DE LA RECHERCHE À L'INDUSTRIE

The basics of modeling (n,xn) cross-sections for actinides.

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(with the help of S. Hilaire & P. Romain)

ESNT workshop

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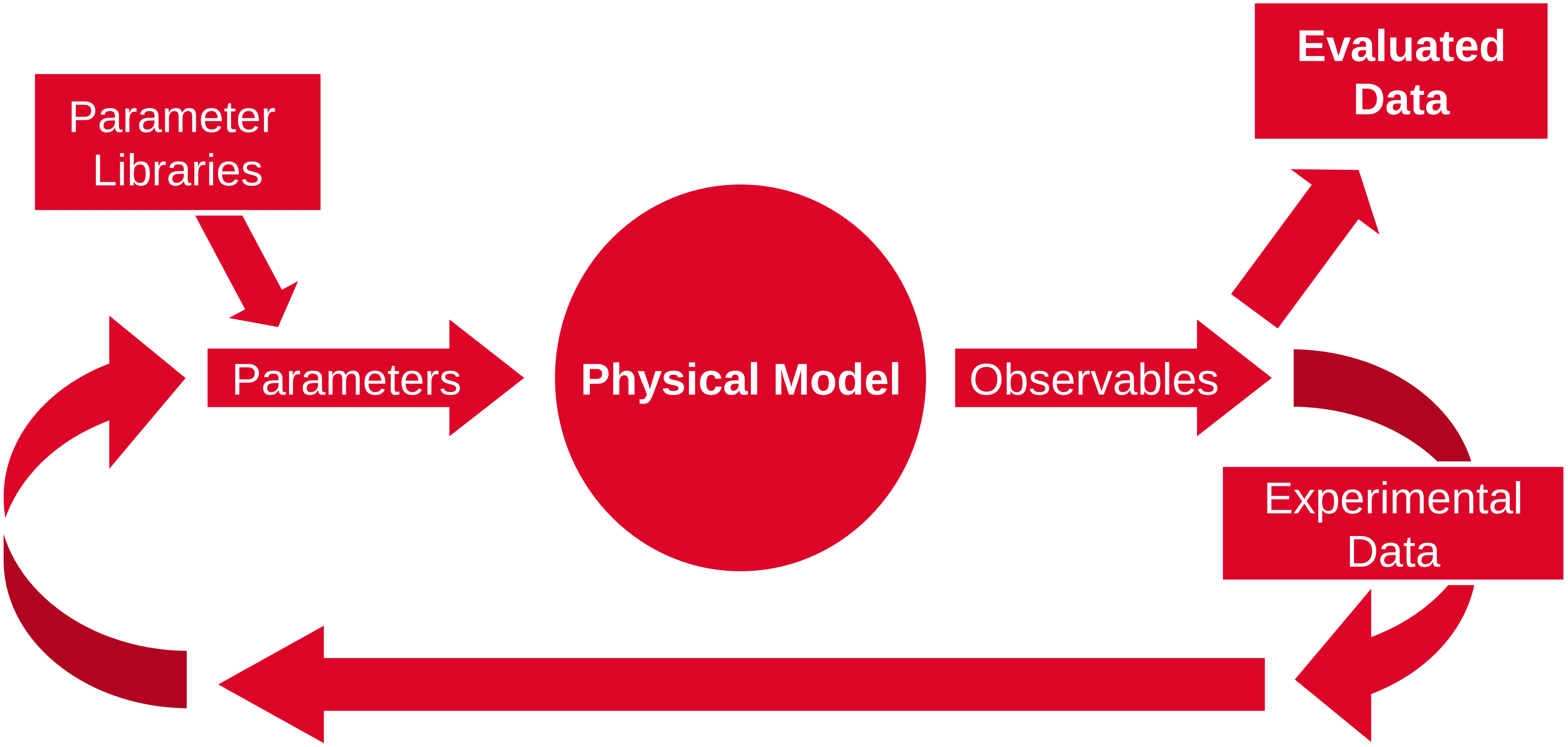
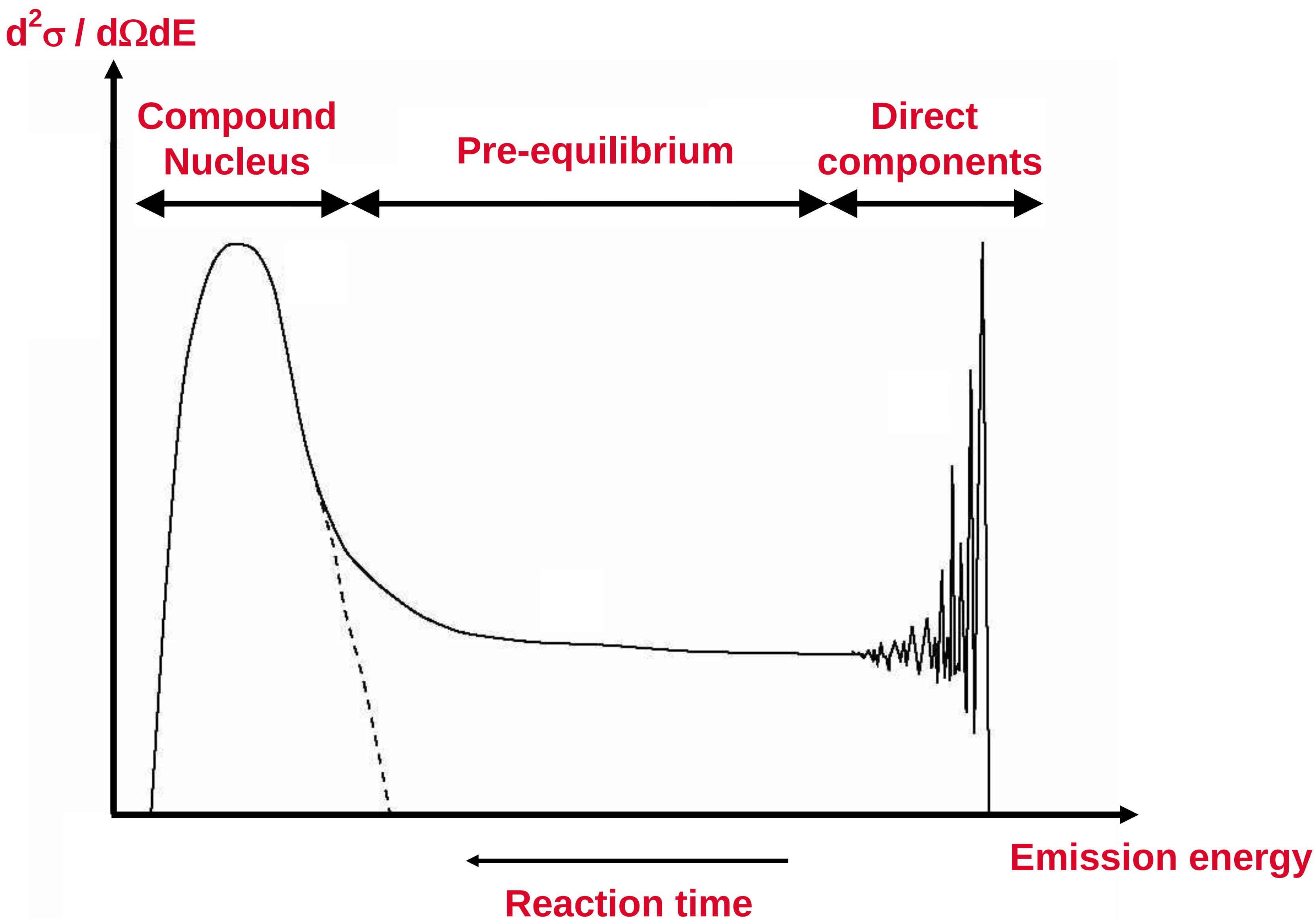
www.cea.fr

Nuclear Reaction Modeling

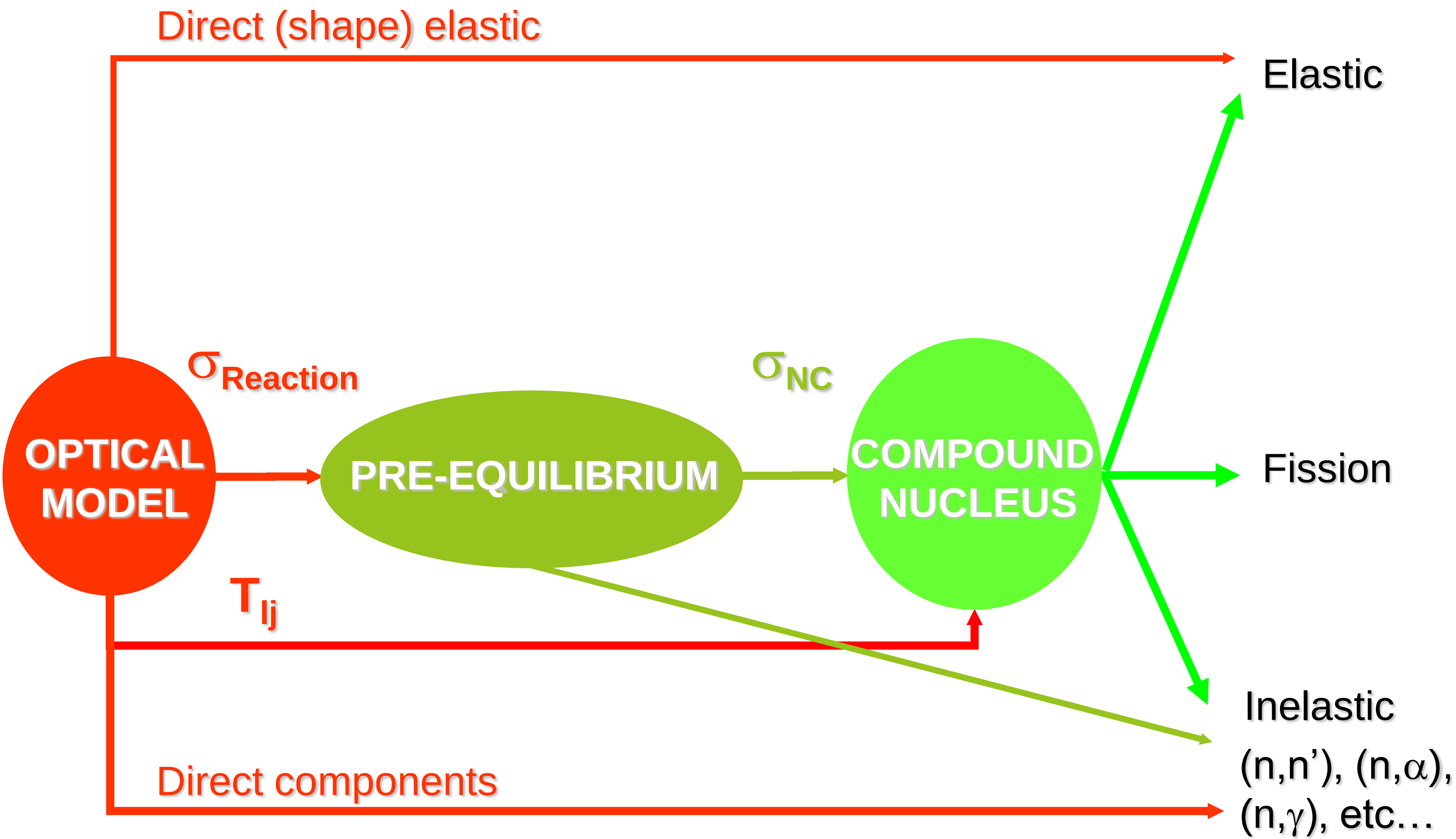
Method which consists of using a physical model (together with sets of parameters) to calculate evaluated data.



Models hierarchy



Models sequence



Optical Model

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

Quantum model → Schrödinger equation

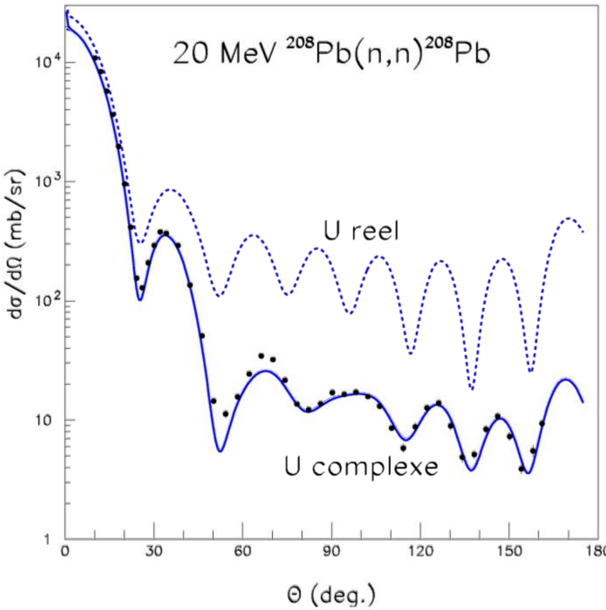
$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + U - E\right)\Psi = 0$$

Complex potential:

$$U = V + iW$$

Refraction (V)

Absorption (iW)



Optical model

$$\sigma_{el} = \sum_{\ell=0}^{\infty} \hat{\ell} \left| S_\ell - 1 \right|^2$$

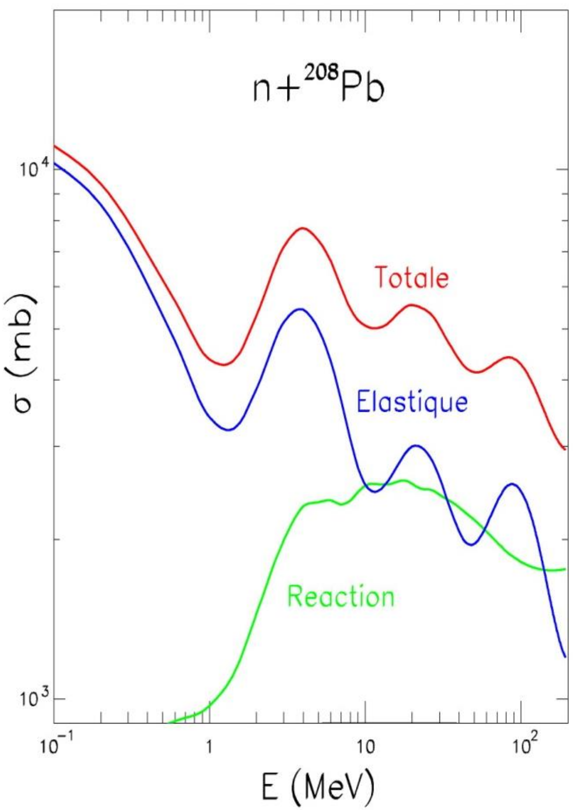
$$\sigma_{abs} = \frac{\pi}{k^2} \sum_{\ell=0}^{\infty} \hat{\ell} \left(1 - \left| S_\ell \right|^2 \right)$$

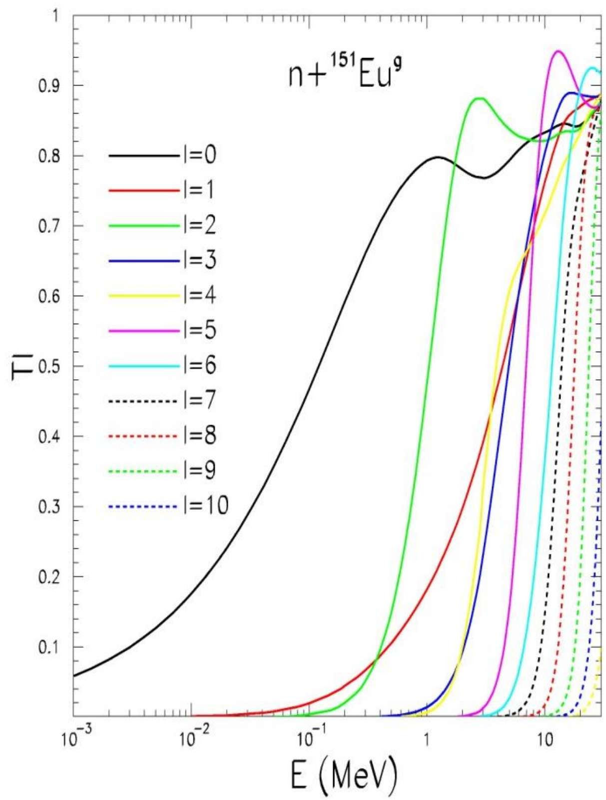
This model yields :

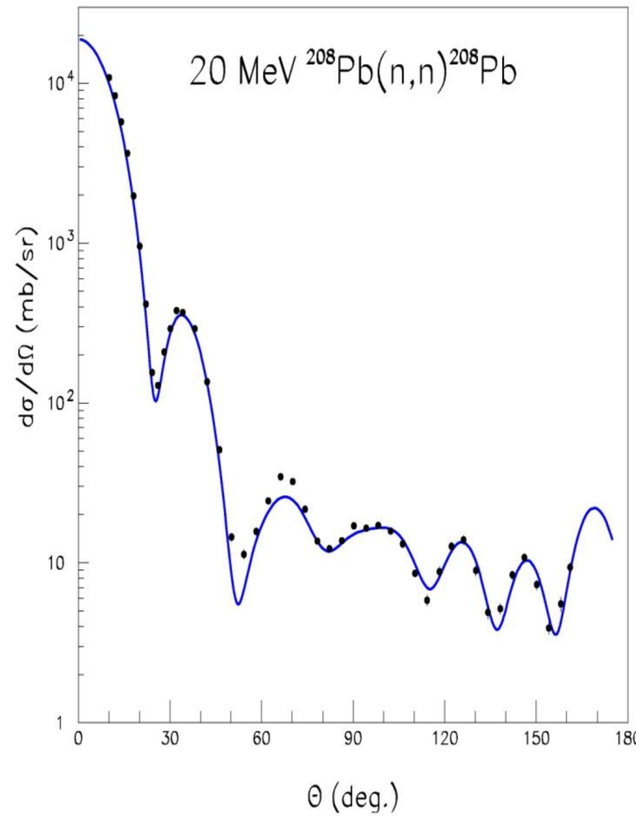
Integrated cross sections

Transmission coefficients (-> spin dist. of C.N.)

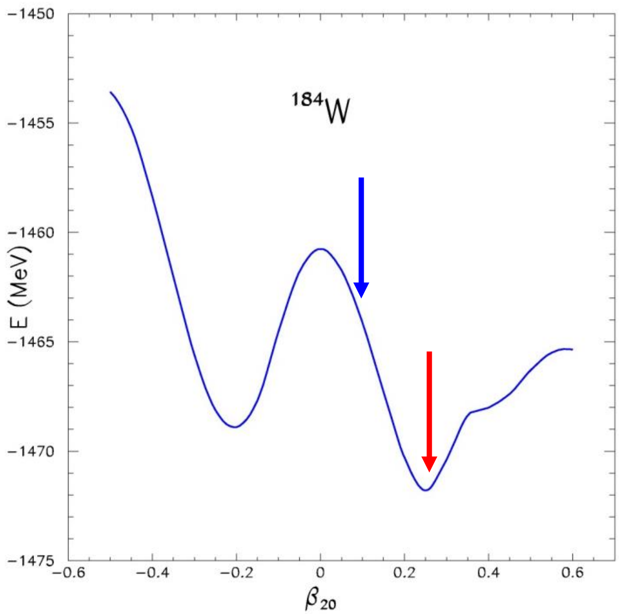
Angular distributions

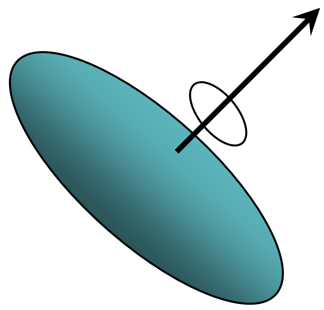


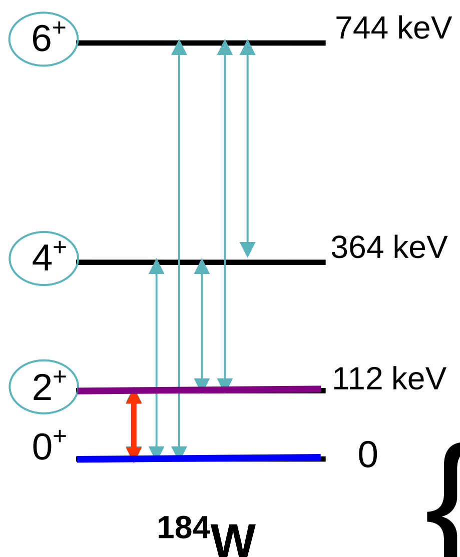




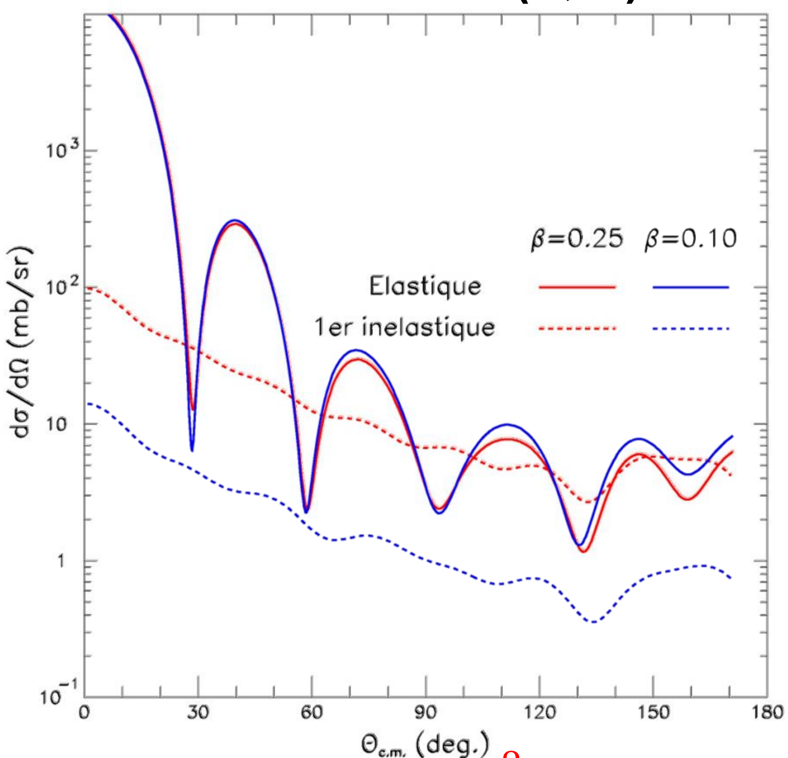
Impact of coupled channels







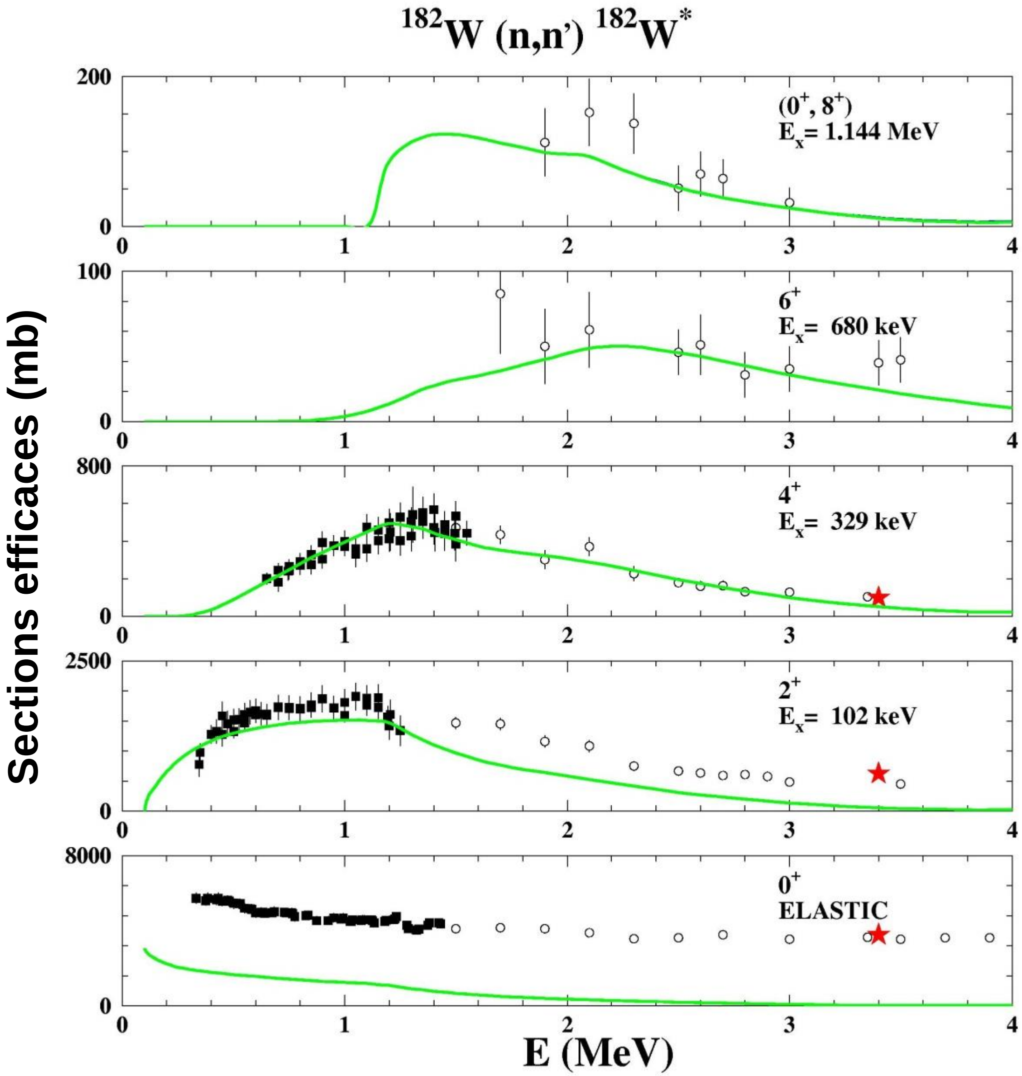
14 MeV ^{184}W(n,n')



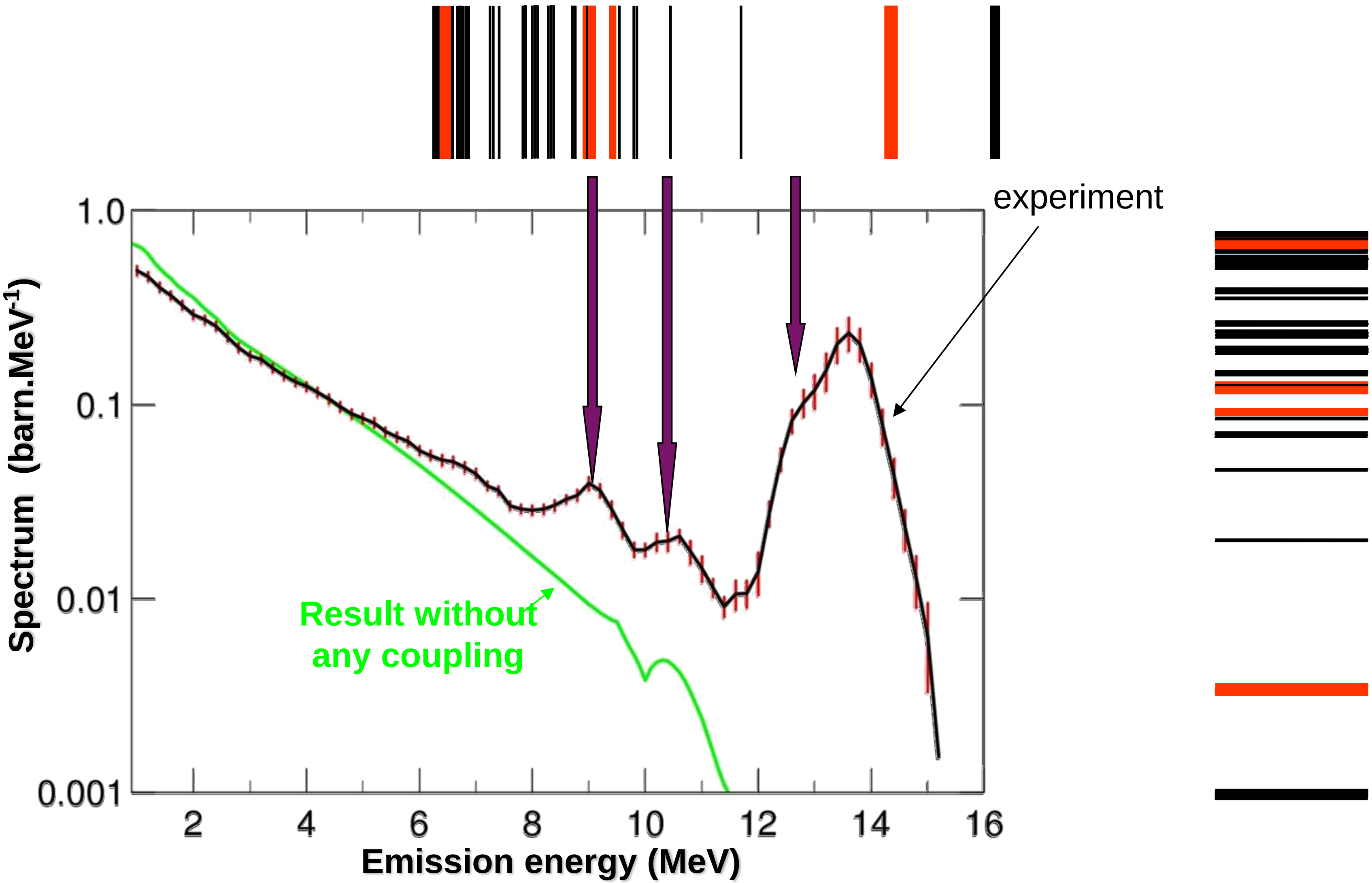
$$\begin{cases} (T+V_{00}-E)\,\Psi_0 = V_{02}\,\Psi_2 \\ (T+V_{22}-E)\,\Psi_2 = V_{20}\,\Psi_0 \end{cases}$$

β

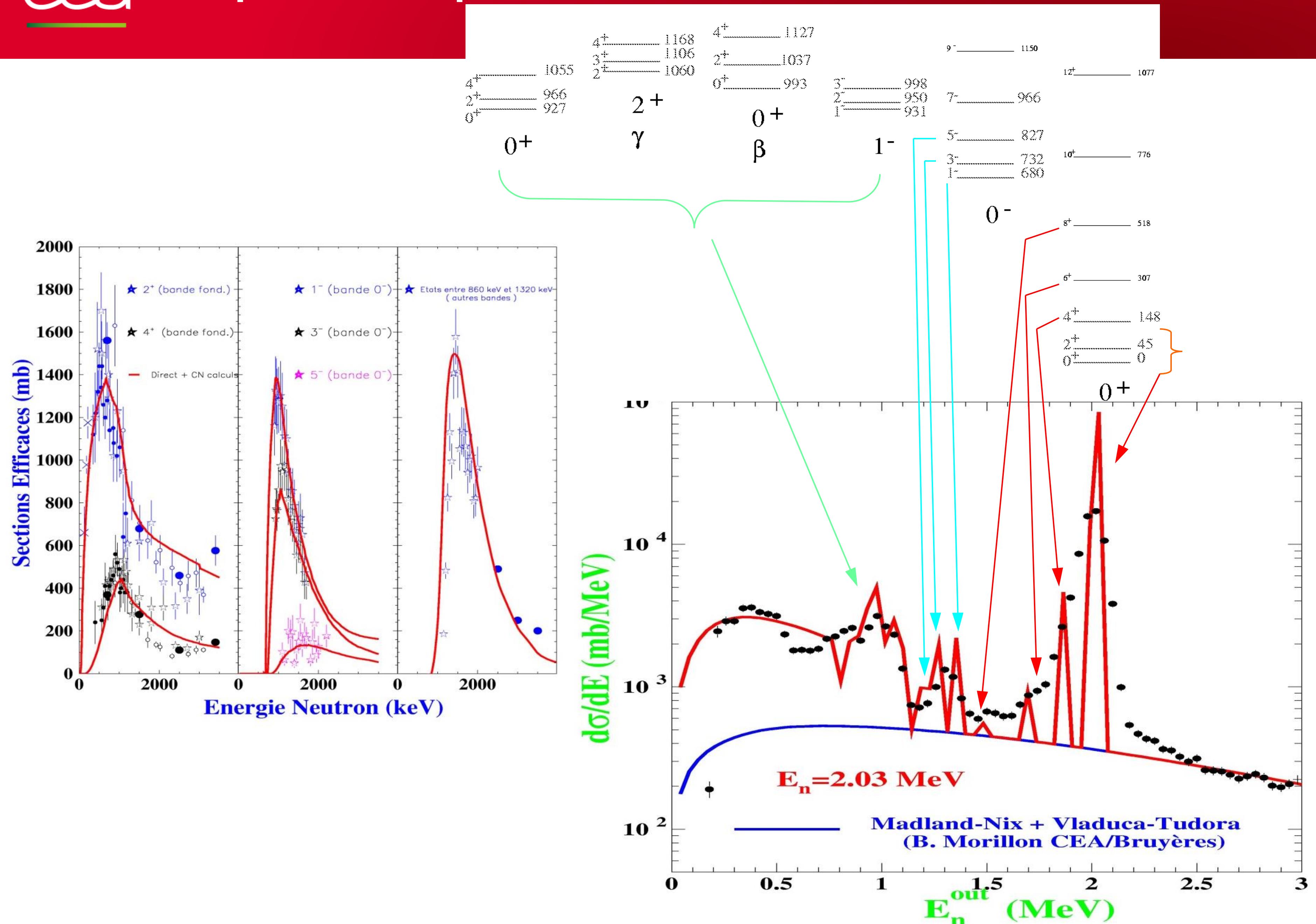
Impact of coupled channels
Direct/compound interplay



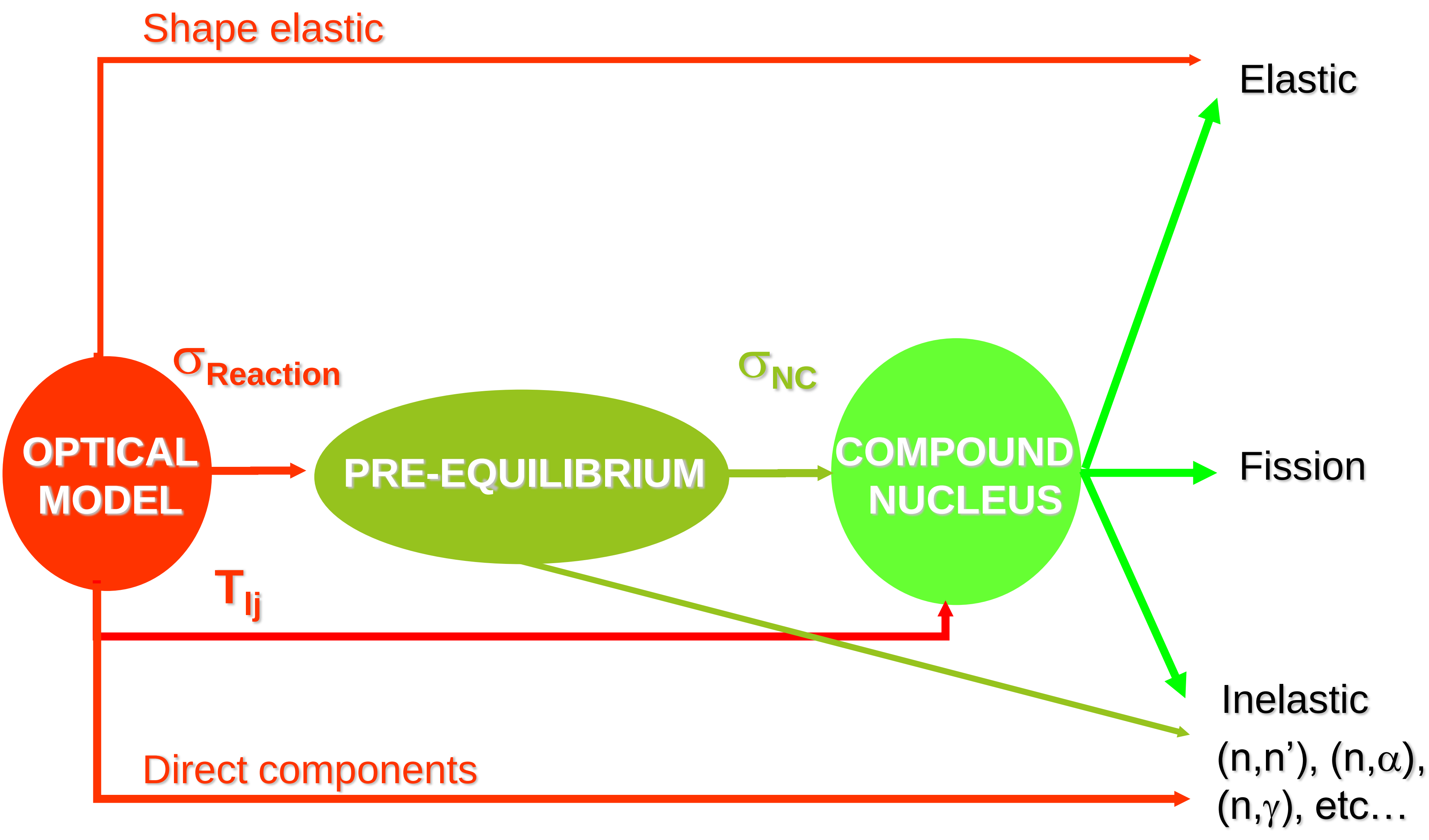
Impact of coupled channels



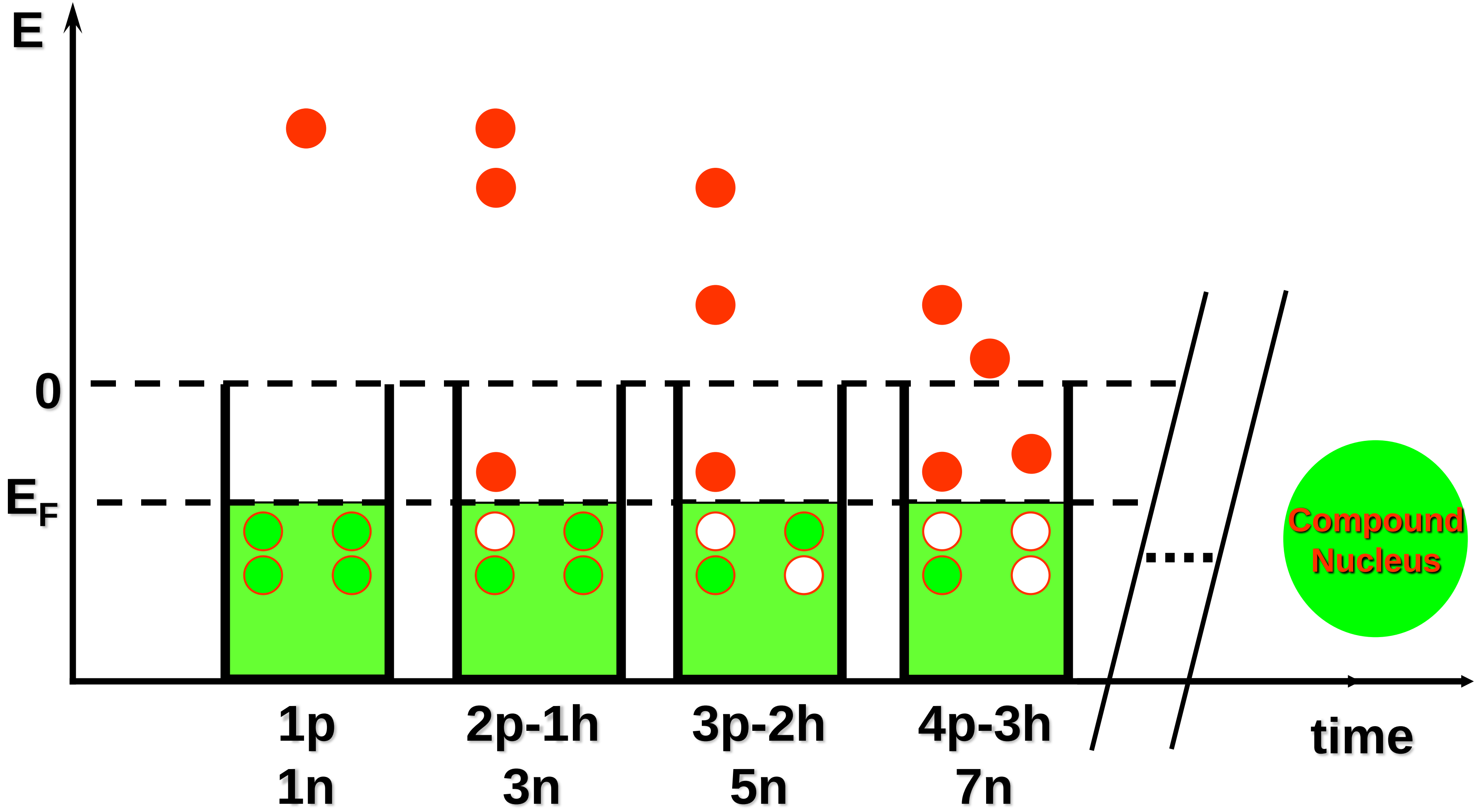
Impact of coupled channel



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 exciton number n.

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

Evolution equation

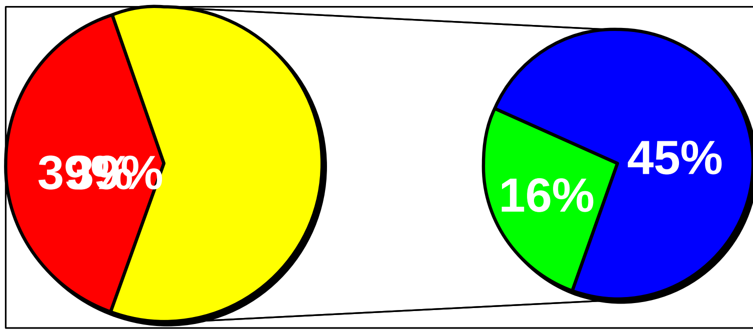
$$\frac{dP(n,E,t)}{dt} = P(n-2,E,t)\,\lambda_{n-2,n}(E) + P(n+2,E,t)\,\lambda_{n+2,n}(E) - P(n,E,t)\left[\lambda_{n,n+2}(E) + \lambda_{n,n-2}(E) + \lambda_{n,emiss}(E)\right]$$

Emission cross section in channel c

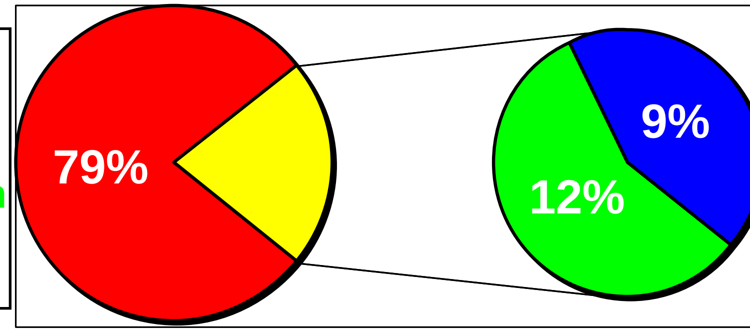
$$\sigma_c(E,\varepsilon_c)\,d\varepsilon_c = \sigma_R \int_0^{t_{eq}} \sum_{n,\Delta n=2} P(n,E,t)\,\lambda_{n,c}(E)\,dt\;\;d\varepsilon_c$$

Pre-equilibrium model

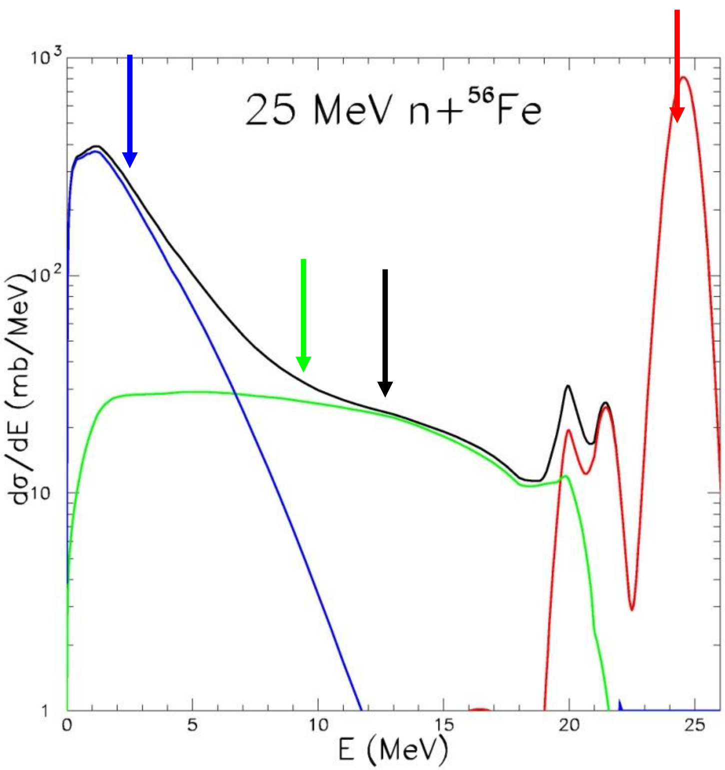
Cross section



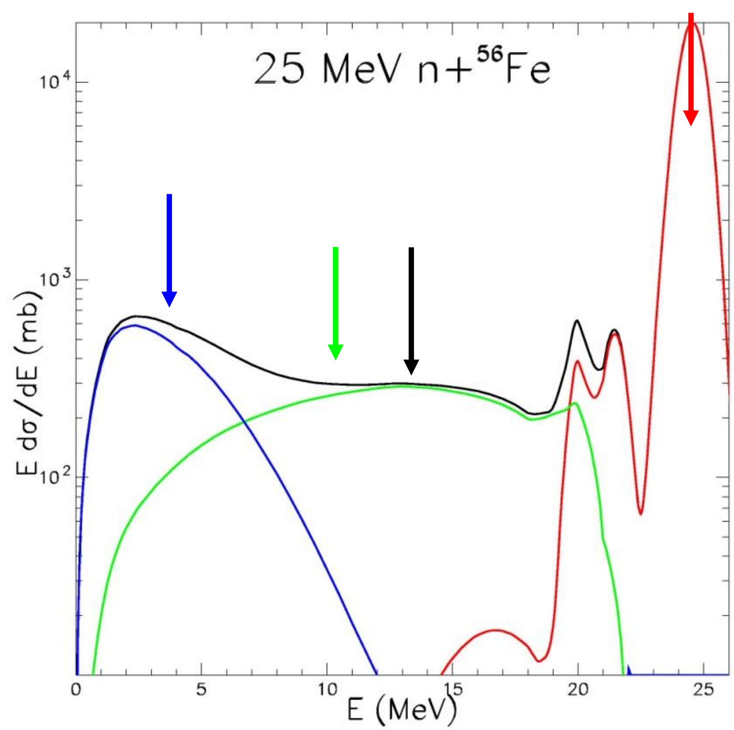
Outgoing energy



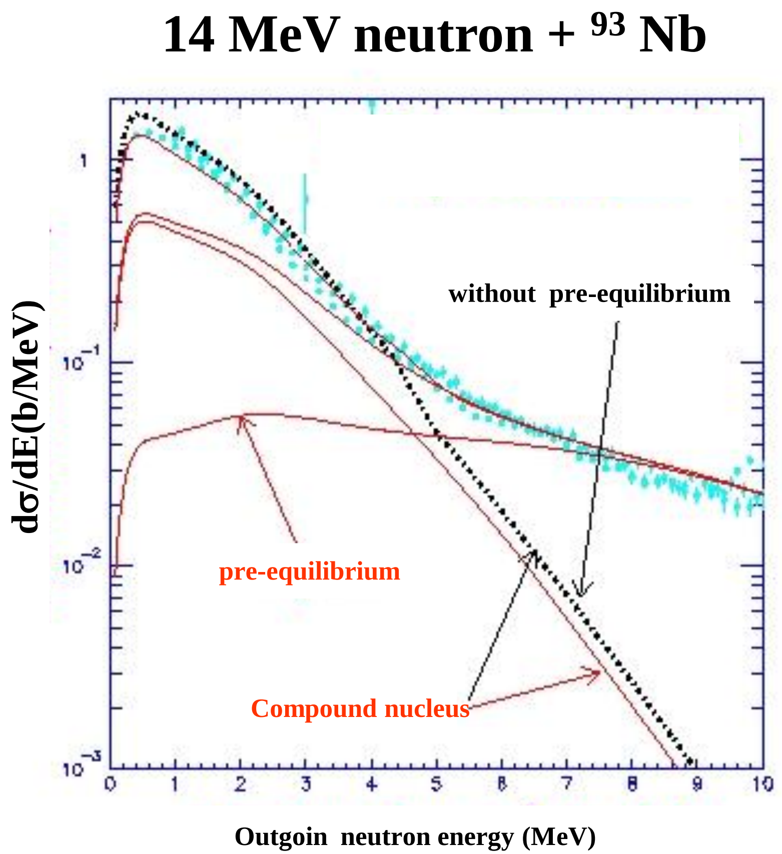
Total
Direct
Pre-equilibrium
Statistical

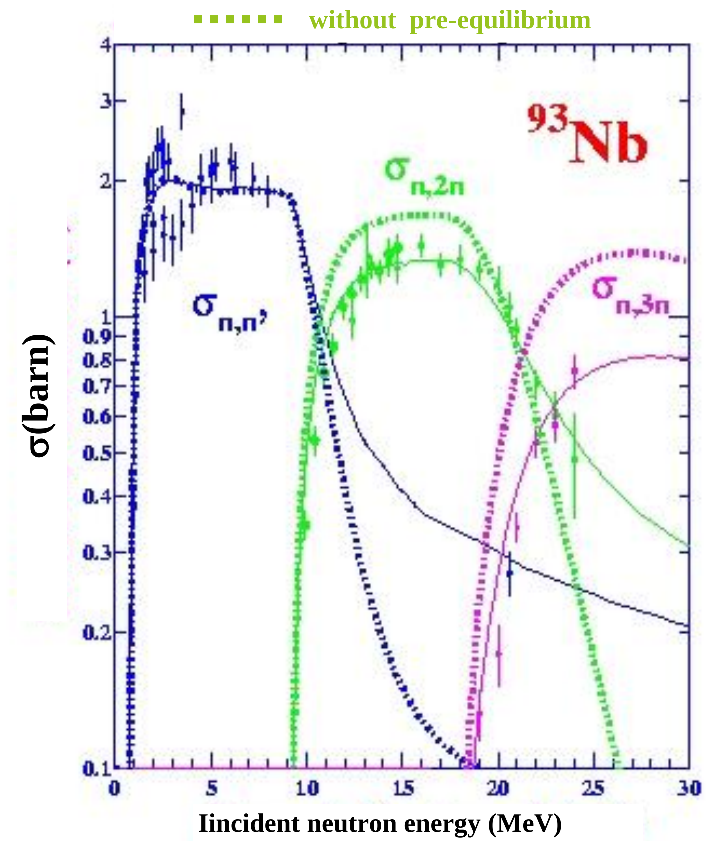


$<E_{Tot}>$= 12.1
$<E_{Dir}>$= 24.3
$<E_{PE}>$= 9.32
$<E_{Sta}>$= 2.5
(MeV)

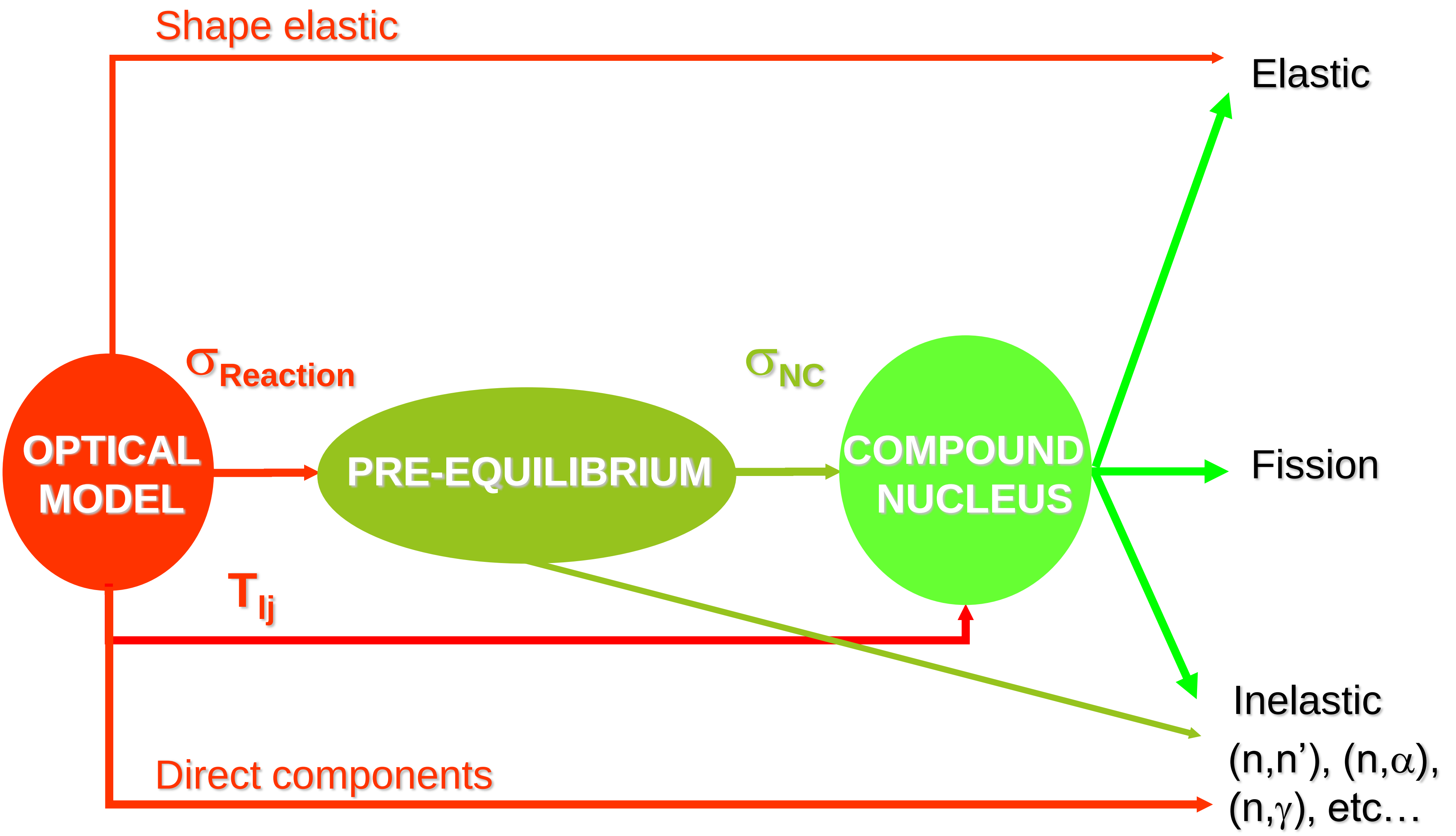


Pre-equilibrium model (with and without)





Models sequence

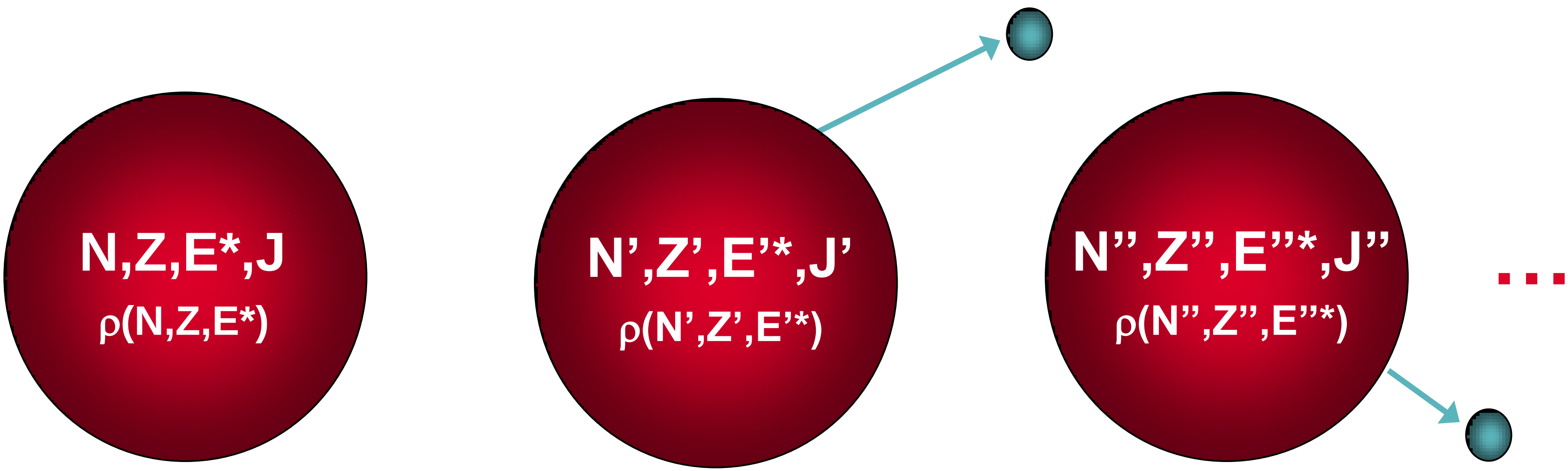


Compound nucleus model

After direct and pre-equilibrium emission

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

N_0	$N_0 - dN_D$	$N_0 - dN_D - dN_{PE}$	$= N$
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 hypothesis

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

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

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

⇒ Hauser- Feshbach formula

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

Compound nucleus model

In realistic calculations, all possible quantum number combinations must be considered

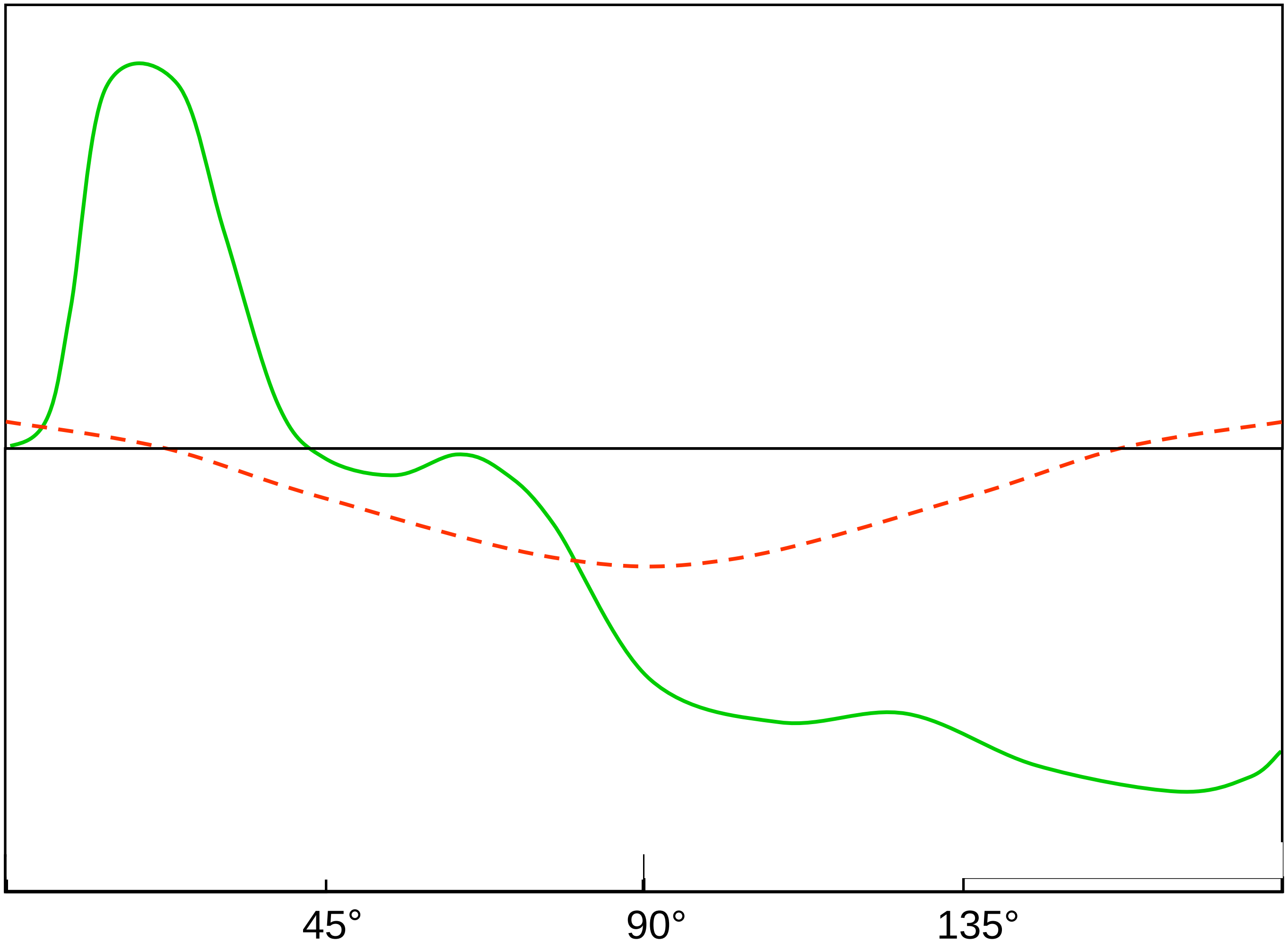
$$\sigma_{ab} = \frac{\pi}{k_a^2} \sum_{J=|I_A - s_a|}^{I_A + s_a + l_a^{max}} \sum_{\pi = \pm} \frac{(2J+1)}{(2I_A+1)(2s_a+1)}$$

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

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

Angular distributions

Compound angular distribution & direct angular distributions



Can be used to disentangle direct and compound components for (n,n) and (n,n')

Channel width fluctuations

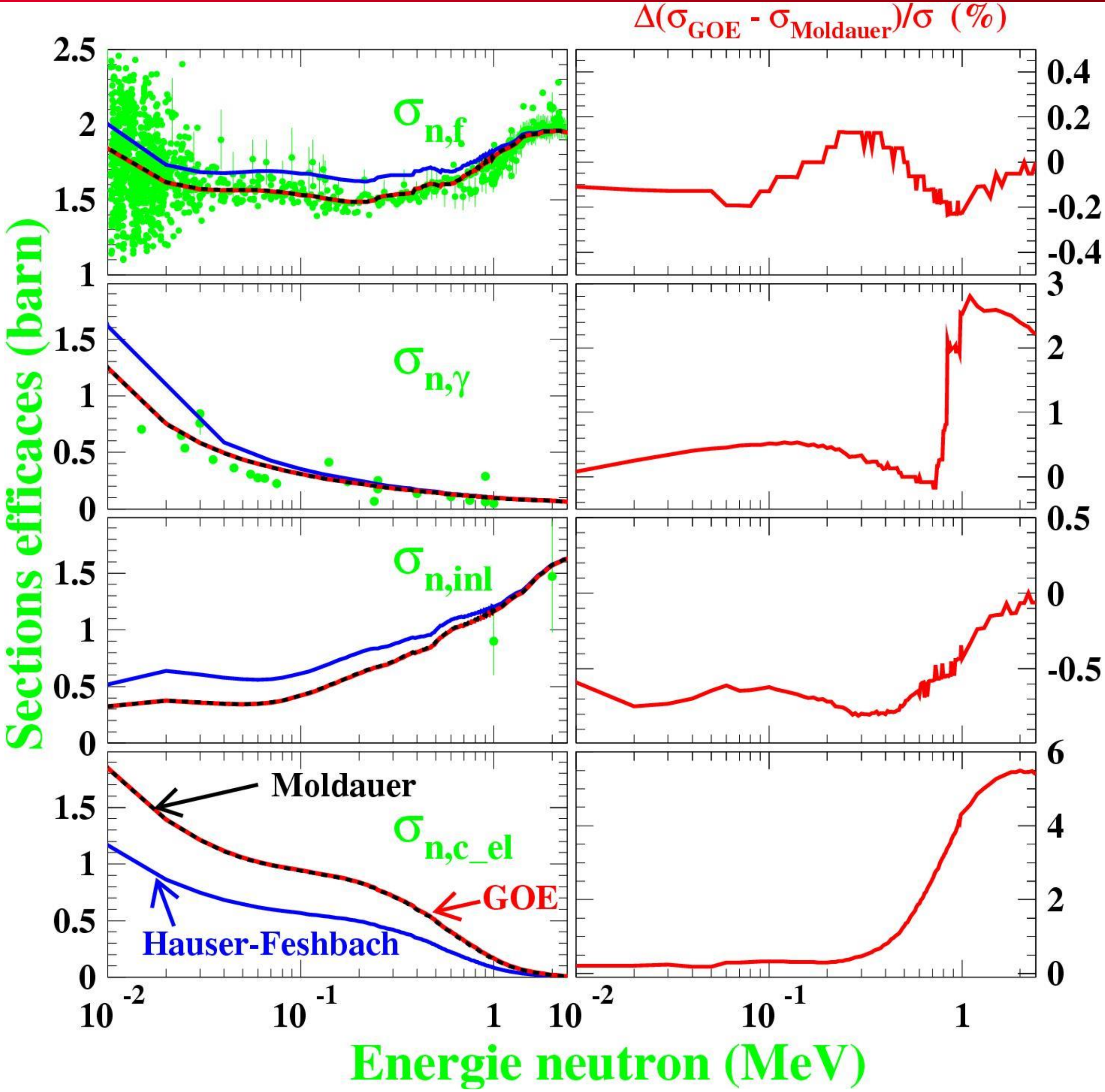
Breit-Wigner resonance integrated and averaged over an energy width corresponding to the incident beam dispersion

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

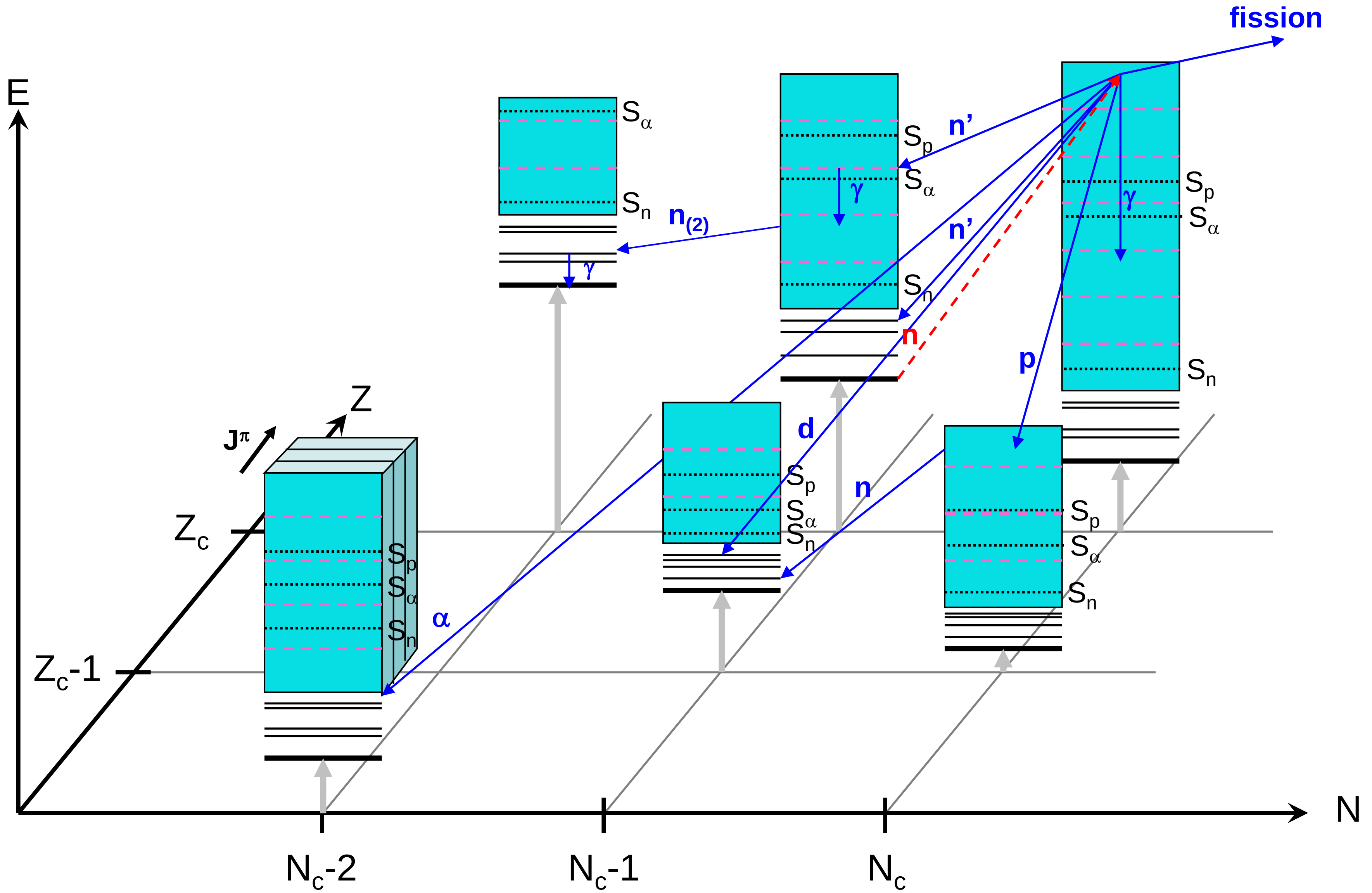
since $T_\alpha \approx \dfrac{2\pi \langle \Gamma_\alpha \rangle}{D}$

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

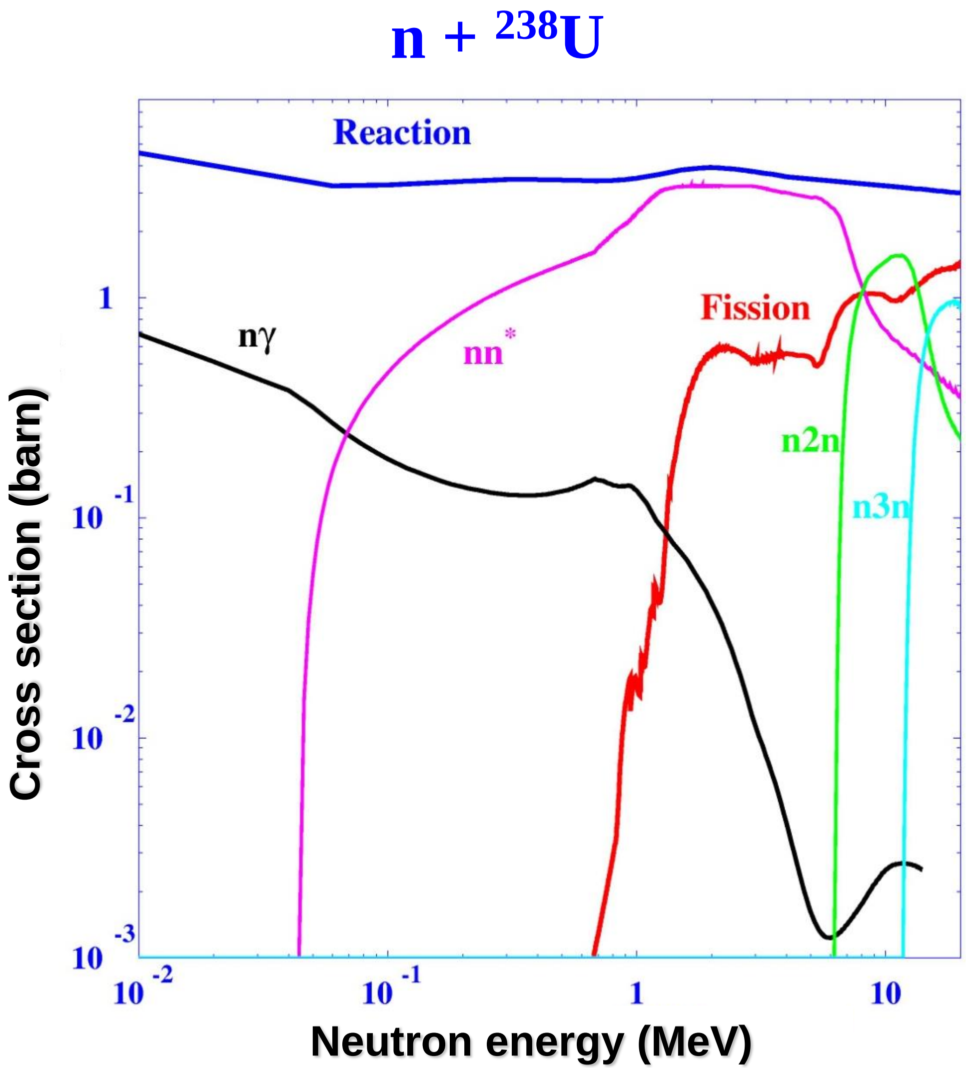
Effect of width fluctuations



Multiple emission processes



Compound nucleus model



Optical model

+

Statistical model

+

Pre-equilibrium model

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

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

Possible decay Channels

- Particle 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.

- Particle emission to a continuum « bin »

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

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

- Emission of photons, fission

Specific treatment

Gamma transmission coefficients

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

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

- 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 $J_f^{\pi f}$:

For $E\lambda$: $\pi_f=(-1)^{\lambda}\,\pi_i$

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

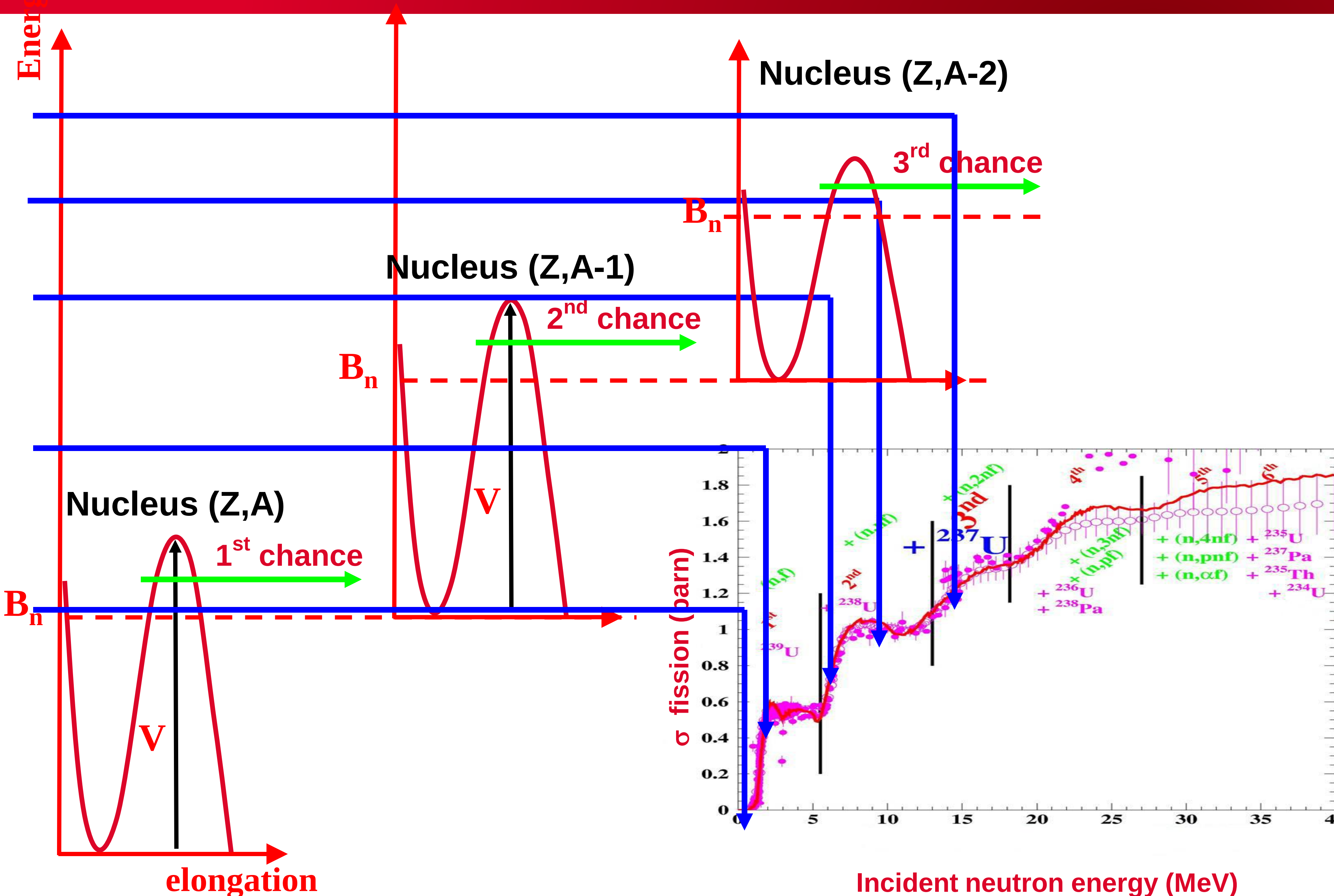
$$|J_i-\lambda| \leq J_f \leq J_i+\lambda$$

Renormalisation technique for thermal neutrons

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

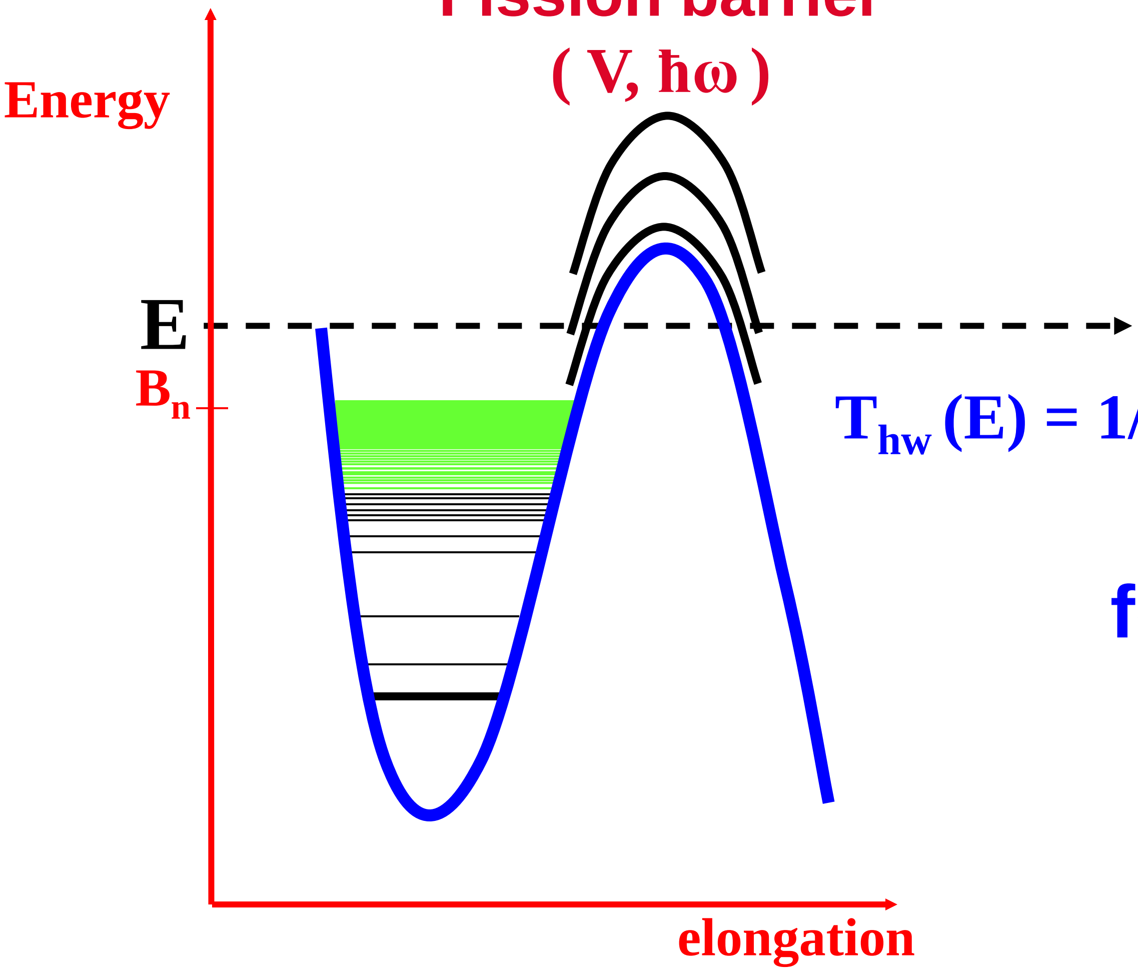
experiment

Multiple chance fission



Fission modeling

Fission barrier
(V, ħω)



Transmission

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

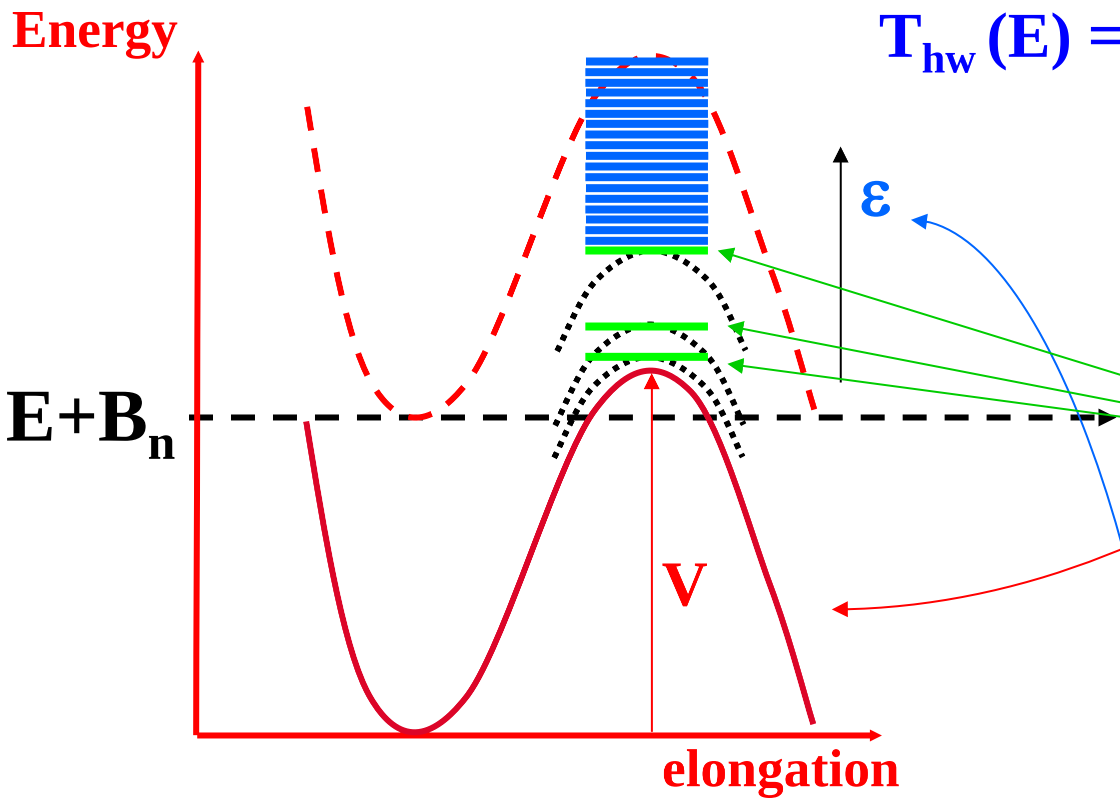
Hill-Wheeler

for one barrier !

+ transition state on top of the barrier !

Bohr hypothesis

Fission transmission coefficients



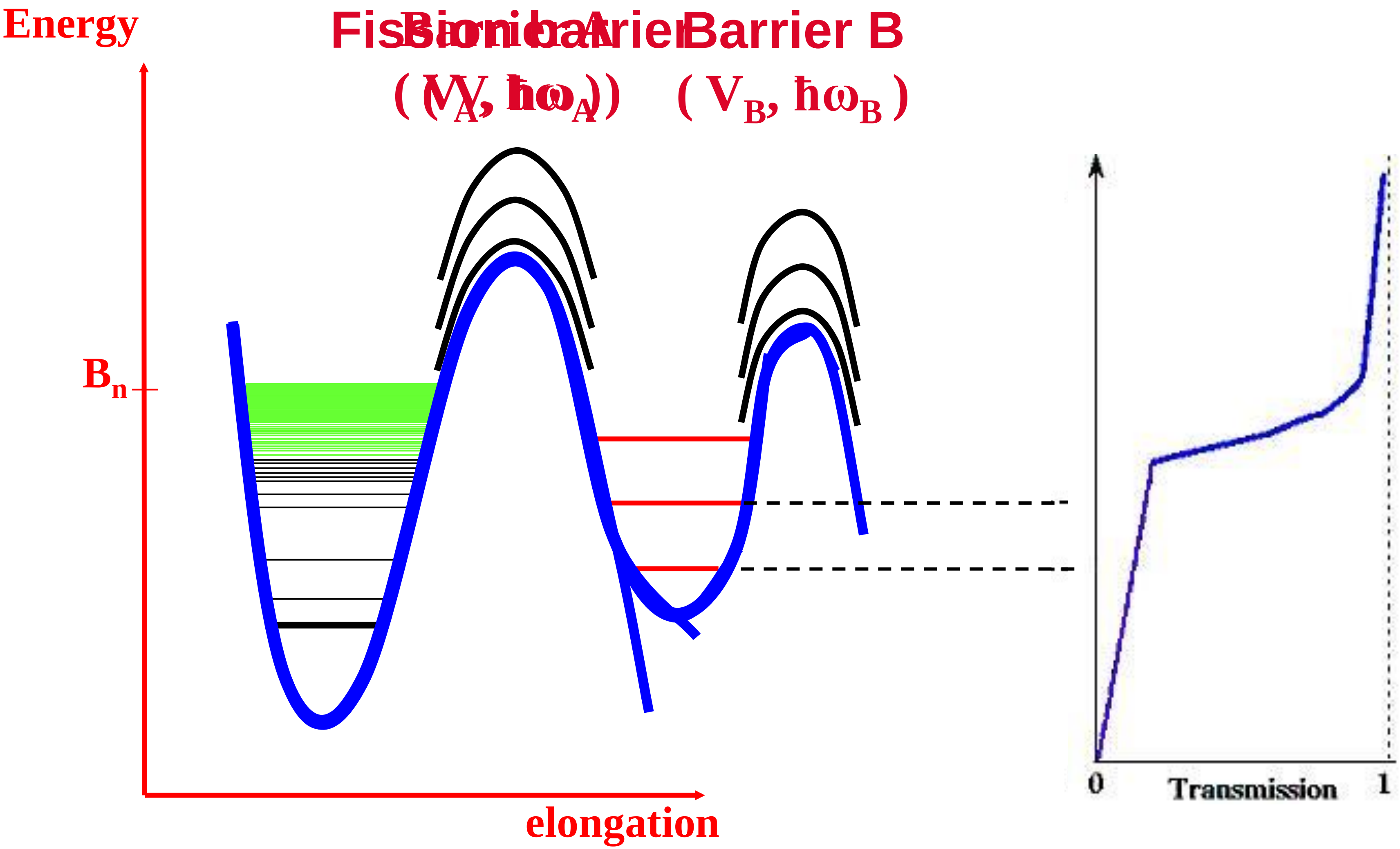
$$T_{hw}(E) = 1/[1 + \exp(2\pi(V - E)/\hbar\omega)]$$

Hill-Wheeler

Discrete transition states with energy ε_d

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

Double-humped barriers



+ transition states on top of each barrier !

+ class II states in the intermediate well !

Fission transmission coefficients

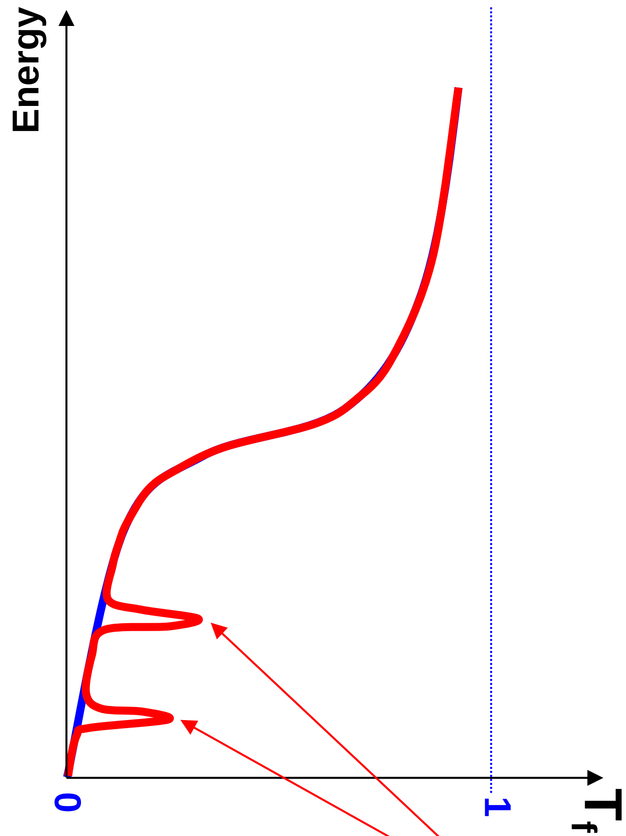
Two barriers A and B

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

Three barriers A, B et C

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

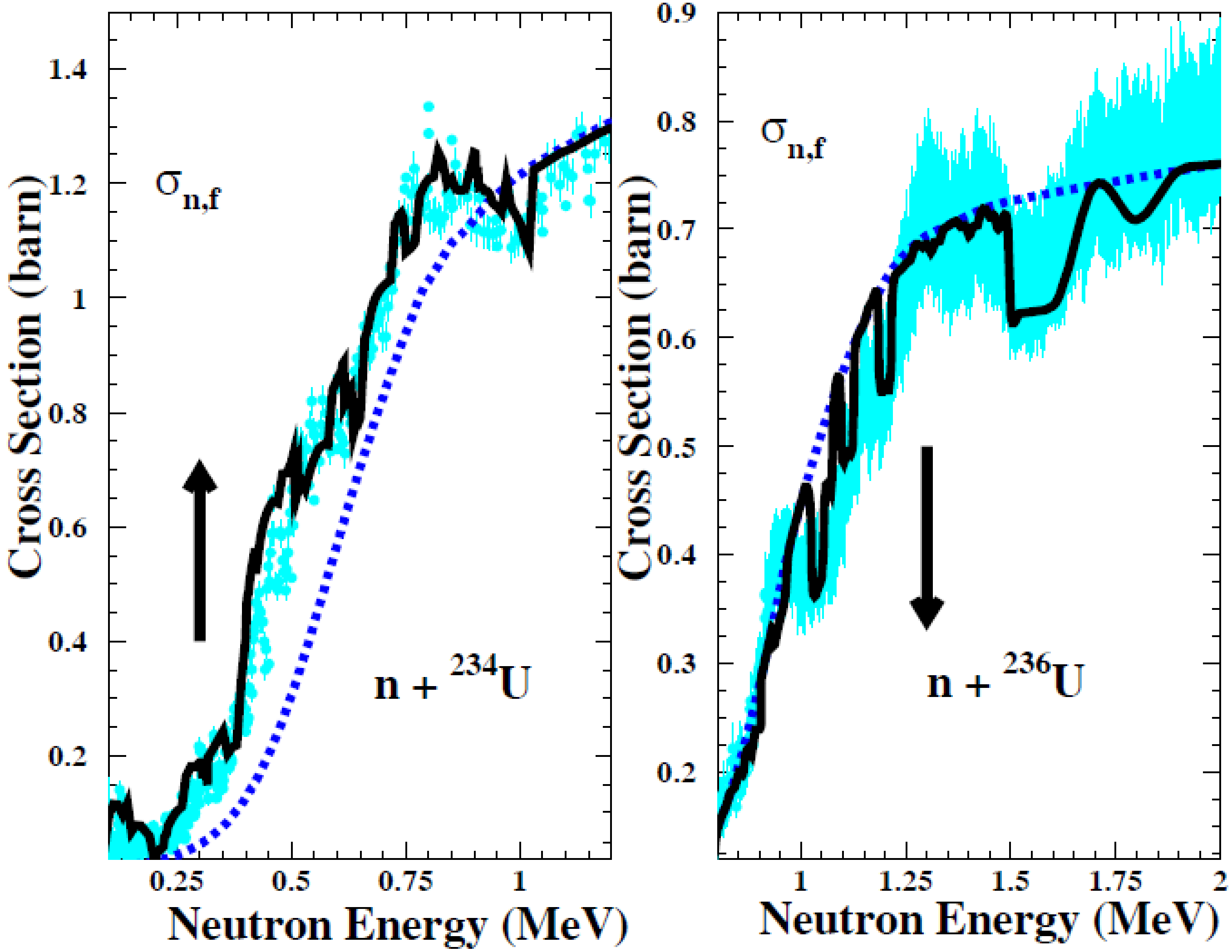
Resonant transmission



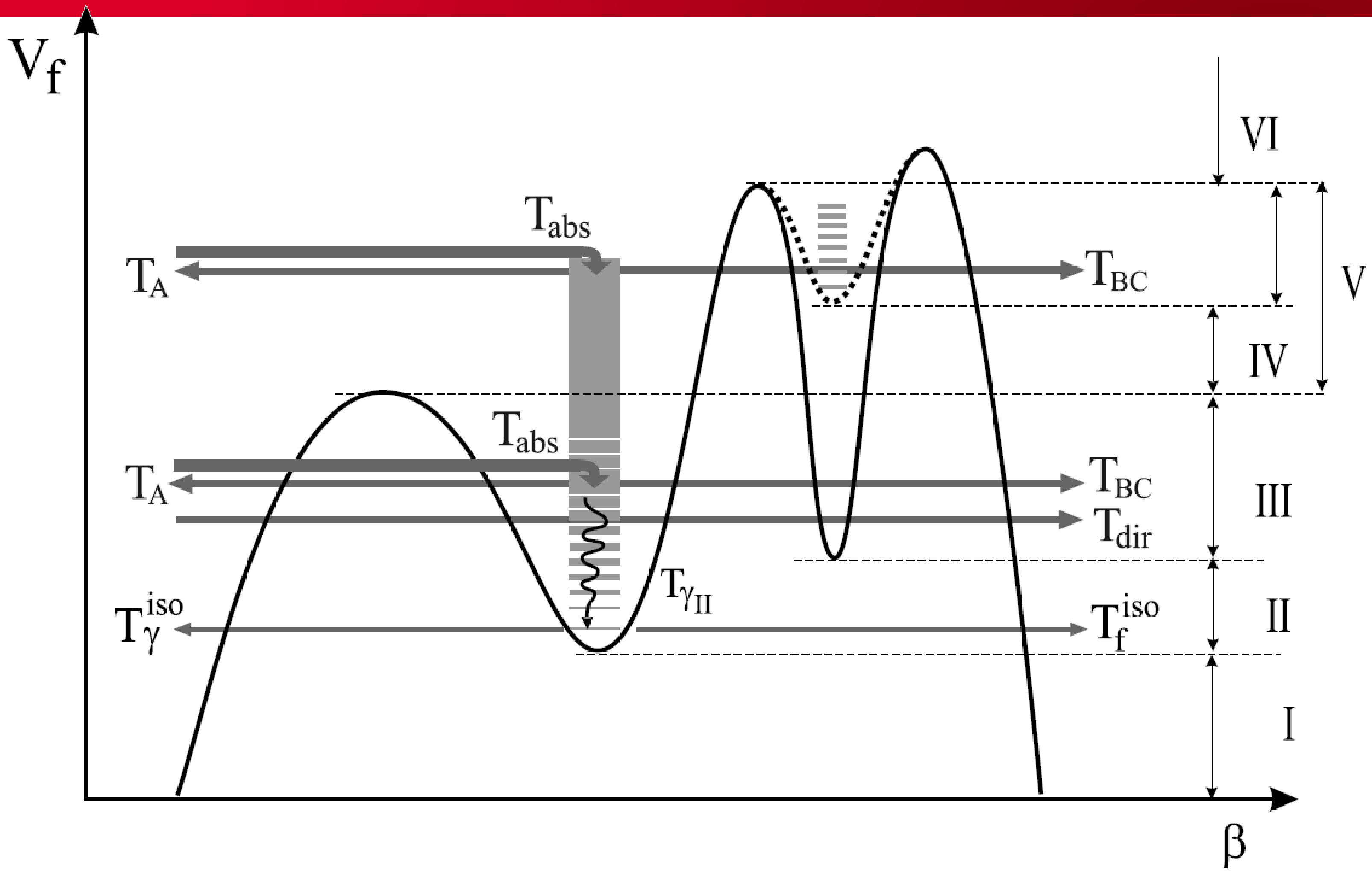
$$T_f = \frac{T_A\, T_B}{T_A + T_B} \qquad \frac{4}{T_A + T_B}$$

More exact expressions in Bauge et al., EPJA 48, 113 (2012)

Effect of class II-III states



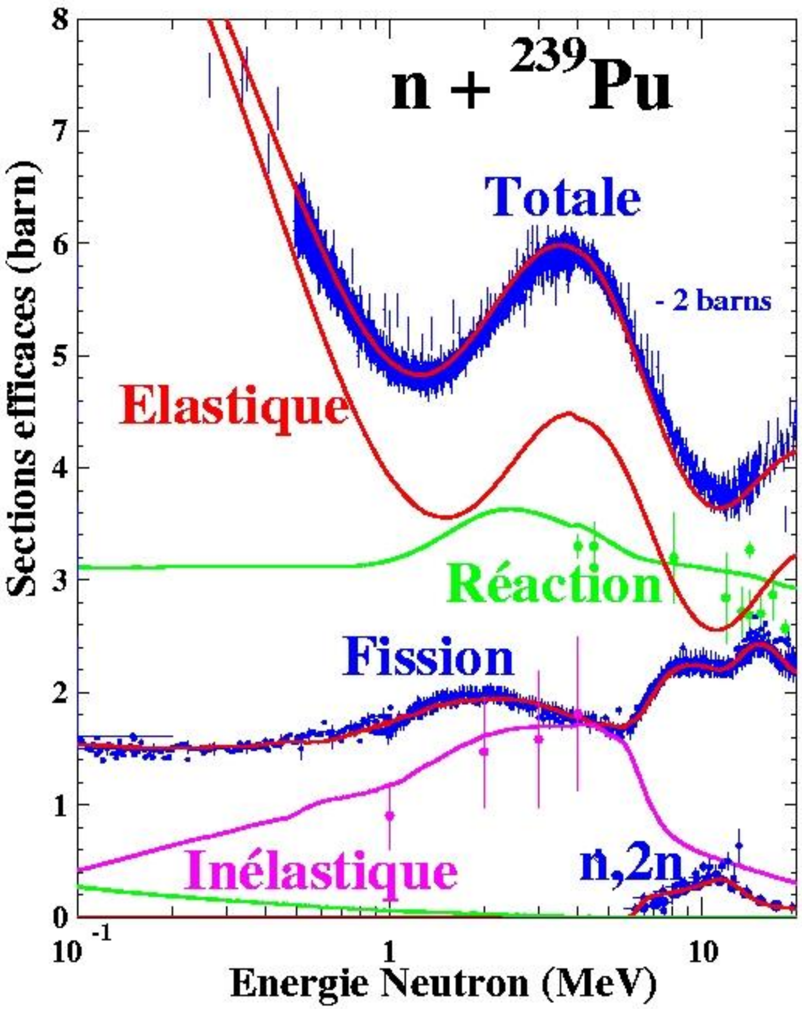
Fission transmission coefficients



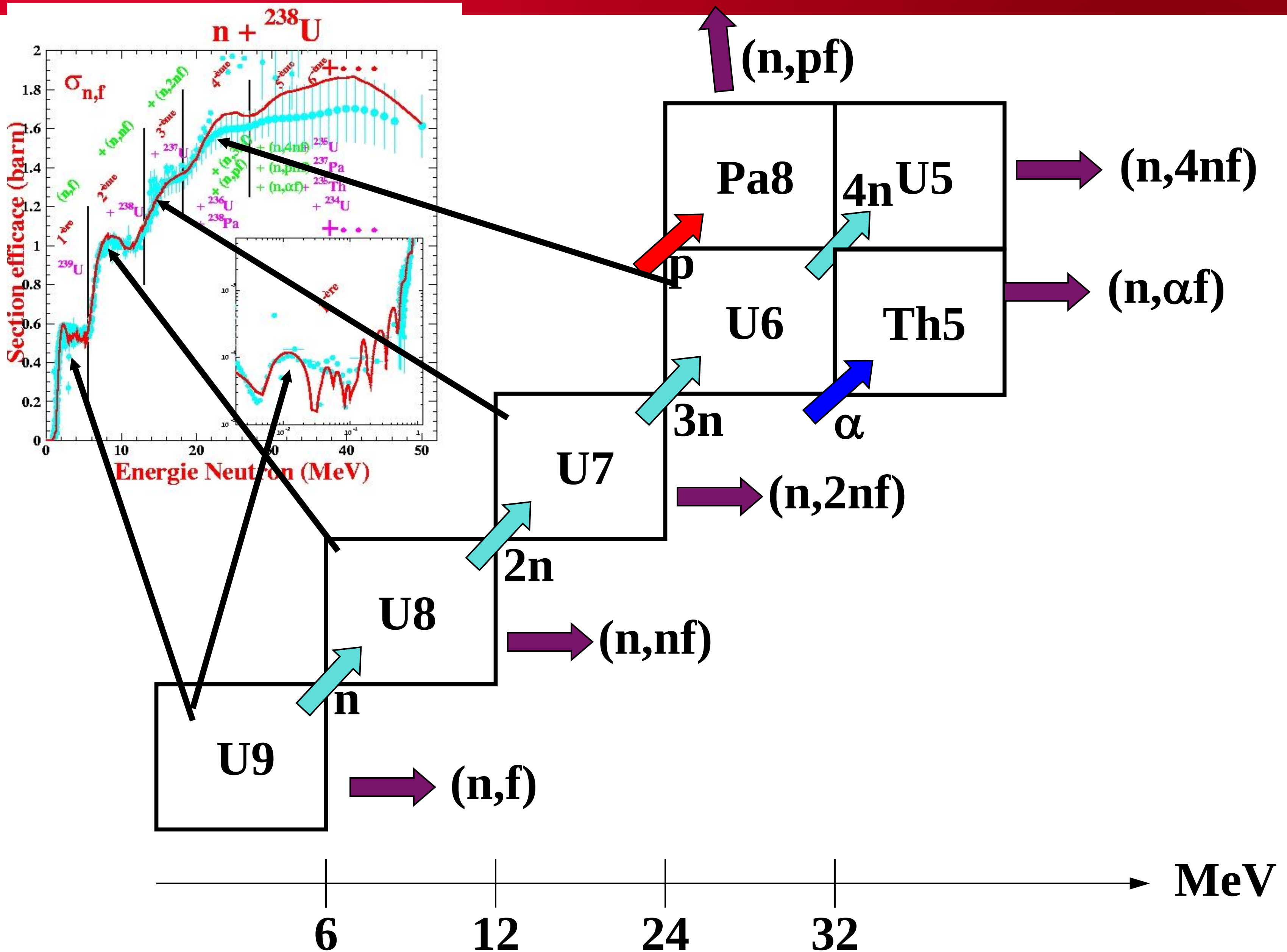
See in Sin et al., PRC 74 (2006) 014608

Bjornholm and Lynn, Rev. Mod. Phys. 52 (1980) 725.

Competition between channels

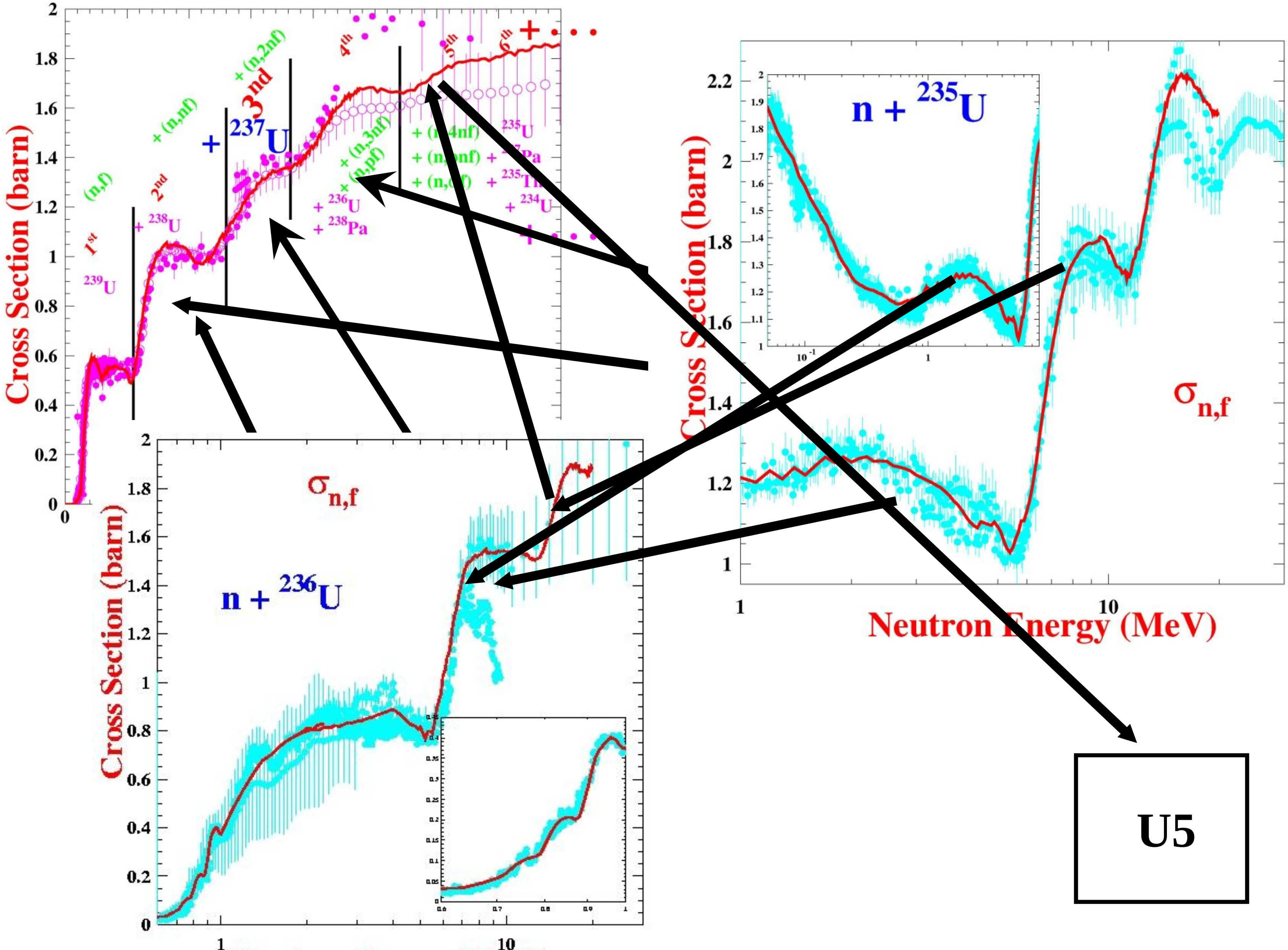


Multi-chance fission : many parameters

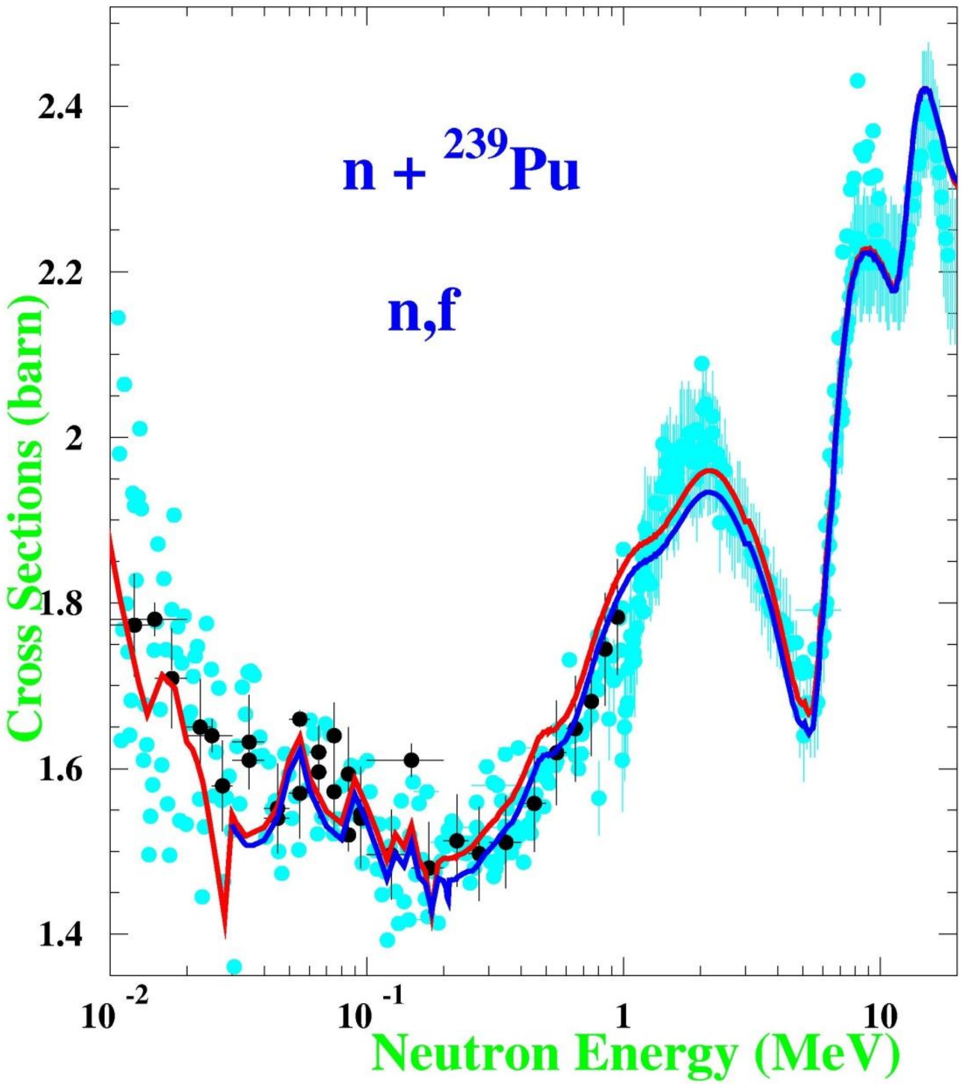


Dealing with numerous parameters : consistant treatment

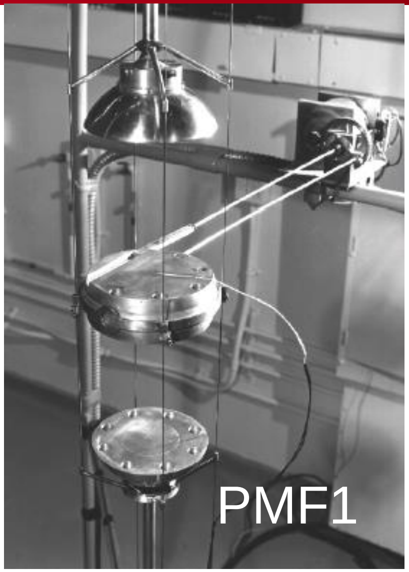
Neutron induced fission on ^{238}U

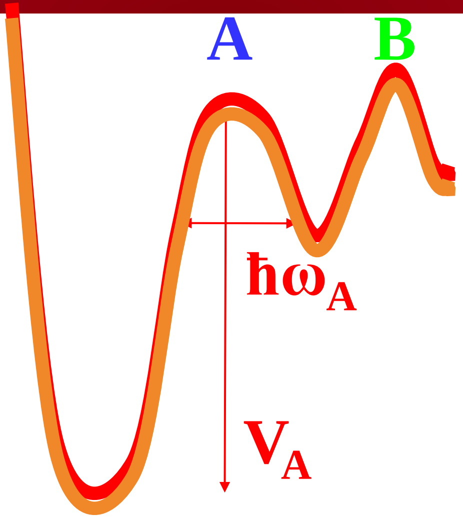


Integral experiments are constraining
Example: JEZEBEL for the ^{239}Pu(n,f) cross section



Courtesy : P Romain (CEA DAM DIF)





-20 keV for V_A
≈ 0.34%

➔1000 pcm on K_{eff} !!!
(measured within 150 pcm)

Summary / things to remember

- Strong **interplay** between direct, pre-equilibrium and compound processes
- Strong **competition** between channels (capture, elastic, inel, (n,2n), fission,…)
- **Many parameters** (OMPs, level densities, γ strength functions, fission barrier parameters(number of humps, height, curvature, transition states, class II-III states,…)) for each C.N.
  - Many choices for each of these parameters (phenomenological or microscopic)
- But **many experimental constraints**
  - **Consistent** adjustment of muti-chance fission, (n,xn) and capture **xs**
  - **Integral** experiments provide strong constraints (D. Bernard)

- Models implemented in TALYS (see S.Hilaire talk)
- More on inelastic models by P. Romain
- More information on pre-equilibrium by M. Dupuis
- R. Capote and T. Kawano will give further insights

- See EPJA **48**, 113 (2012) for a more complete review of many of the above topics.