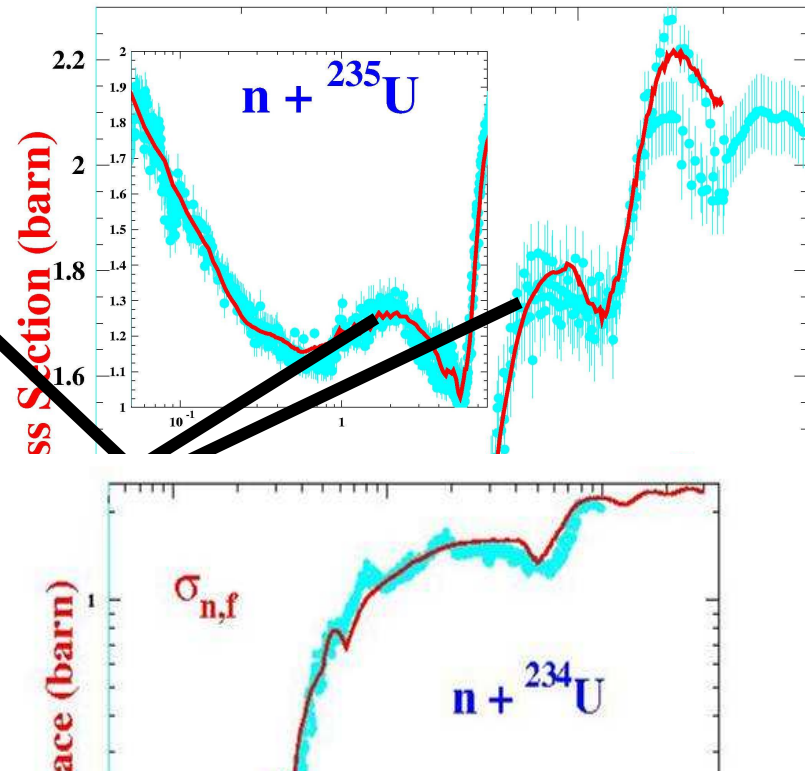
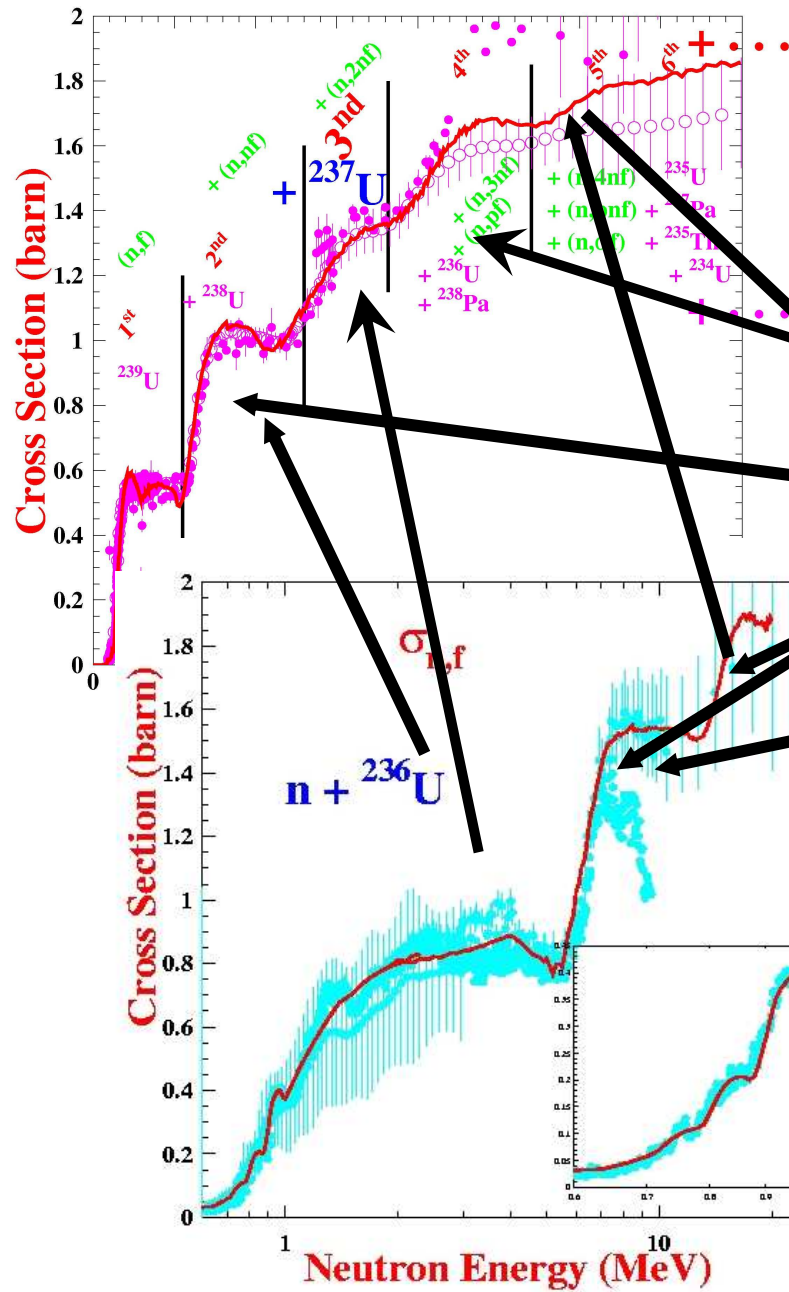


Effects of class II states on opening of second chance fission









Avec le même passe-partout ^{238}U
on visite plusieurs réservoirs :

- $\sigma_{\text{CN}} (n+^{238}\text{U}) \rightarrow n, \text{nf}$
- $\sigma_{\text{CN}} (n+^{237}\text{U}) \rightarrow n, \text{f}$
- $\sigma_{\text{abs}} (\gamma+^{238}\text{U}) \rightarrow \gamma, \text{f}$



**In our approach
at**

BRuyères-le-Châtel (BRC) :

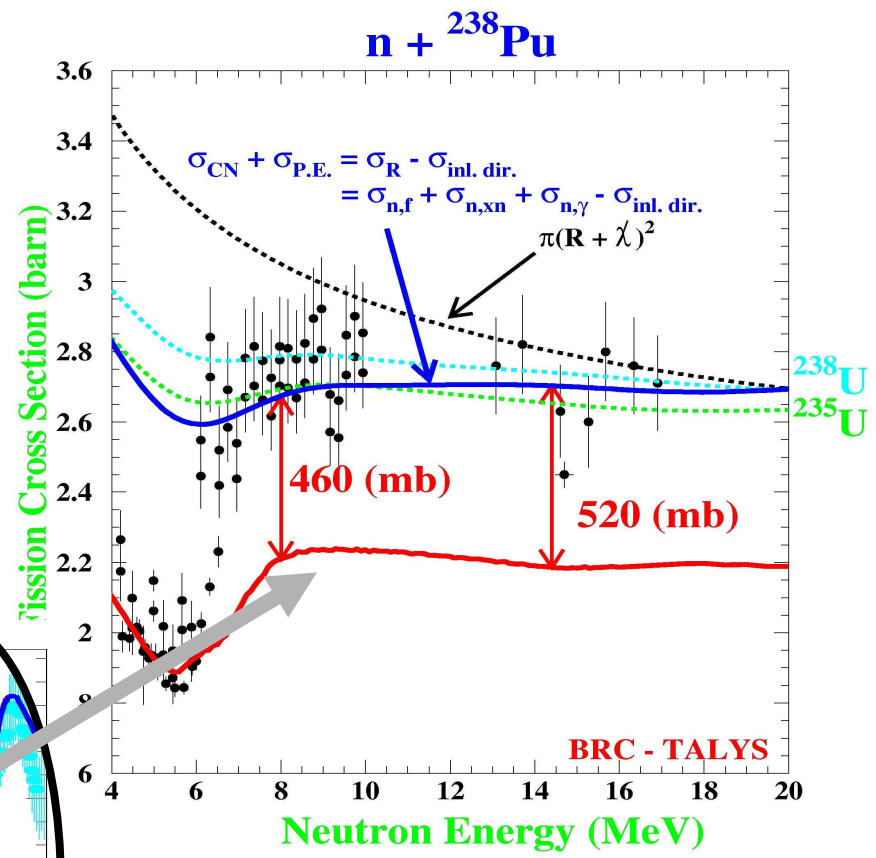
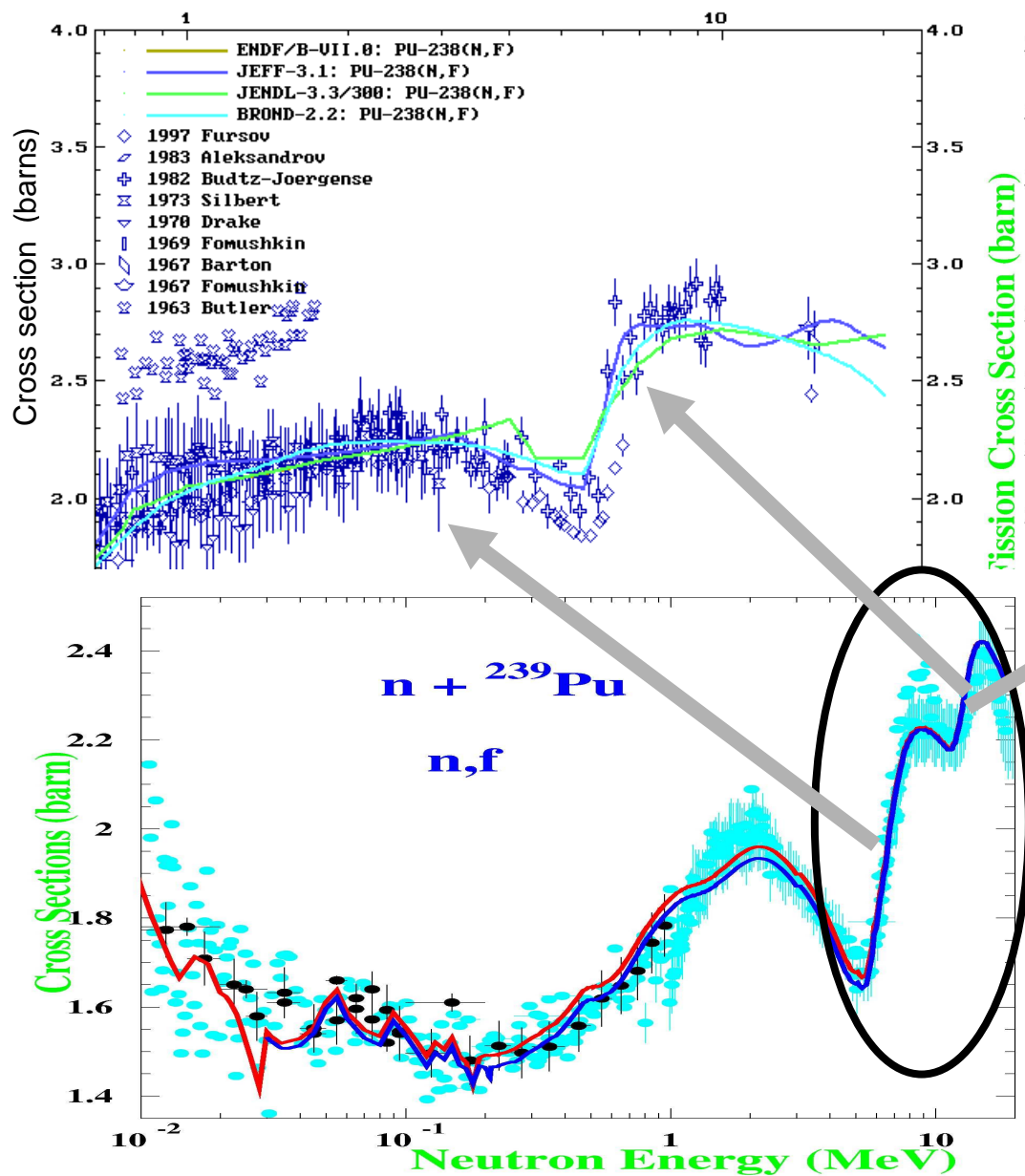
FULL MODEL

approach

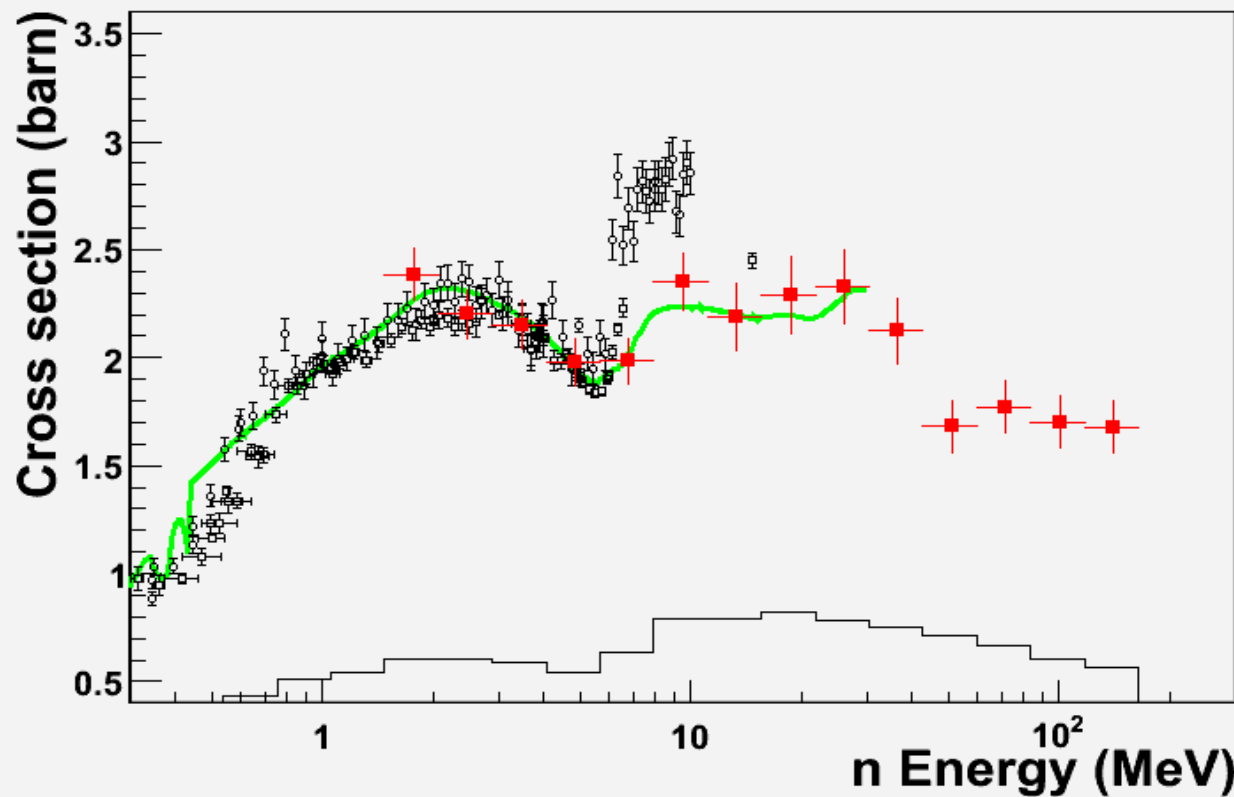
=

consistency

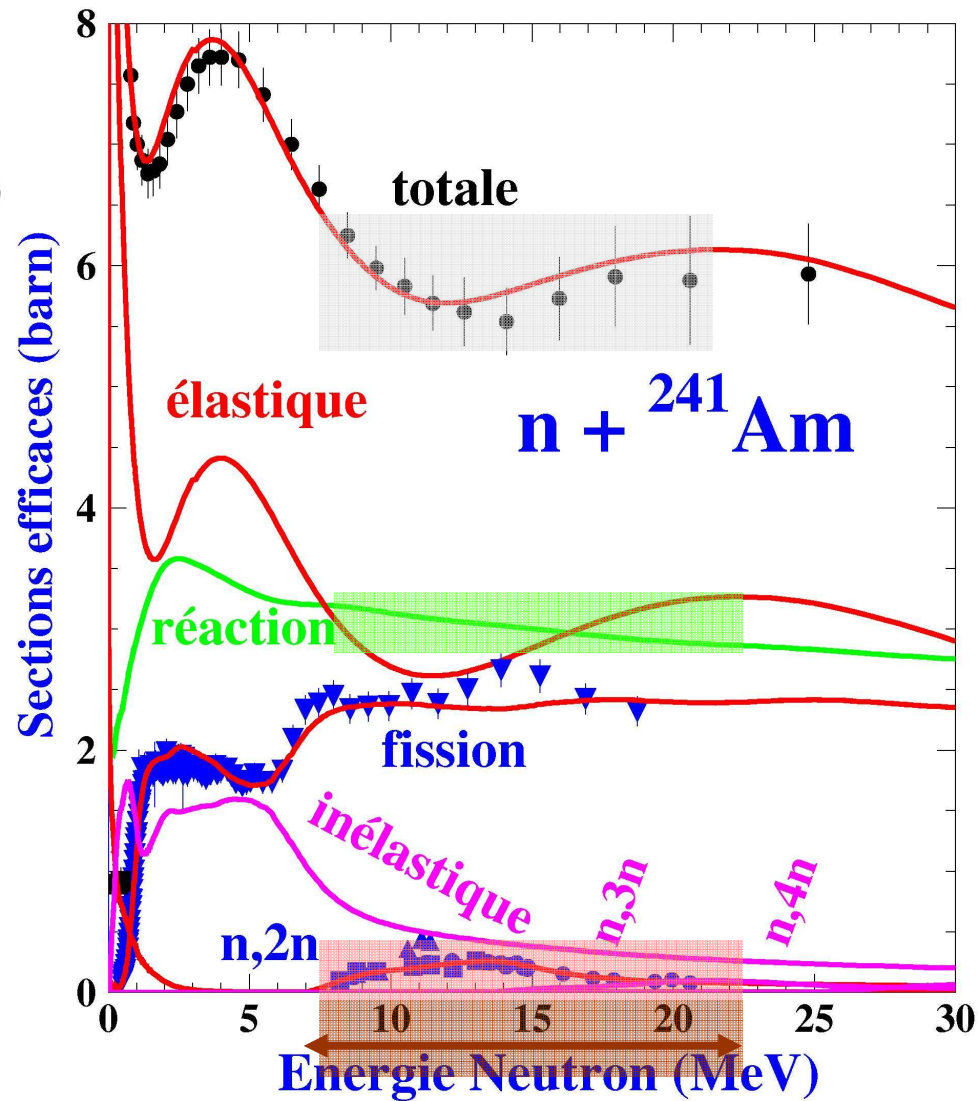
Problem in $^{238}\text{Pu}(n,f)$



From T. Granier et al.

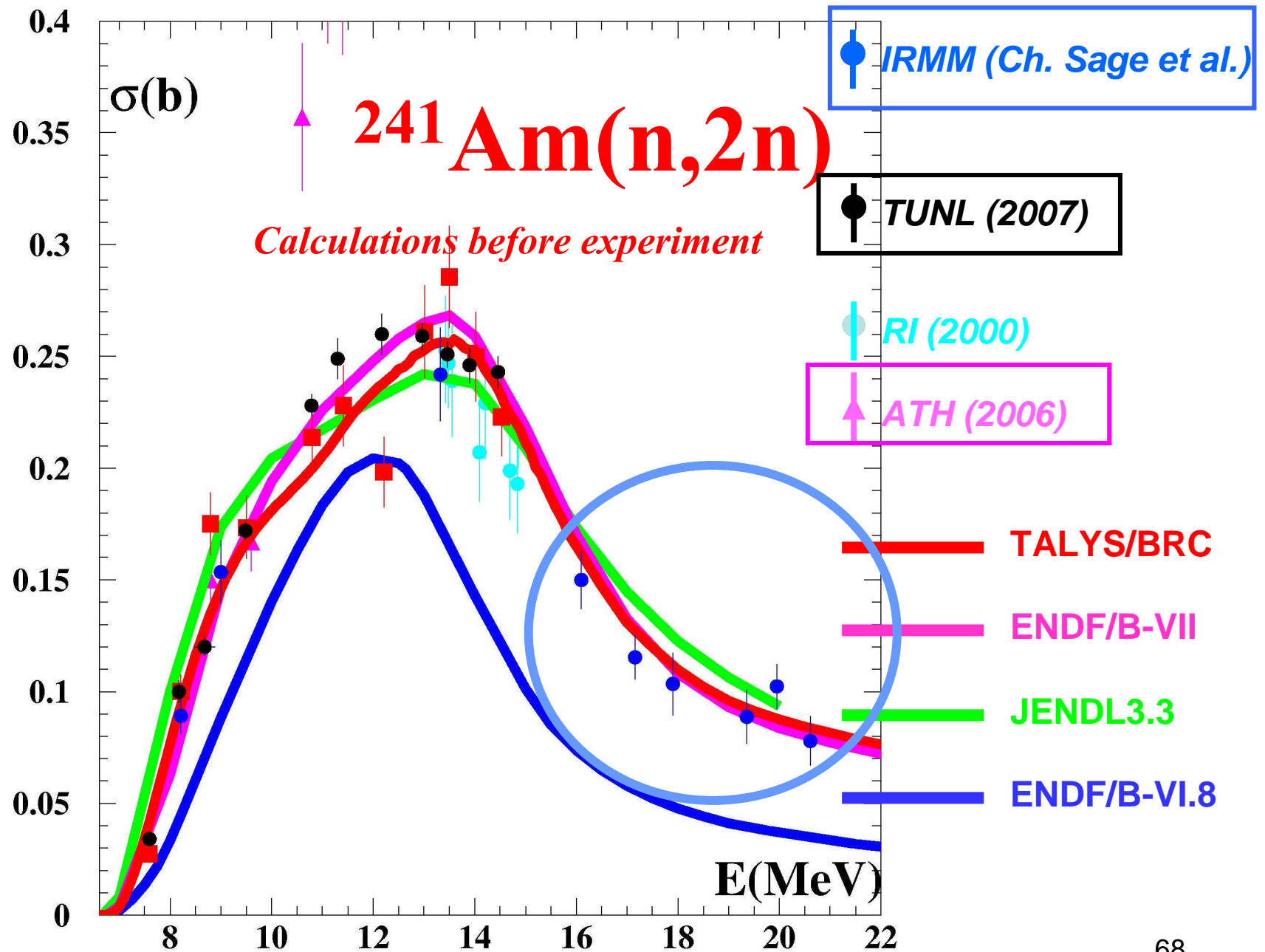


From T. Granier *et al.*



$\approx 4.5\%$ de σ_{tot}

$\approx 8.5\%$ de σ_{R}





TALYS
adventures
in
wonderland



The End

THANKS