First simultaneous evaluation of fission probabilities and neutron-induced cross sections for the Pu fissile isotopes

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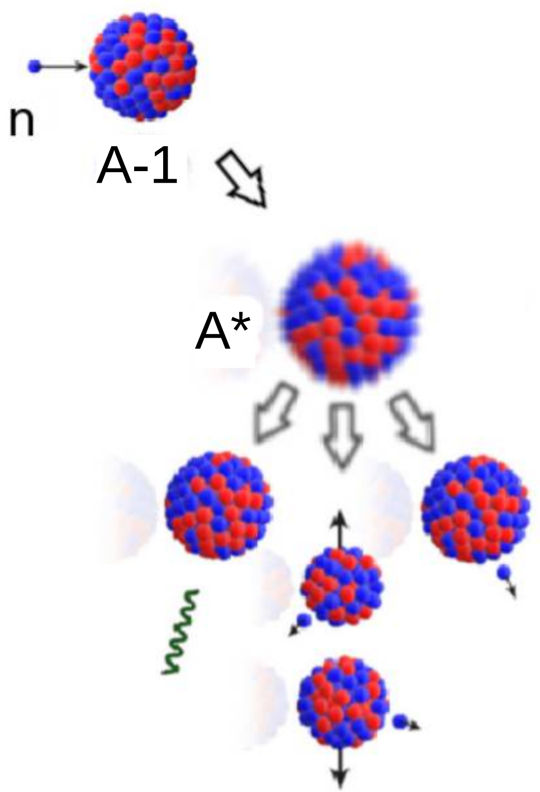
In memory of Olivier

A unique and coherent description : why ?

n-induced reaction



n-induced reactions

- Fundamental physics
- Nuclear astrophysics
- Applications

} **σ(n,c')** for as many nuclei as possible

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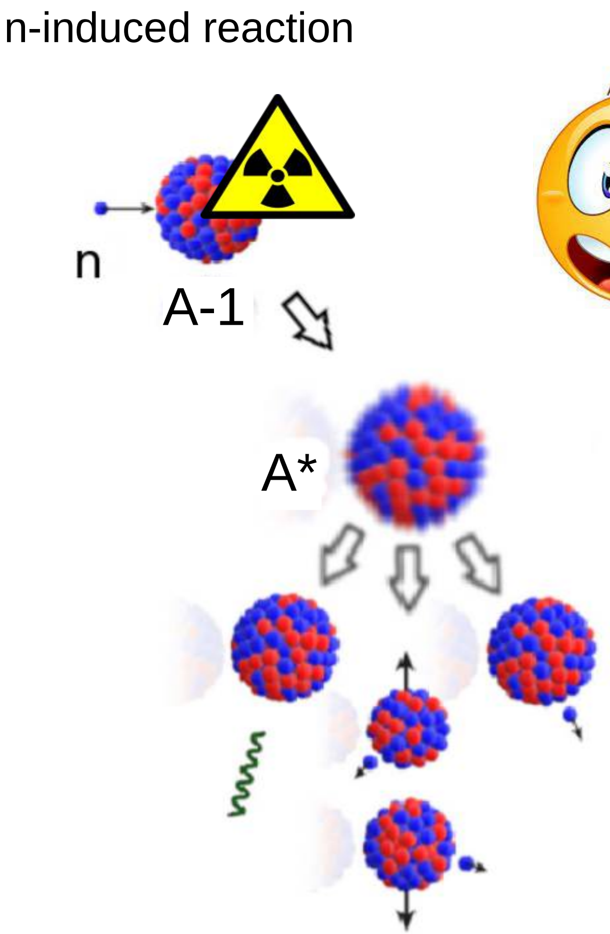

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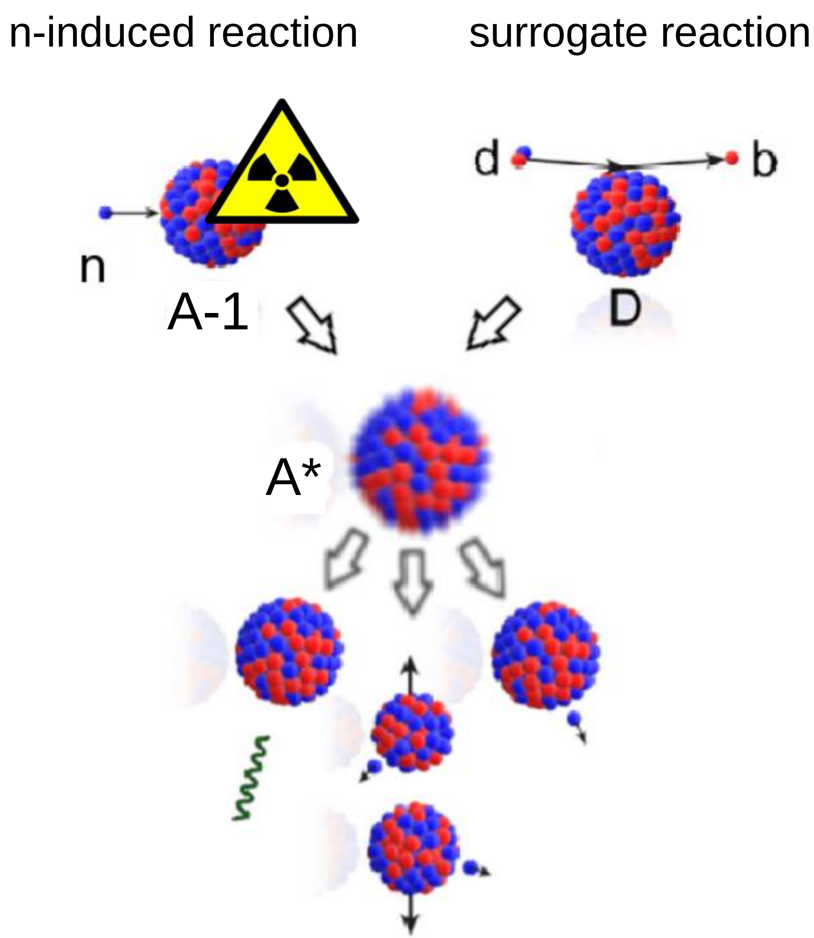

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Surrogate reactions : → deexcitation **probabilities**

- Short-lived nuclei σ(n,c')
- Fission barriers and resonance structures **@E*<S$_n$**

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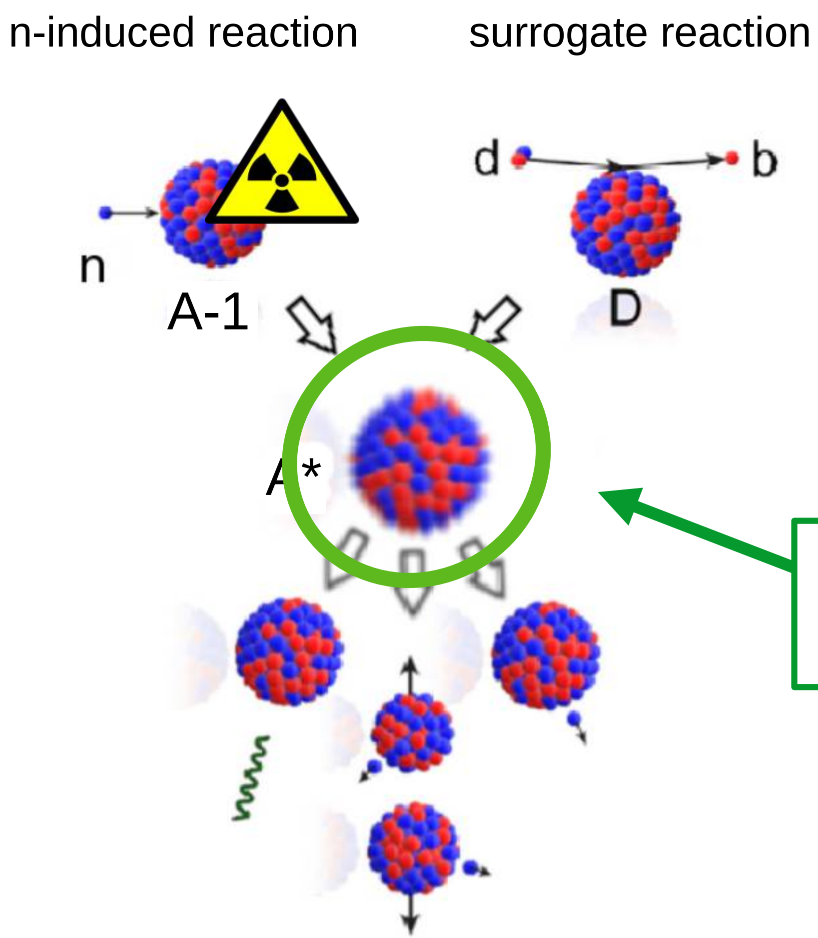

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Two reaction mechanisms - the same system?

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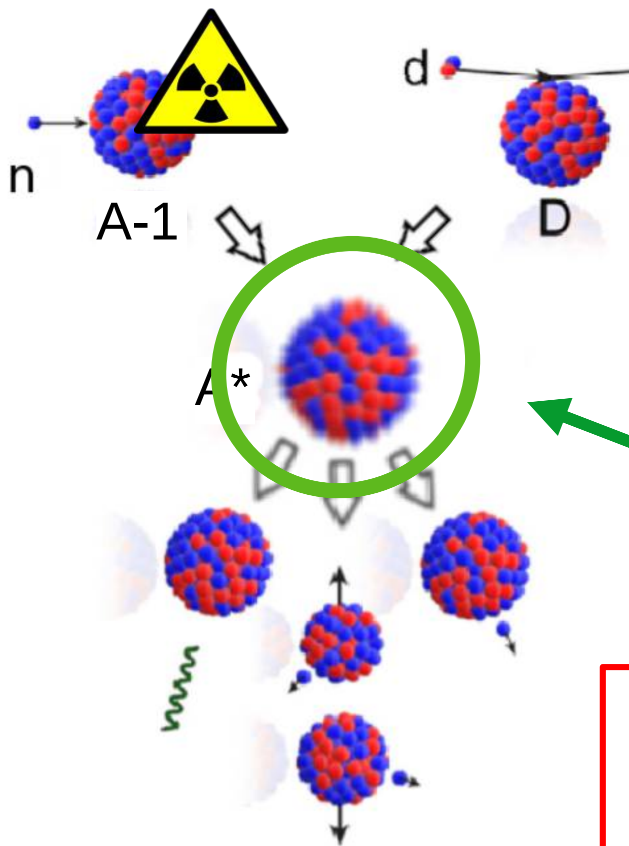
n-induced reaction surrogate reaction



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Two reaction mechanisms - the same system?

Theoretical framework to **simultaneously** describe **both** reactions with a **unique set** of nuclear parameters

AVXSF-LNG code + R-matrix formalism

O. Bouland, PRC 100, 064611 (2019)

A unique and coherent description : how ?

Average CROSS Section Fission – Lynn and Next Generation

O. Bouland, PRC 100, 064611 (2019)
O. Bouland & PM, Nucl. Data Sh. 193, 105 (2024)

Ingredients :

- Hauser Feshback theory

$$\overline{\sigma_{n,c'}}(E_n) = \sigma^{CN}(E_n) * \sum_{J^\pi} [\boldsymbol{J^\pi} \, populated \, distrib(E_n) * BR_{c'}^{J^\pi}(E_n)]$$

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Improvement

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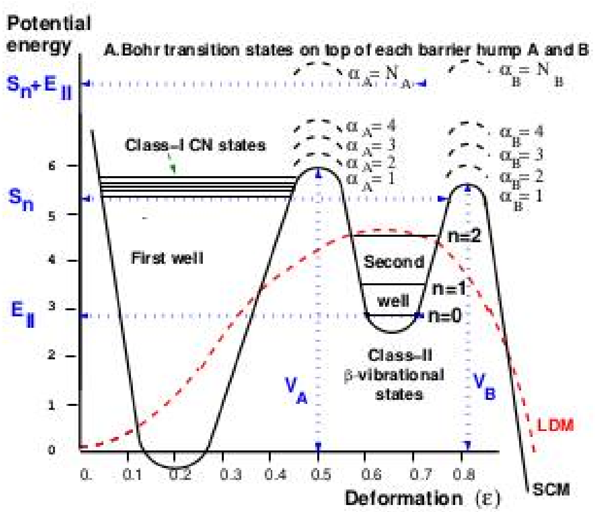
  - **Fission** → double-humped fission barrier



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- Exit channel description/competition:
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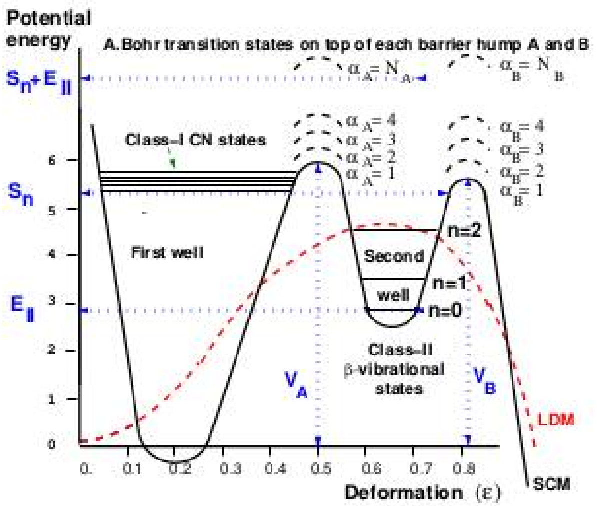
  - **Fission** → double-humped fission barrier →

HF equations : **Monte Carlo method**
Correlations between class-I and II state width fluctuations and the shape of fission barrier **are NOT washed out**

Improvement



<σ(n,c')>$_{MC}$ differs **up to 10%** from the analytical solution

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- Surrogate-reaction probabilities modeling → J^π n-induced $\neq$ **surrogate** reaction

- Exit channel description/competition:
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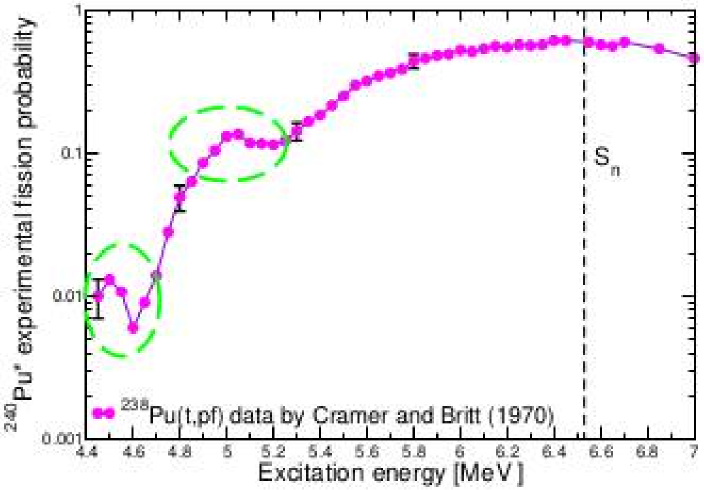
  - **Fission** → double-humped fission barrier → HF equations : **Monte Carlo method**

→ Model fission probabilities in **β-vibrational resonance** region



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- Surrogate-reaction probabilities modeling ➡ J^π n-induced $\neq$ **surrogate** reaction

- Exit channel description/competition: ➡ HF equations : **Monte Carlo method** **+** Model the **β-vibrational resonance** region

Improvement

- **Unique input parameters database** for n-induced and surrogate reactions

A school case : $^{240}Pu^*$

Model applied to the **Pu** **fissile** isotopes [4-8MeV E_n] → $^{237\text{-}244}Pu^*$

WHY

^{239}Pu : key nucleus → high quality evaluation → **challenge** for theoretical calculation of surrogate reactions to get a good agreement

$P_f \rightarrow \sigma(n,f)$

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P_f ⟶ σ(n,f)

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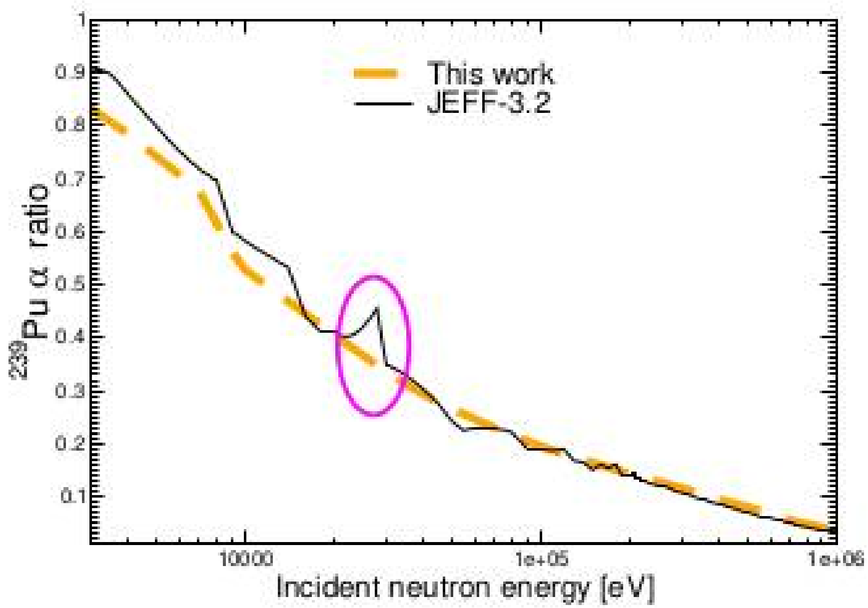

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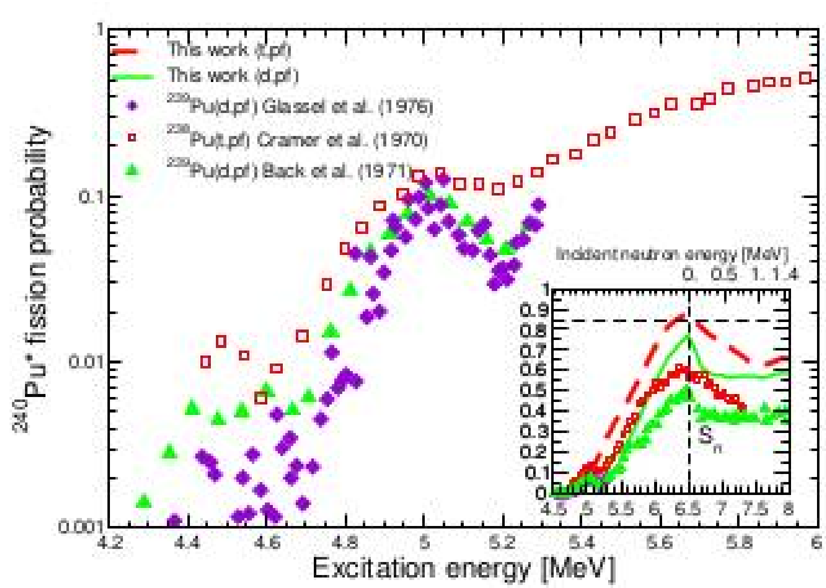
(t,p) and (d,p) data sets



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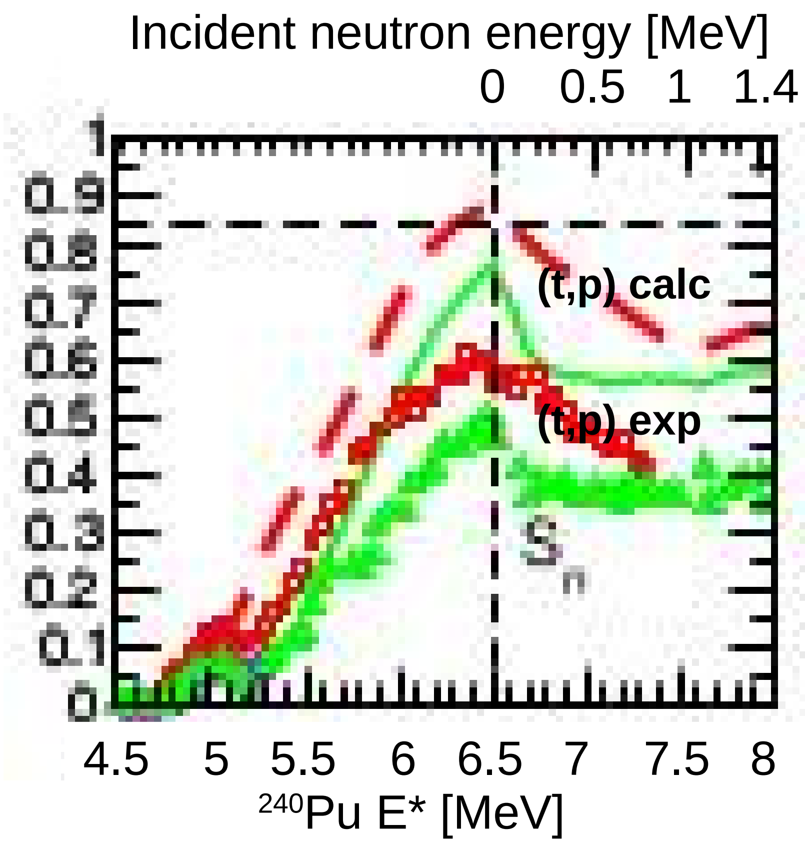
P_f exp = **0.6±0.06** Cramer et al. (1970)

P_f calc = **0.89±??**



Do we need to renormalize experimental data of 30% ???

Is the model affected by 30% uncertainty ?

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Most **sensitive input parameters** at S_n+1eV

- ✔ V_A and V_B
- ✔ s-wave n strength function S_0
- ✔ class-I mean spacing D
- ✔ Total γ average width Γ_γ

} RIPL-3
S. Bjornholm et al, Rev. Mod. Phys. 52, 725 (1980)

- ✔ Populated CS J^π distribution

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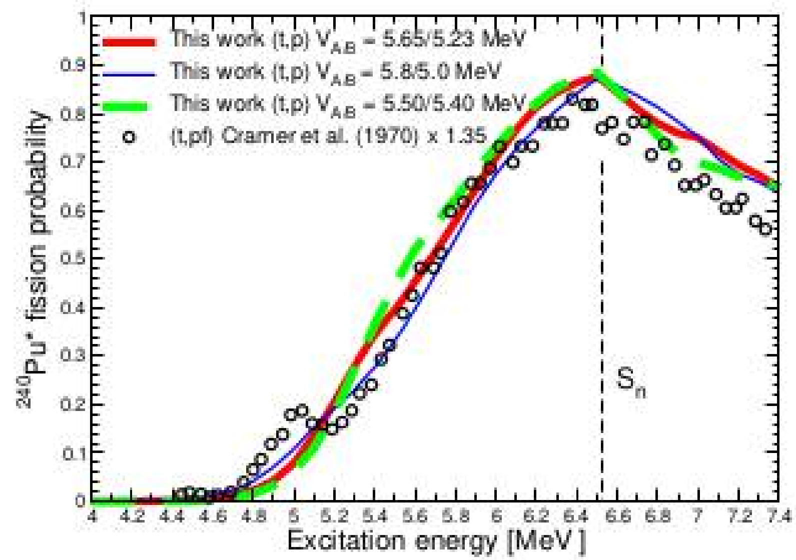

$(V_A,V_B) = (5.65, 5.23)$ MeV

- In **agreement** with theoretical predictions of $V_B<V_A$
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- P_f at S_n **not sensitive** to (V_A,V_B)

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a. Com

et al. (1970)

Mos

✔ V/

Fission barrier heights can be confidently extracted from **surrogate reaction data** for fissile isotopes

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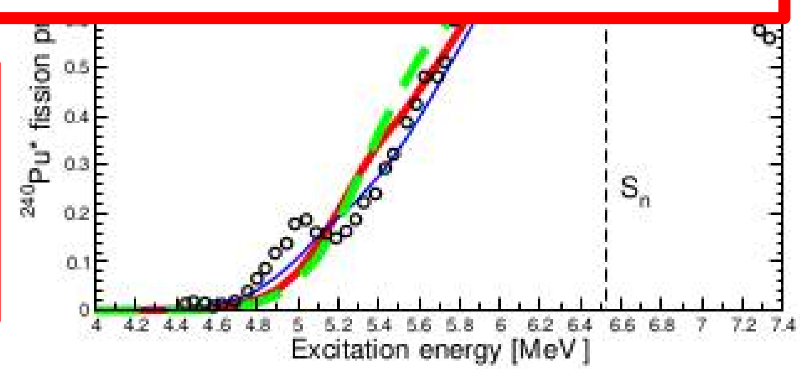

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Direct perturbation within reference uncertainties

Δ_{max}~ 2.1 % between calculations with REF and "our" parameters

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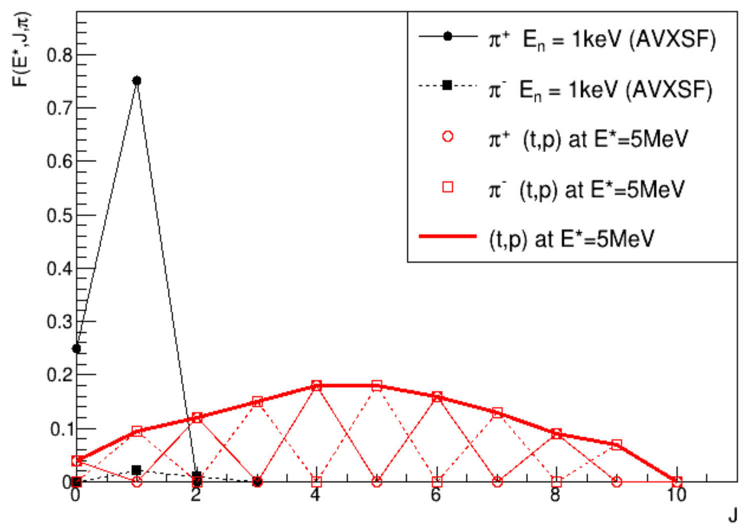

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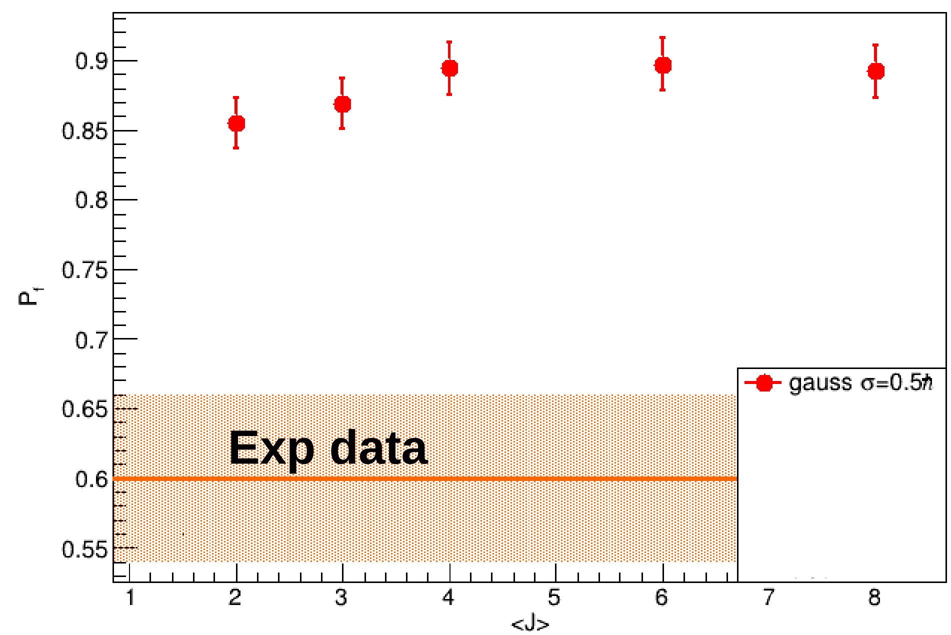
  - **Gaussian**



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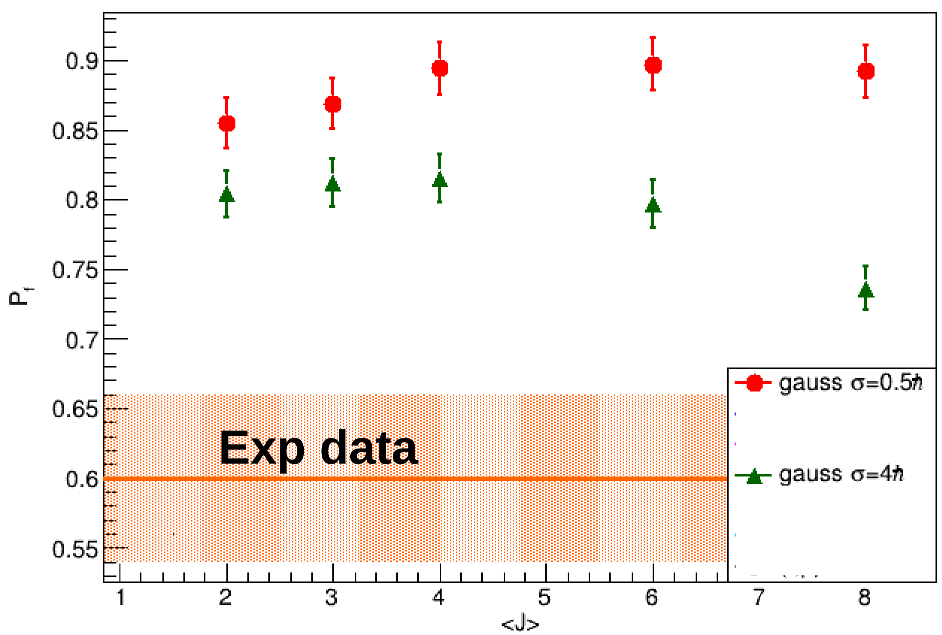

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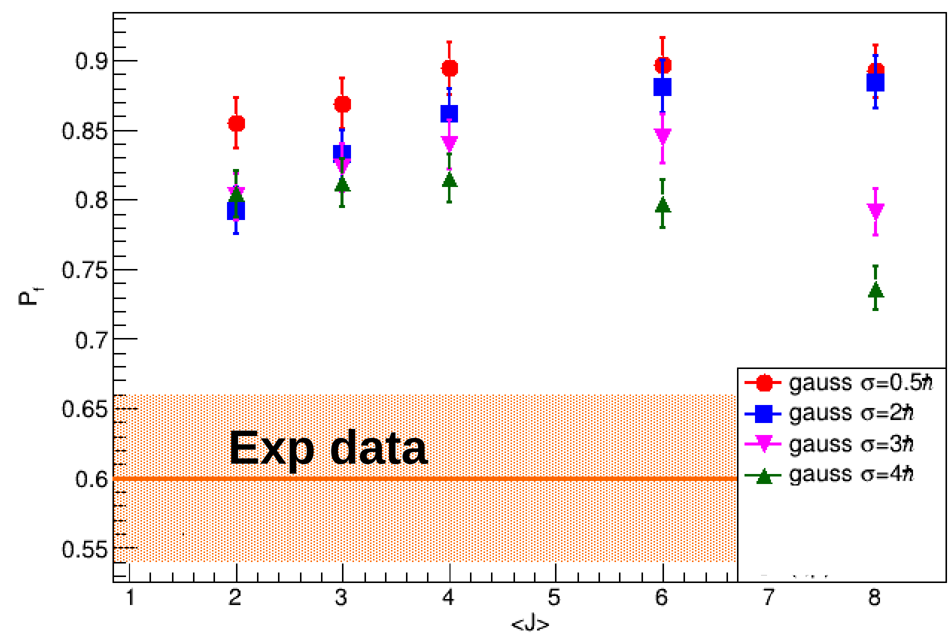

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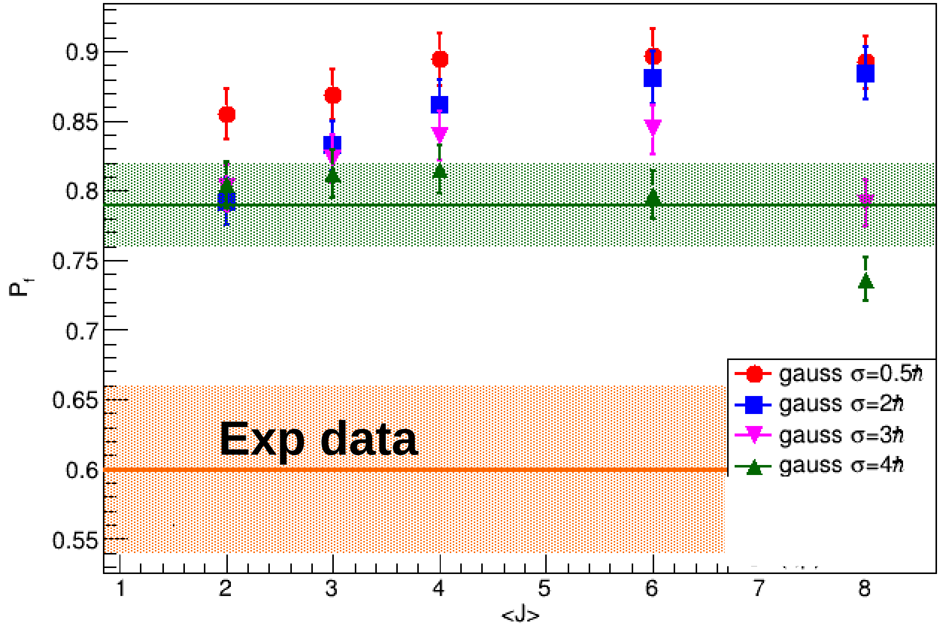

- Gaussian
- **Gaussian but no <J> and σ assumption**

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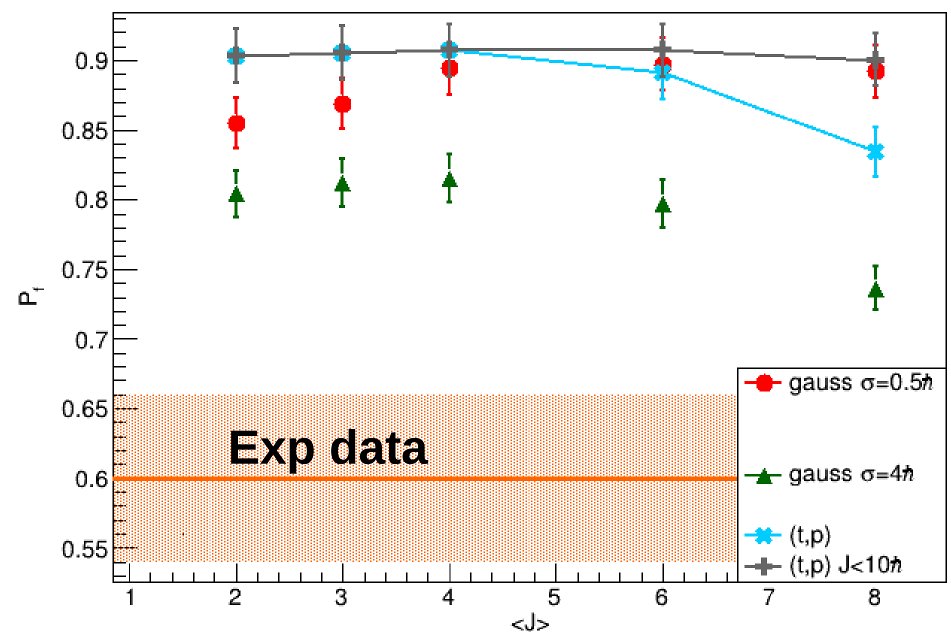
  - **from Back et al. (1974) w/ and w/o cuts for J≤10h**



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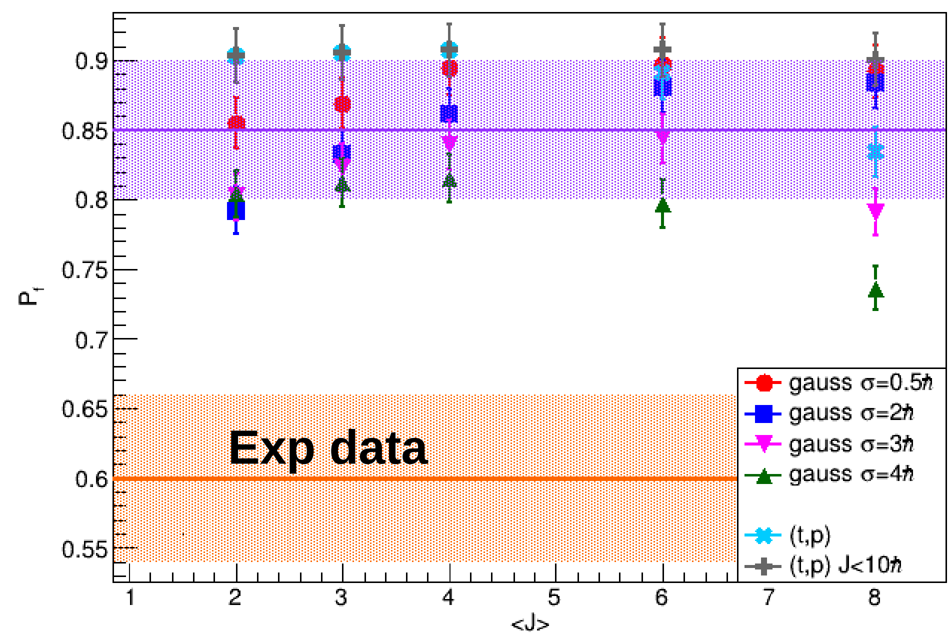

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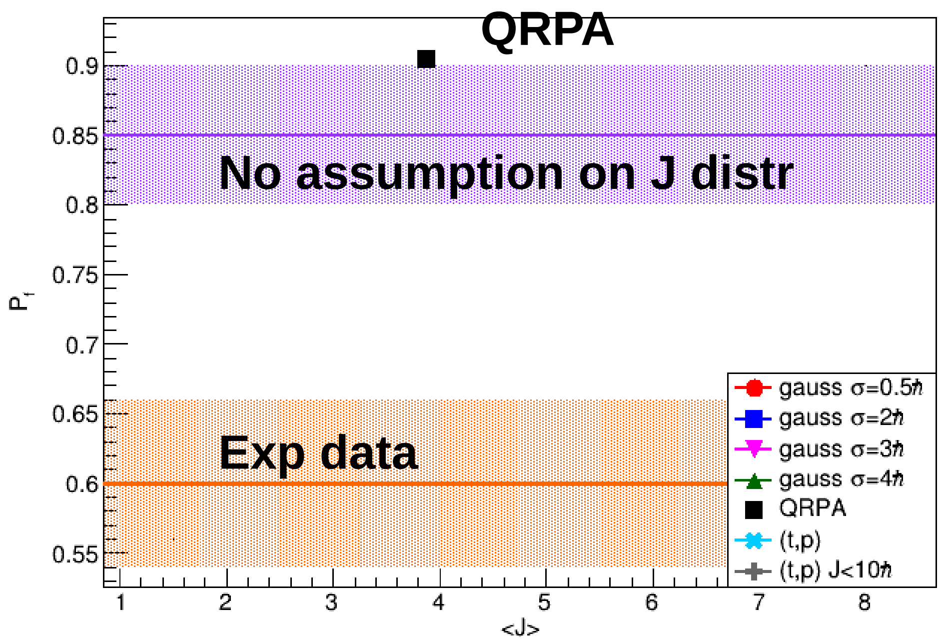
  - **QRPA calculation of J distribution** (<J>=3.9h σ=3.2h)



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a. Com

et al. (1970)

Mos

✔ V

✔ P

Weak sensitivity of P_f at S_n to the chosen **J^π CS distribution**

[for (t,p) reactions !!]

The **total uncertainty** on the calculated P_f at S_n is **6.3%**

-
-

for σ_10h

- no assumption Δ_{max}~ 6 %

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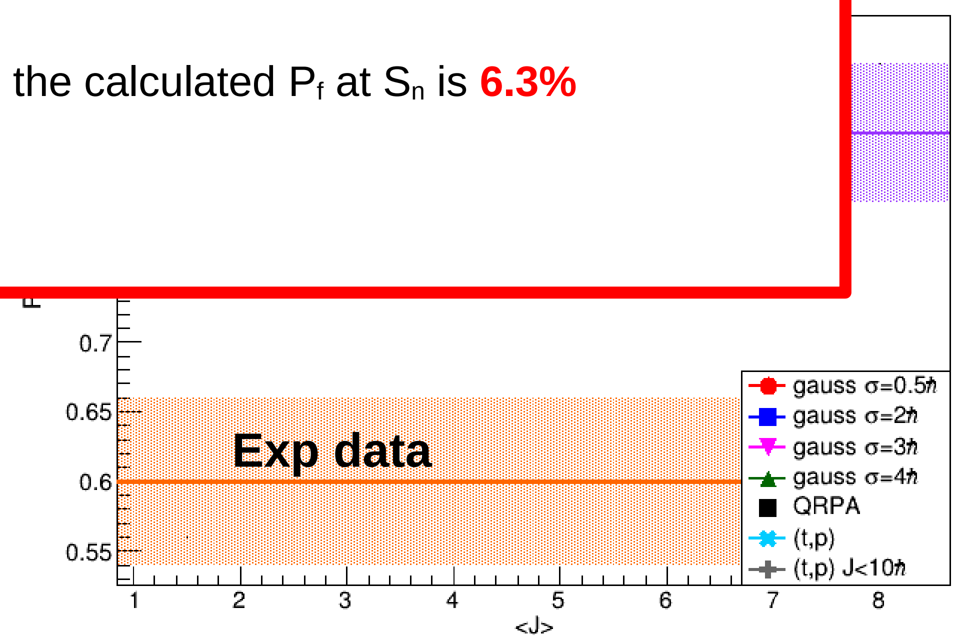

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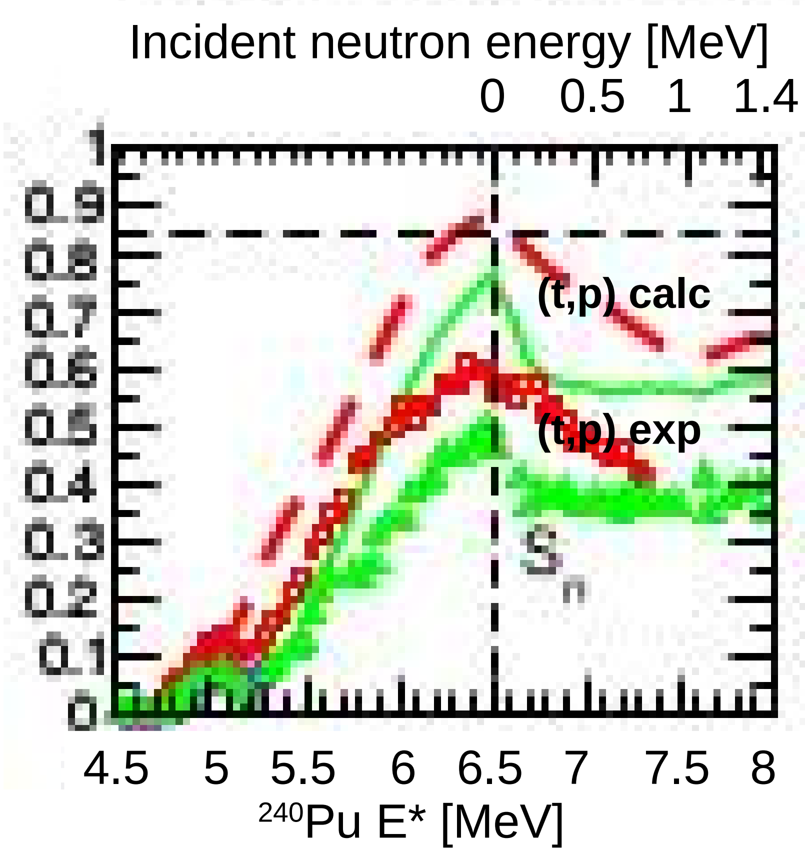
P_f calc = **0.89±0.06**

Need for a 30% **renormalization** of exp data



A school case : $^{240}Pu^*$

1. Test on **n-induced data** : does the model reproduce $\frac{\sigma(n,\gamma)}{\sigma(n,f)}$? ✔

2. Let's look at **surrogate reactions**

   a. Comparison of experimental and calculated **P_f at S_n**

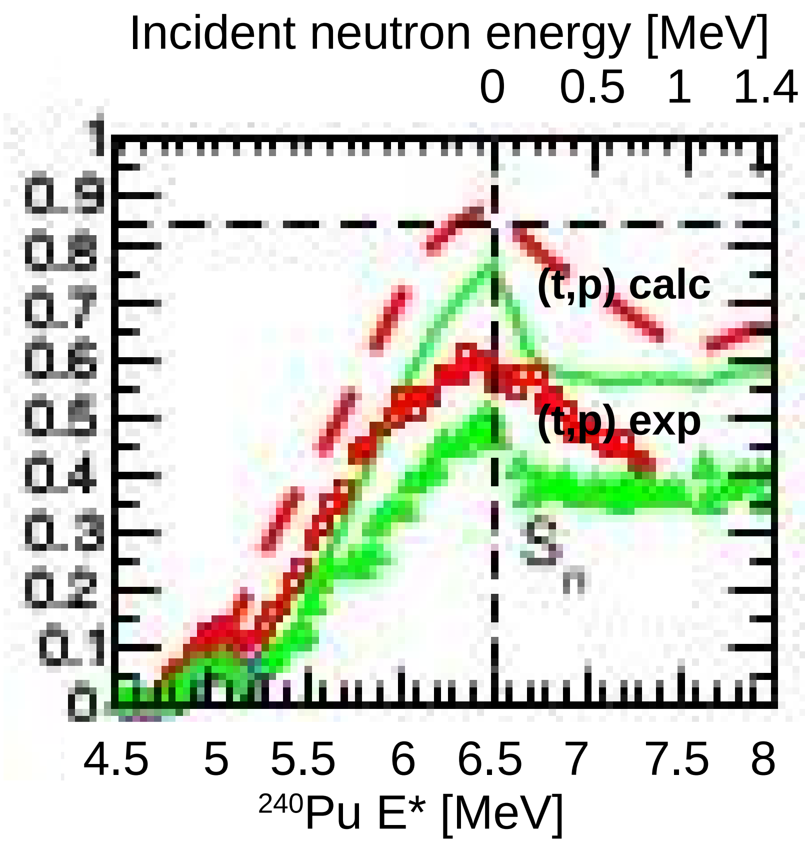
P_f exp = **0.6±0.06** Cramer et al. (1970)

P_f calc = **0.89±0.06**

Need for a 30% **renormalization** of exp data

Estimated systematic uncertainty
~30%

Back et al. (1974)



A school case : $^{240}Pu^{*}$

1. Test on **n-induced data** : does the model reproduce $\frac{\sigma(n,\gamma)}{\sigma(n,f)}$? ✔

2. Let's look at **surrogate reactions** +++

   a. Comparison of experimental and calculated **P_f at S_n** ➡ Need for a **renormalization** of exp data

   b. **Barrier height** estimates +++

A school case : ^{240}Pu*

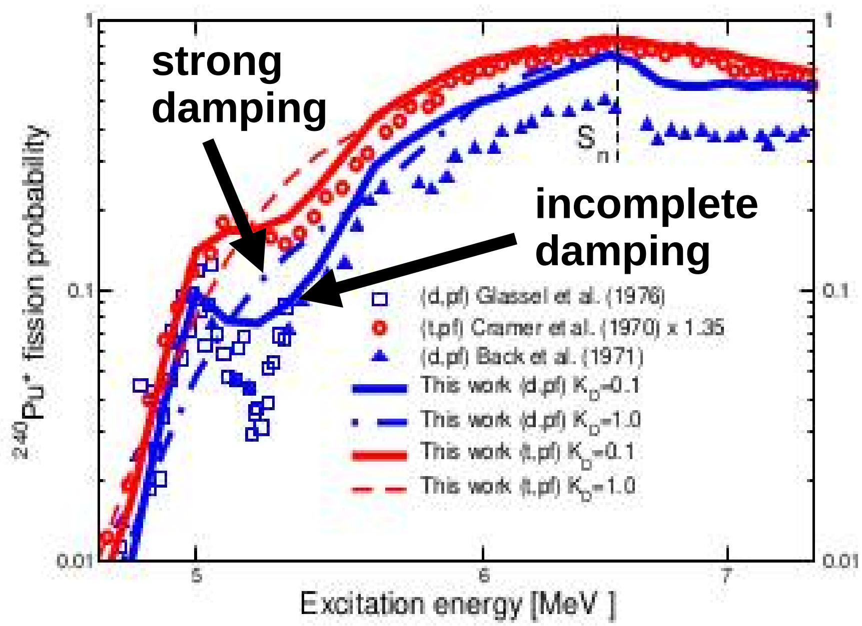
1. Test on **n-induced data** : does the model reproduce $\frac{\sigma(n,\gamma)}{\sigma(n,f)}$? ✔

2. Let's look at **surrogate reactions** +++

   a. Comparison of experimental and calculated **P_f at S_n** ➡ Need for a **renormalization** of exp data

   b. **Barrier height** estimates +++

   c. **Intermediate resonance** structures ➡ **damping strength** of β-vibrations



Does the damping strength of β-vibrations modify σ_{calc}(n,f)?

A school case : $^{240}Pu^*$

1. Test on **n-induced data** : does the model reproduce $\frac{\sigma(n,\gamma)}{\sigma(n,f)}$? ✔

2. Let's look at **surrogate reactions** +++

   a. Comparison of experimental and calculated **P_f at S_n** ➡ Need for a **renormalization** of exp data

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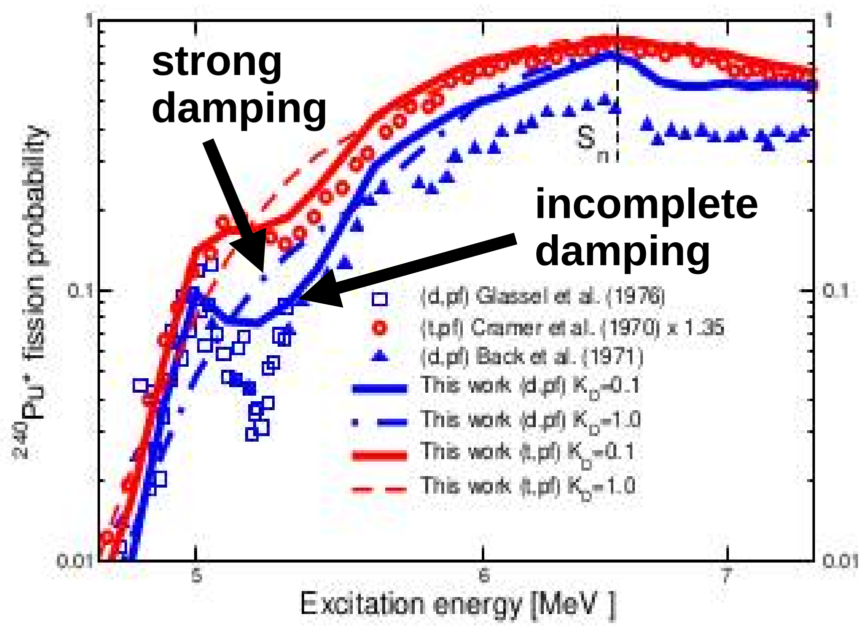
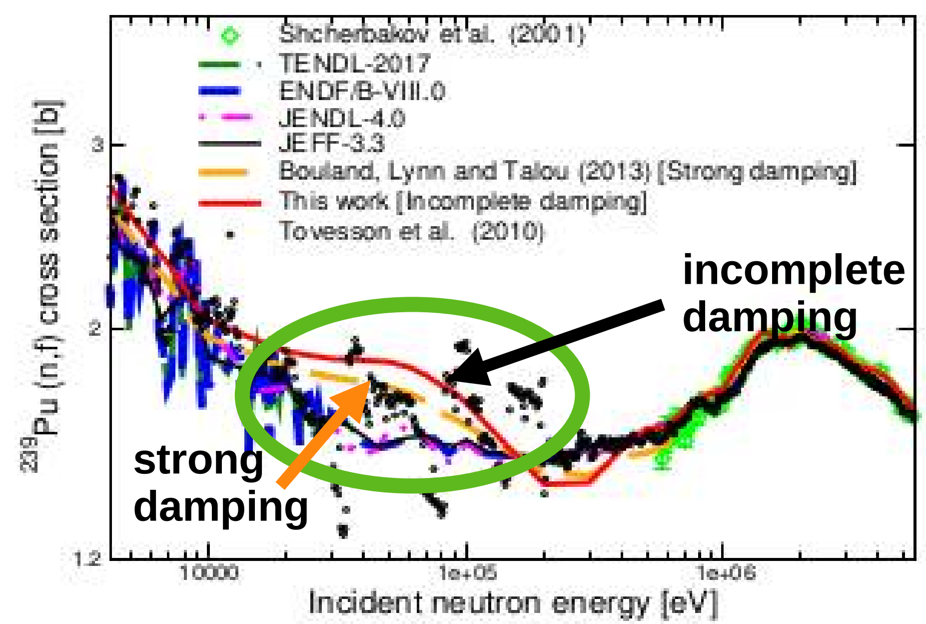




A school case : $^{240}Pu^*$

1. Test on **n-induced data** : does the model reproduce $\frac{\sigma(n,\gamma)}{\sigma(n,f)}$? ✔

2. Let's look at **surrogate reactions** +++

a. Com ... exp data

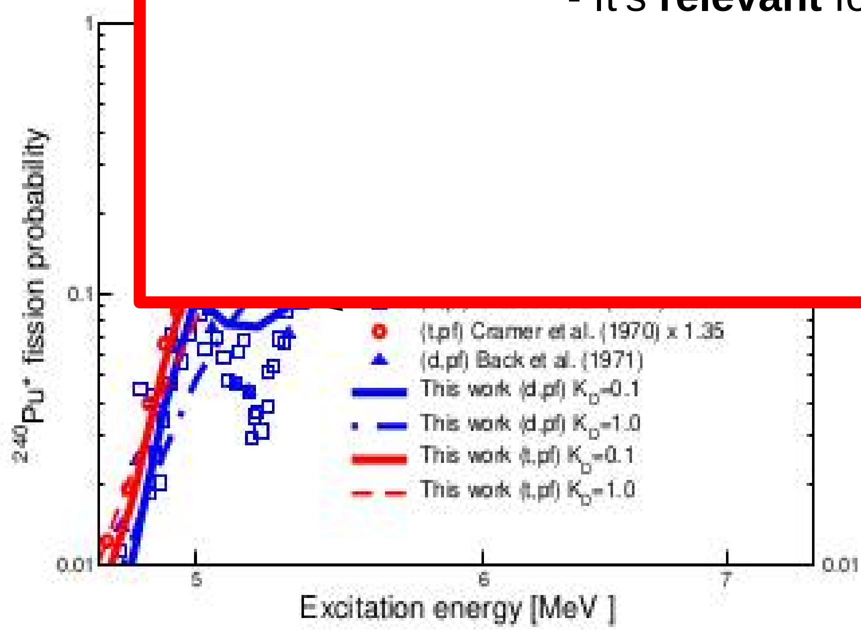
b. **Barr**

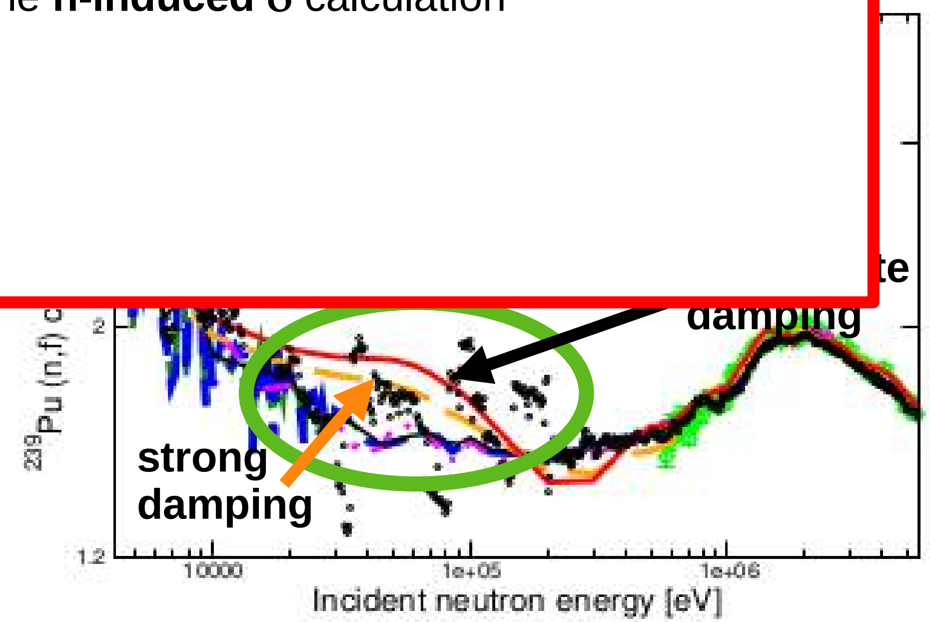
c. **Inter**

The **damping strength of β-vibration** :

- can be extracted from **surrogate** reaction data

- It's **relevant** for the **n-induced σ** calculation





A school case : $^{240}Pu^*$

1. Test on **n-induced data** : does the model reproduce $\frac{\sigma(n,\gamma)}{\sigma(n,f)}$? ✔

2. Let's look at **surrogate reactions** +++

   a. Comparison of experimental and calculated **P_f at S_n** ➡ Need for a **renormalization** of exp data

   b. **Barrier height** estimates +++

   c. **Intermediate resonance** structures ➡ **damping strength** of β-vibrations +++

   d. Intermediate resonances in **individual J^π P_f** ➡ The small contribution of 1^+ P_f explains the s-wave σ(n,f)

Conclusions and perspectives

WHY

Challenge : high quality evaluations of σ(n,f) for heavy nuclei

- high target accuracy
- **fissile** nuclei

Conclusions and perspectives

WHY

Challenge : high quality evaluations of σ(n,f) for heavy nuclei { high target accuracy / **fissile** nuclei }

↑

HOW

Use **surrogate reaction** data to refine **nuclear model parameters**

Conclusions and perspectives

WHY

Challenge : high quality evaluations of σ(n,f) for heavy nuclei

- high target accuracy
- **fissile** nuclei

Simultaneous and **coherent** analysis of P_f and σ(n,f)

HOW

Use **surrogate reaction** data to refine **nuclear model parameters**

Conclusions and perspectives

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- high target accuracy
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Simultaneous and **coherent** analysis of P_f and σ(n,f)

HOW

Use **surrogate reaction** data to refine **nuclear model parameters**

- ✔ Uncertainty on calculated P_f ~6.3%
- ✔ Estimate fission barrier heights
- ✔ Estimate damping strength of β-vibrations
- ✔ Consistency test of existing surrogate and n-induced reaction data

Conclusions and perspectives

WHY

Challenge : high quality evaluations of σ(n,f) for heavy nuclei { high target accuracy; **fissile** nuclei }

Simultaneous and **coherent** analysis of P_f and σ(n,f)

HOW

Use **surrogate reaction** data to refine **nuclear model parameters**

- ✔ Uncertainty on calculated P_f ~6.3%
- ✔ Estimate fission barrier heights
- ✔ Estimate damping strength of β-vibrations
- ✔ Consistency test of existing surrogate and n-induced reaction data

FUTURE

Simultaneous analysis / measurement of **ALL deexcitation channels**

Modeling of and experimental comparison to (n,2n) data

First simultaneous evaluation of fission probabilities and neutron-induced cross sections for the Pu fissile isotopes

Thank you for your attention

In memory of Olivier

237Pu*

238Pu*

242Pu*

244Pu*

Standard HF + fission

Monte Carlo

Theory improvements

Input parameters

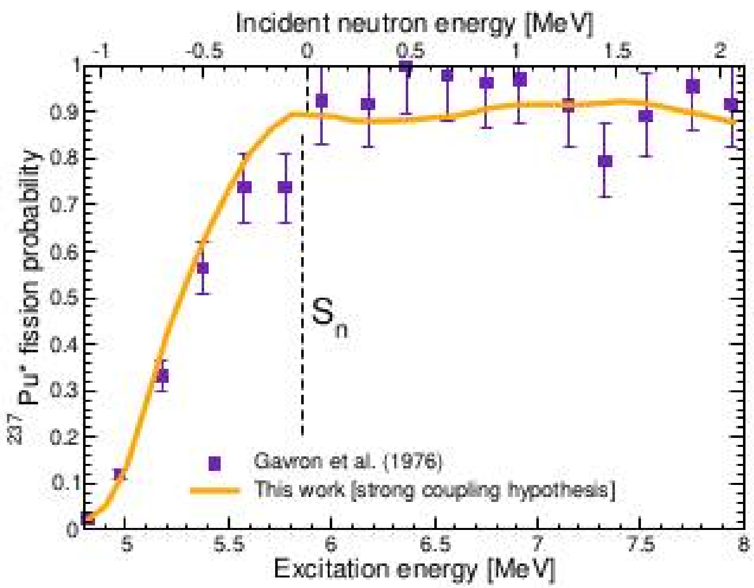
237 Pu*

The fissile Pu isotopic chain : $^{237-244}Pu^*$

$^{237}Pu^*$

$t_{1/2}$ (^{236}Pu)= 2.85y   very few n-induced σ data   Gerasimov et al. (1997)
Gromova et al. (1990)

^{237}Np(^{3}He,t) data available   Gavron et al. (1976)



- ✔ No evidence of intermediate structures ➡ Strong β-vibration damping
- ✔ (V_A,V_B) = (5.70, 5.10)MeV < S_n ➡ Fissile nucleus
- ✔ Truncated gauss distribution centered around ^{237}Pu(gs) (J=7/2)

Very **good agreement** of exp and calc P_f

The fissile Pu isotopic chain : $^{237-244}Pu^*$

$^{237}Pu^*$

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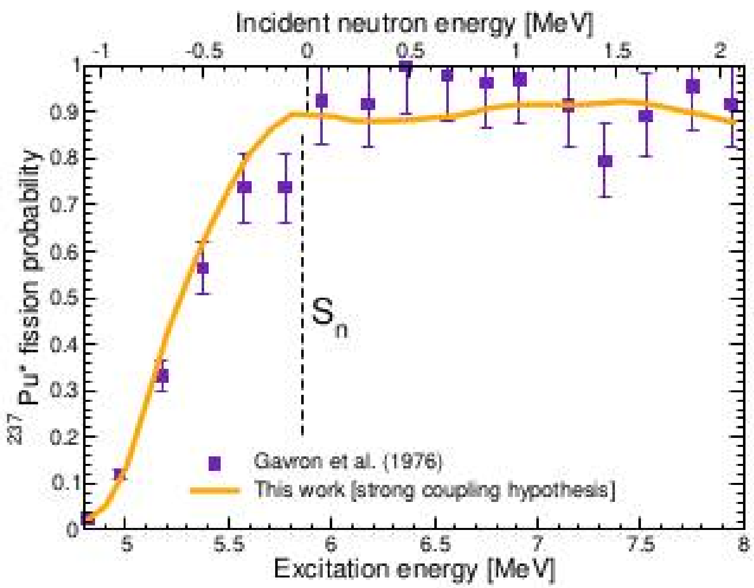
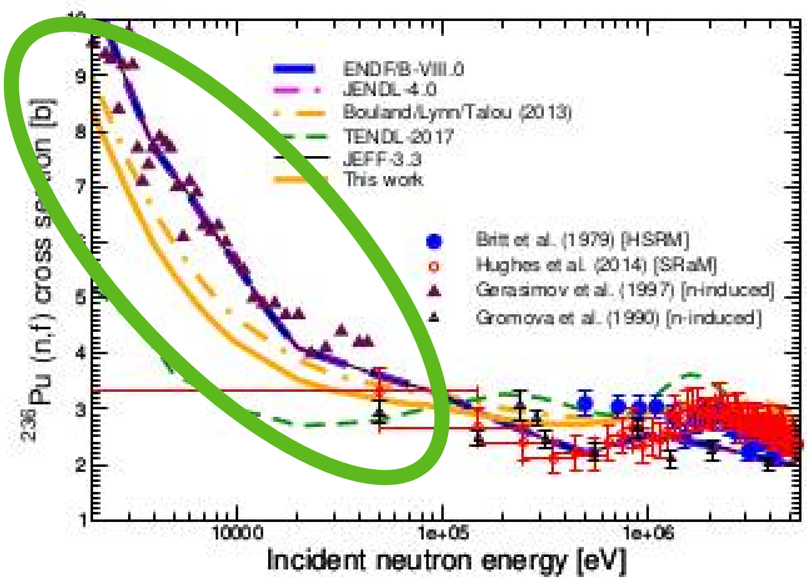




Very **good agreement** of exp and calc P_f

Doubts on Gerosimov's data below 50keV => **on evaluations** [but P_f dependence on J^{π} of (^{3}He,t) not investigated]

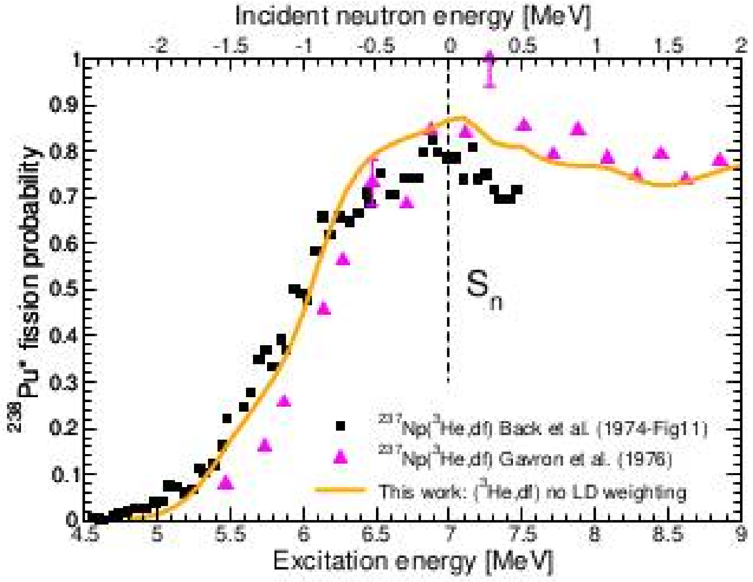
238 Pu*

The fissile Pu isotopic chain : $^{237-244}Pu^*$

$^{238}Pu^*$

$t_{1/2}$ (^{237}Pu)= 45d   no n-induced σ data

$^{237}Np(^{3}He,d)$ data available   Back et al. (1974)
Gavron et al. (1976)



- ✔ No evidence of intermediate structures ➡ Strong b-vibration damping
- ✔ $(V_A,V_B) = (5.65, 5.45)$MeV < S_n ➡ Fissile nucleus
- ✔ Truncated gauss distribution centered around ^{237}Pu(gs) (J=7/2)

Very **good agreement** of exp and calc P_f

The fissile Pu isotopic chain : $^{237-244}$Pu*

^{238}Pu*

$t_{1/2}$ (^{237}Pu)= 45d   no n-induced σ data

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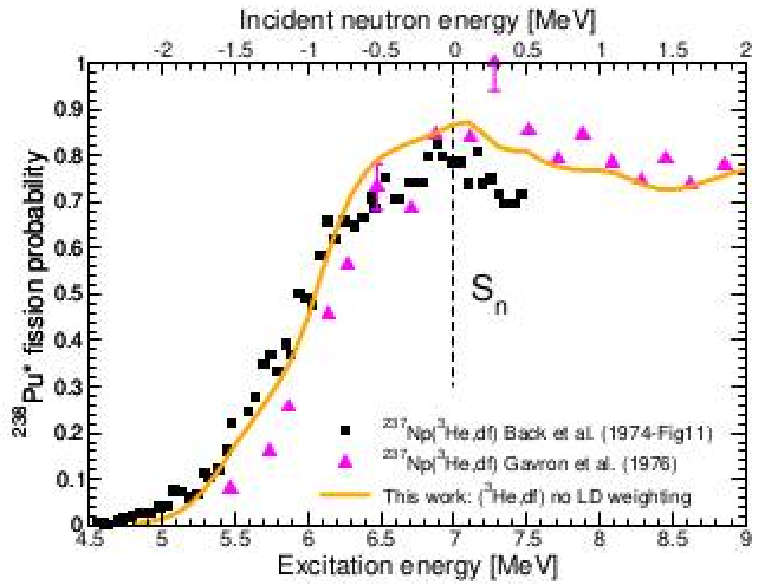
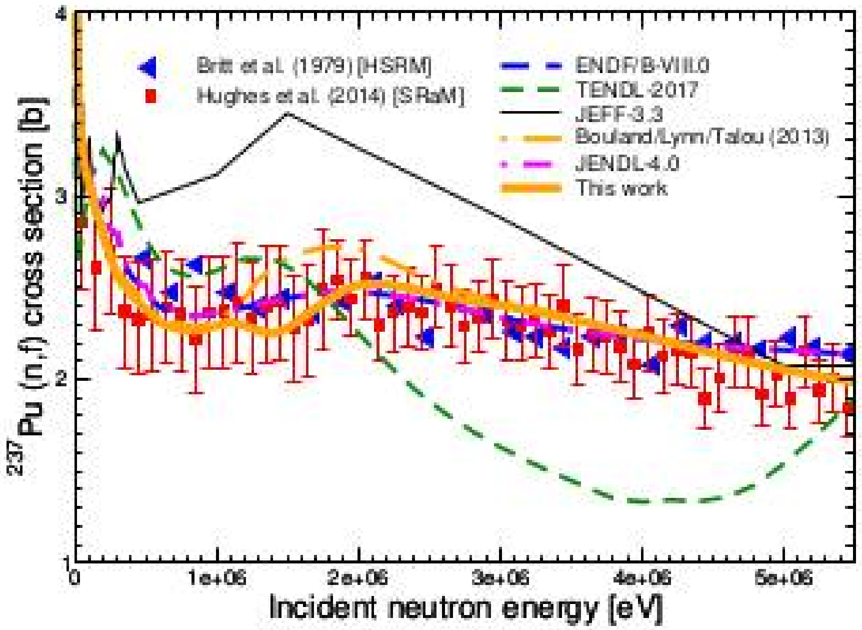




Very **good agreement** of exp and calc P_f **Not in agreement** w/ JEFF 3.3

242 Pu*

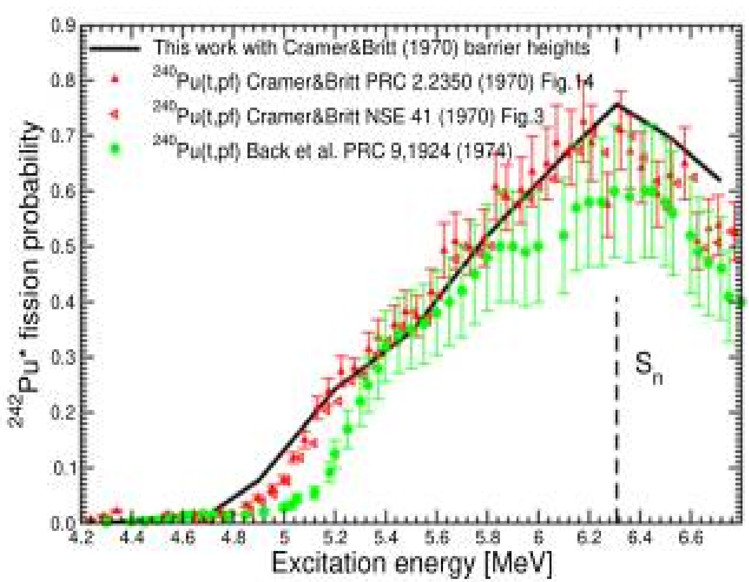
The fissile Pu isotopic chain : $^{237-244}Pu^*$

$^{242}Pu^*$

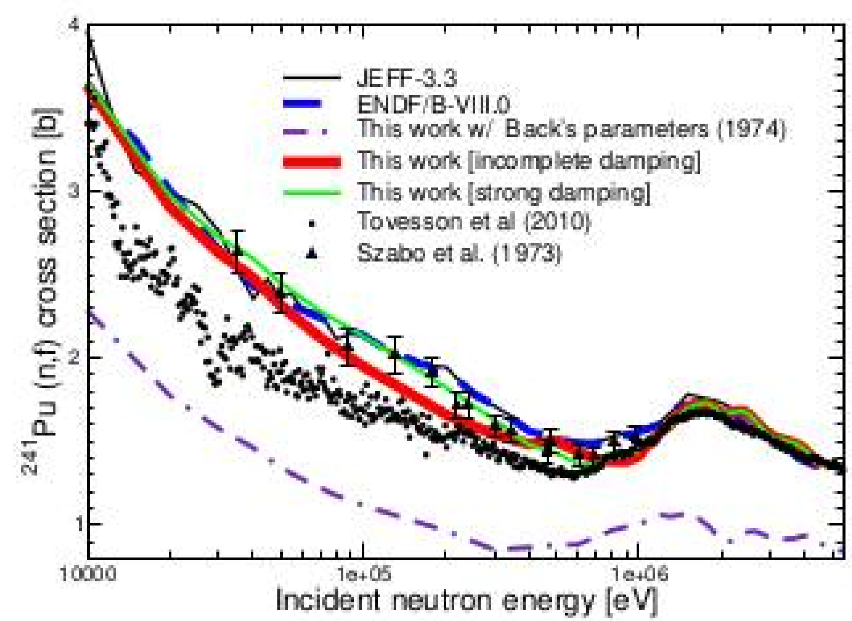
11% of total Pu mass in mixed oxide fuel

n-induced data — Tovesson et al. (2010), Szabo et al. (1973)

$^{240}Pu(t,p)$ data available — Back et al. (1974), Cramer et al (1970)



- ✔ Good agreement at Sn with Cramer at al.
- ✔ Renormalization needed for Back's data
- ✔ (V_A,V_B) values from Back et al. do not reproduce s(n,f), while values from literature and ours do (5.30,5.30)MeV
- ✔ Doubts on Tovesson's n-induced data
- ✔
- ✔ In agreement with evaluations



The fissile Pu isotopic chain : $^{237-244}Pu^{*}$

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11% of total Pu mass in mixed oxide fuel

n-induced data — Tovesson et al. (2010), Szabo et al. (1973)

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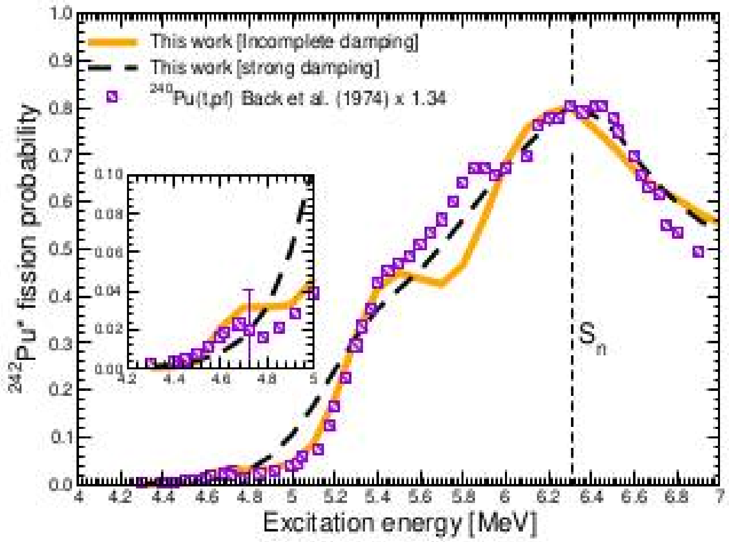

IS at 5.4MeV reproduced with incomplete damping

- ✔ Good agreement at Sn with Cramer at al.
- ✔ Renormalization needed for Back's data
- ✔ (V_A,V_B) values from Back et al. do not reproduce s(n,f), while values from literature and ours do (5.30,5.30)MeV
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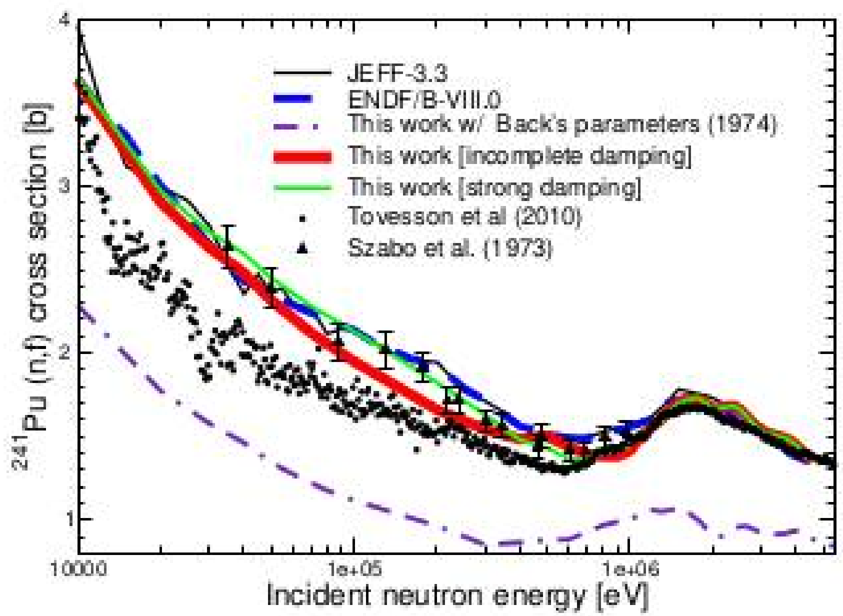


244 Pu*

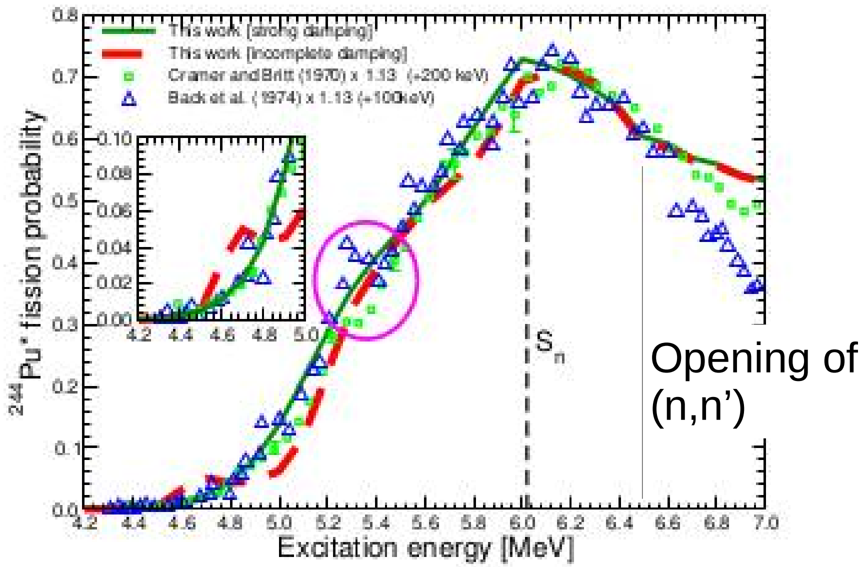
The fissile Pu isotopic chain : $^{237-244}Pu^*$

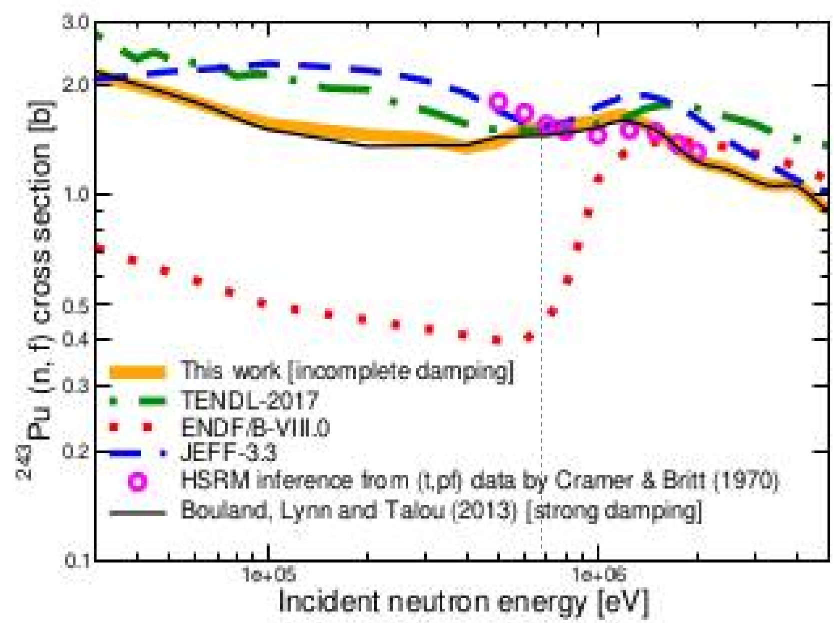
$^{244}Pu^*$

$t_{1/2}$ (^{243}Pu)= 4.95h   no n-induced σ data

^{242}Pu(t,p) data available   Cramet et al. (1970)
Back et al. (1974)

- ✔ Renormalization needed (13%)
- ✔ (V_A,V_B)=(5.30,5.25)MeV in agreement with theoretical calc ($V_A \sim V_B$) but significantly different from other authors
- ✔ Too little info on IS at 5.3MeV
- ✔ s(n,f) En>700keV : good agreement
  En<700keV :
  a) absence of width fluctuation correction factor in exp data
  b) $\sigma(n,f)_{calc} < \sigma_{TENDL}$ et σ_{JEFF}
  c) $\sigma(n,f)_{calc}$ not in agreement with ENDF (choice of (V_A,V_B))?





Standard HF + fission

Standard HF theory

Average n-induced reaction cross section $\sigma_{n,c'}(E_n)=\sum_{J^\pi}[\sigma_n^{CN}(E_n,J^\pi)B_{c'}^{J^\pi}(E_x)W_{n,c'}^{J^\pi}(E_x)]$

In-out-going channel width fluctuation correction factor

N-induced CN partial formation cross section $\sigma_n^{CN}(E_n,J^\pi)=\pi\lambda g_J\sum_{s=|I-\frac{1}{2}|}^{I+\frac{1}{2}}\sum_{l=|J-s|}^{J+s}T_n^{J^\pi(ls)}(E_n)$

Incoming n transmission coefficient $T_n^{J^\pi}(E_n)=1-\exp(-2\pi S_l(E_n))$

n strength function

Heavy nuclei + low En => we can use s- and p- wave Sl extracted from the analysis of the energy-resolved resonance region and from the fit of average cross sections below 300keV

$S_l=1.044*10^{-4}$ even-l waves

$S_l=2.48*10^{-4}$ odd-l waves

Standard HF theory : exit channels

Transmission coefficients :

- n channel : $T_n^{J^\pi}(E_x) = 1 - \exp(-2\pi S_l(E_x))$

- other channels : $T_\gamma^{J^\pi} = 2\pi \frac{\langle \Gamma_\gamma^{J^\pi} \rangle}{D_{J^\pi}}$

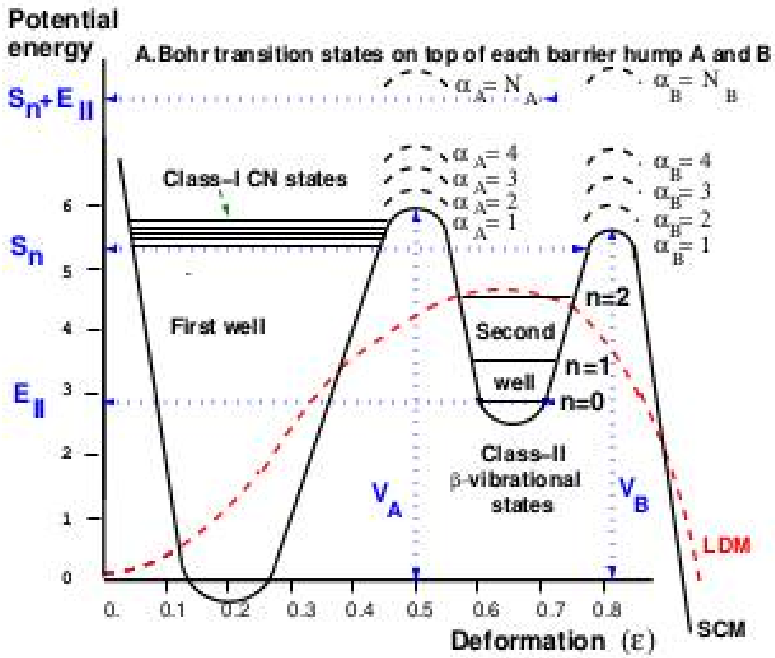
$\langle \Gamma_\gamma^{J^\pi} \rangle$ Average capture width

D_{J^π} Average resonance spacing for a given (Jp)

obtained with the combinatorial quasiparticle-vibration-rotation (QPVR) model

- fission :

Standard HF theory : fission exit channel



Total width for class-I states :
(elastic + inelastic + gamma)

$$\Gamma_{\lambda I\,tot} \approx \Gamma_{\lambda I n} + \Gamma_{\lambda I n'} + \Gamma_{\lambda I \gamma}$$

Total width for class-II states :

$$\Gamma_{\lambda II\,tot} \approx \Gamma_{\lambda II \downarrow} + \Gamma_{\lambda II \uparrow} + \Gamma_{\lambda II \gamma}$$

where the class-II fission width is

$$\langle \Gamma_{\lambda II(\uparrow)} \rangle = \frac{D_{\lambda II}}{2\pi} T_B$$

Transmission coeff through outer barrier

and the class-II coupling width is

$$\langle \Gamma_{\lambda II(\downarrow)} \rangle = \frac{D_{\lambda II}}{2\pi} T_A$$

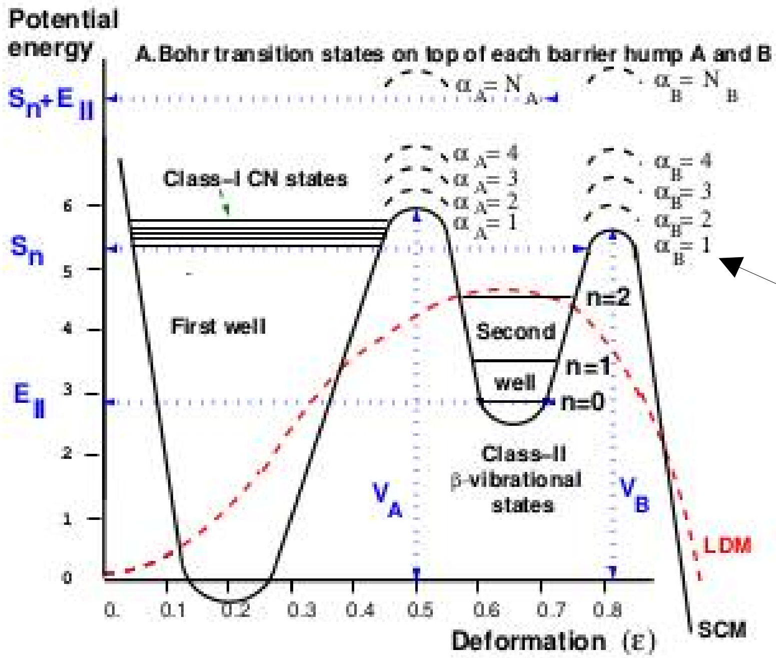
Standard HF + Aage Bohr fission theory

$$\sigma_{n,f}(E_n) = \sum_{J^\pi} \{ \sigma_n^{CN}(E_n, J^\pi) [\sum_{\alpha_B \in J^\pi} B_f^{\alpha_B}(E_x) W_{II}^{\alpha_B}(E_x)] W_{n,f}^{J^\pi}(E_x) \}$$

Class-II width fluctuation correction

Impact the calculation of <σ(n,f)> for Pu

Standard HF theory : fission exit channel



Total width for class- II states :

$$\Gamma_{\lambda II\, tot} \approx \Gamma_{\lambda II\downarrow} + \Gamma_{\lambda II\uparrow} + \Gamma_{\lambda II\,\gamma}$$

$$\sigma_{n,f}(E_n) = \sum_{J^\pi} \{ \sigma_n^{CN}(E_n, J^\pi) [\sum_{\alpha_B \in J^\pi} B_f^{\alpha_B}(E_x) W_{II}^{\alpha_B}(E_x)] W_{n,f}^{J^\pi}(E_x) \}$$

Fission BR for a specific outer barrier transition state

$$B_f^{\alpha_B} = T_f(\alpha_B) / T_{total}$$

Depending on the E* the average formulation of B changes :

At low E* the discrete structure of class-II states impact the fission transmission coefficient T_f =>

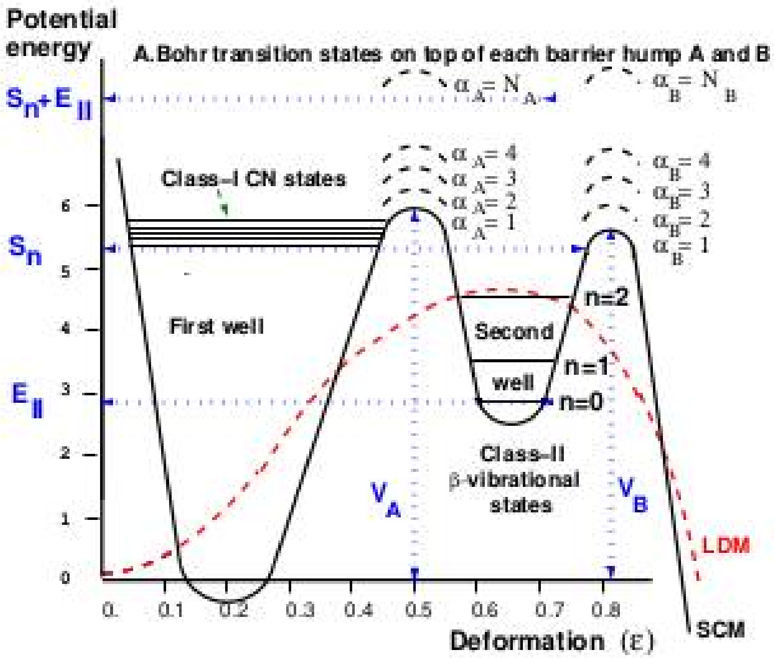
$$B_f^{\alpha_B} = f\left(\frac{T_I}{T_f}\right)$$

T_I : Damping transmission coefficient in the first well = sum of particle and gamma emission transmission coefficients

Impact the calculation of <σ(n,f)> for Pu

Monte Carlo

Monte Carlo form of HF equations



$$\sigma_{n,f}(E_n)=\sum_{J^\pi}\{\sigma_n^{CN}(E_n,J^\pi)[\sum_{\alpha_B\in J^\pi}B_f^{\alpha_B}(E_x)W_{II}^{\alpha_B}(E_x)]W_{n,f}^{J^\pi}(E_x)\}$$

a) Analytical solution

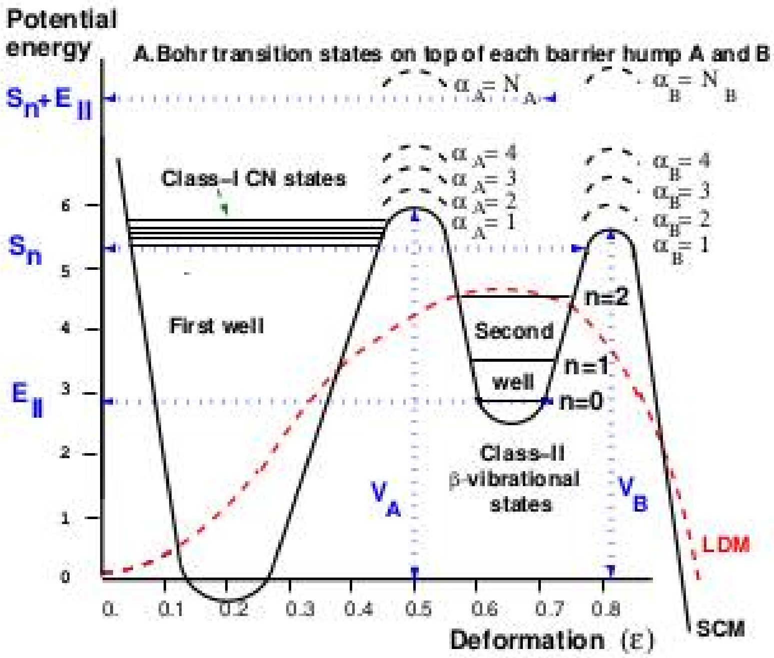
no correlation between statistical class I and II state width fluctuations and the shape of the barrier

a) Monte Carlo algorithm

Calculate average observables accounting for statistical nuclear data fluctuations under the relevant IS

Impact the calculation of <σ(n,f)> for Pu

Monte Carlo route



$$\sigma_{n,f}(E_n)=\sum_{J^\pi}\{\sigma_n^{CN}(E_n,J^\pi)[\sum_{\alpha_B\in J^\pi} B_f^{\alpha_B}(E_x)W_{II}^{\alpha_B}(E_x)]W_{n,f}^{J^\pi}(E_x)\}$$

1) R-matrix average parameters for each (En,CN, residue) are calculated using :

- HF **transmission coefficients**
- mean **level spacing**

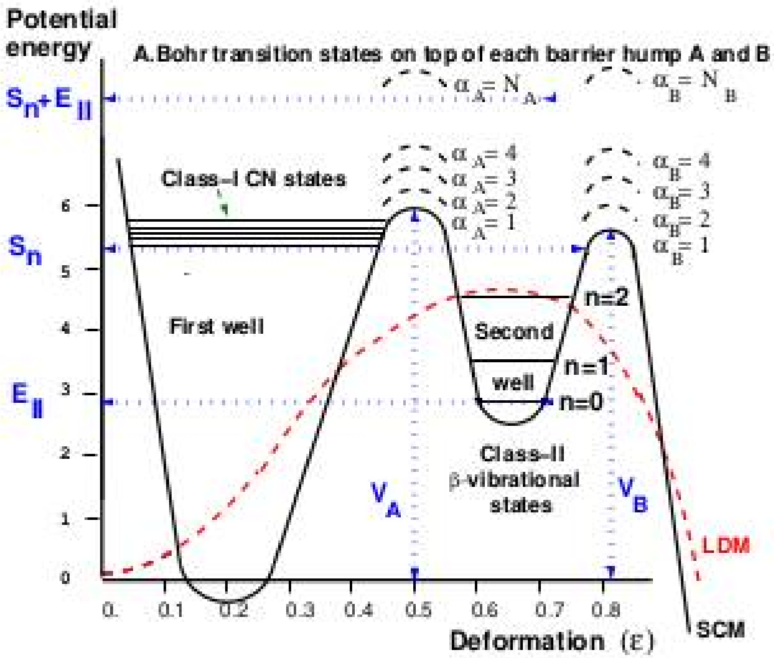
$\Rightarrow \langle \Gamma_{\lambda II(\downarrow)} \rangle$

$\langle \Gamma_{\lambda II(\downarrow)} \rangle$ used to evaluate the average of the squared coupling matrix elements

$$\langle\langle \lambda_{II}|H_c|\lambda_I\rangle^2\rangle=\Gamma_{\lambda II(\downarrow)}\frac{D_I}{2\pi}$$

They describe the **coupling** across the inner barrier **of each** class-II state, λ_{II}, to its neighboring class-I levels, $\lambda_{I\,i}$

Monte Carlo route



$$\sigma_{n,f}(E_n)=\sum_{J^\pi}\{\sigma_n^{CN}(E_n,J^\pi)[\sum_{\alpha_B\in J^\pi}B_f^{\alpha_B}(E_x)W_{II}^{\alpha_B}(E_x)]W_{n,f}^{J^\pi}(E_x)\}$$

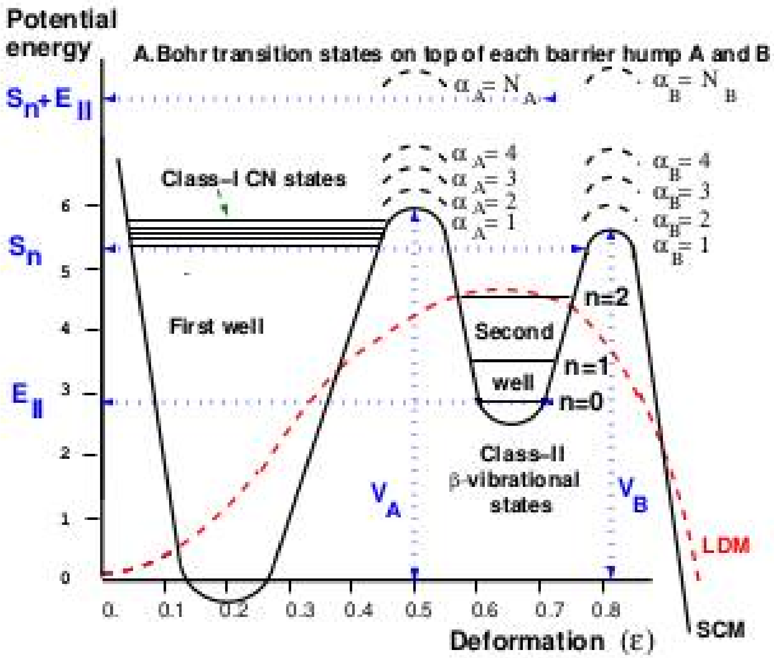
1) $\langle\langle\lambda_{II}|H_c|\lambda_I\rangle^2\rangle=\Gamma_{\lambda II(\downarrow)}\frac{D_I}{2\pi}$

2) **class-I state energies** are generated from a Wigner distribution corrected for long-range correlations using $D_{\lambda I}$

$D_{\lambda I}$ calculated using either Gilbert and Cameron's law, or the **QPVR level density model**

Impact the calculation of <σ(n,f)> for Pu

Monte Carlo route



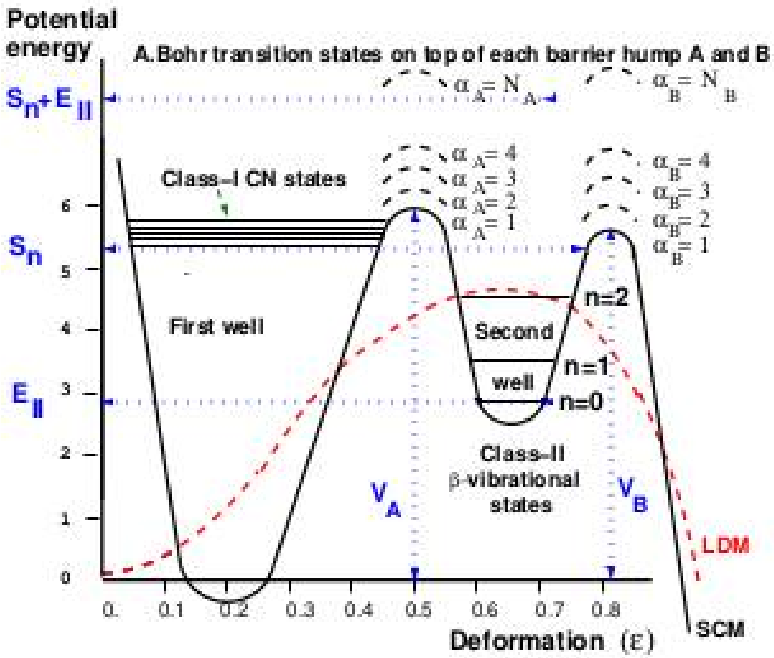
$$\sigma_{n,f}(E_n)=\sum_{J^\pi}\{\sigma_n^{CN}(E_n,J^\pi)[\sum_{\alpha_B\in J^\pi} B_f^{\alpha_B}(E_x)\,W_{II}^{\alpha_B}(E_x)]\,W_{n,f}^{J^\pi}(E_x)\}$$

1) $\langle\langle\lambda_{II}|H_c|\lambda_I\rangle^2\rangle=\Gamma_{\lambda II(\downarrow)}\dfrac{D_I}{2\pi}$

2) **class-I state energies** are generated using $D_{\lambda I}$ from the **QPVR level density model**

3) **class-II state energies** are generated using $D_{\lambda II}$ diagonalizing a 5x5 diagonal matrix, whose diagonal and non-diagonal elements follow a Poissonian and a Gaussian distribution, respectively

Monte Carlo route



$$\sigma_{n,f}(E_n)=\sum_{J^\pi}\{\sigma_n^{CN}(E_n,J^\pi)[\sum_{\alpha_B\in J^\pi} B_f^{\alpha_B}(E_x)\,W_{II}^{\alpha_B}(E_x)]\,W_{n,f}^{J^\pi}(E_x)\}$$

1) $\langle\langle\lambda_{II}|H_c|\lambda_I\rangle^2\rangle=\Gamma_{\lambda II(\downarrow)}\frac{D_I}{2\pi}$

2) **class-I state energies** are generated using $D_{\lambda I}$ from the **QPVR level density model**

3) **class-II state energies** are generated using $D_{\lambda II}$

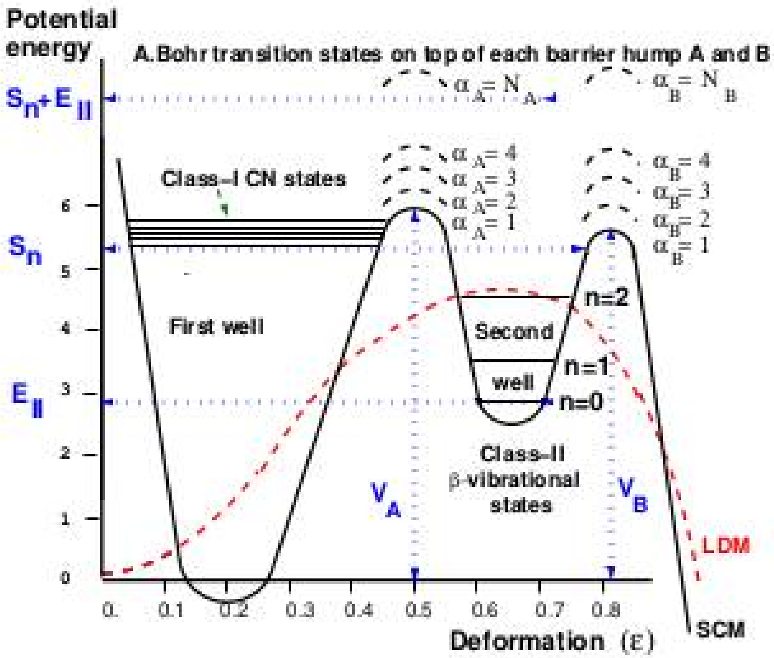
4) class-I n emission $\Gamma_{\lambda I n}+\Gamma_{\lambda I n'}$
class-II coupling $\Gamma_{\lambda II\downarrow}$
class-II fission $\Gamma_{\lambda II\uparrow}$
individual $\langle\lambda_{II}|H_c|\lambda_I\rangle$

width amplitudes

sampled from a gaussian distribution around their mean value $\bar{p}$ and $\sigma=\sqrt{2\bar{p}}$

$\Gamma_{\lambda I\gamma},\Gamma_{\lambda II\gamma}$. Do not fluctuate => average value for each studied E*

Monte Carlo route



$$\sigma_{n,f}(E_n)=\sum_{J^\pi}\{\sigma_n^{CN}(E_n,J^\pi)[\sum_{\alpha_B\in J^\pi}B_f^{\alpha_B}(E_x)W_{II}^{\alpha_B}(E_x)]W_{n,f}^{J^\pi}(E_x)\}$$

1) $\langle\langle\lambda_{II}|H_c|\lambda_I\rangle^2\rangle=\Gamma_{\lambda II(\downarrow)}\frac{D_I}{2\pi}$

2) **class-I state energies** are generated using $D_{\lambda I}$ from the **QPVR level density model**

3) **class-II state energies** are generated using $D_{\lambda II}$

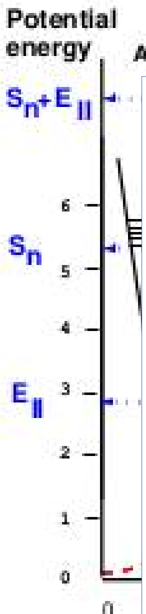
4) $\Gamma_{\lambda I n}+\Gamma_{\lambda I n'},\Gamma_{\lambda II\downarrow},\Gamma_{\lambda II\uparrow},\langle\lambda_{II}|H_c|\lambda_I\rangle$ **sampled** from gaussian, $\Gamma_{\lambda I\gamma},\Gamma_{\lambda II\gamma}$ average value for each E*

5) get the **median energy of class-II states** sampled energy → λ_{II}^{median}

$\Gamma_{\lambda II\,tot}^{median}$ compared to class-I state mean level spacing $D_{\lambda I}$

Class-II state that mainly contribute to the fission width of the corresponding final R-matrix eigenstates

Monte Carlo route



$\Gamma^{median}_{\lambda II\ tot} < 4\, D_{\lambda I}$. **Narrow class-II state hypothesis** : exact calculation of class-I and class-II admixture coefficients in the final R-matrix eigenstates performed

$\Gamma^{median}_{\lambda II\ tot} \geq 4\, D_{\lambda I}$. **Broad « median » class-II state** : its major contribution to the R-matrix eigenstates is computed from the calculated average class-I and class-II parameters and from the class-II coupling width. Second-order contribution is calculated assuming a Lorentzian pattern into the final R-matrix eigenstates

$)]W^{J^\pi}_{n,f}(E_x)\}$

$D_{\lambda I}$ from the

$D_{\lambda II}$

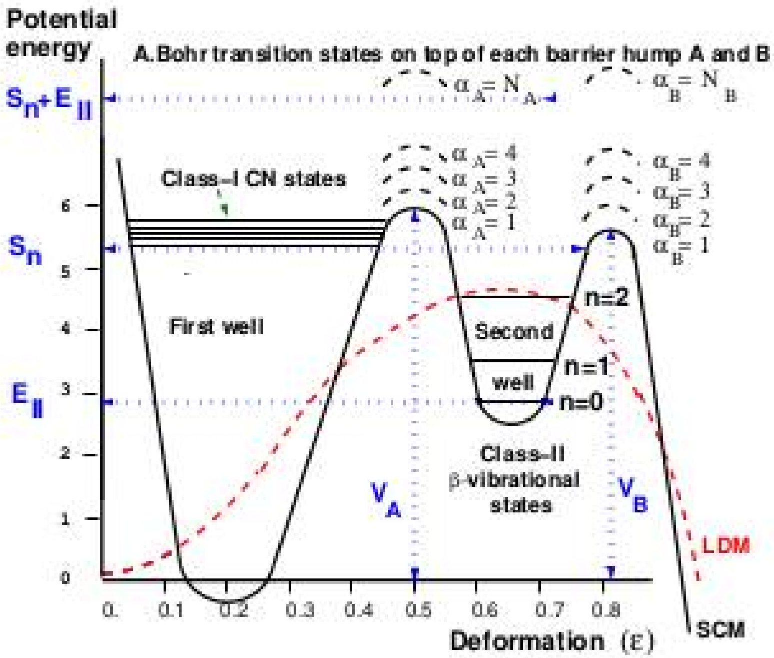
4) $\Gamma_{\lambda II}$ … r each E*

5) get the **median energy of class-II states** sampled energy → λ^{median}_{II}

$\Gamma^{median}_{\lambda II\ tot}$. compared to class-I state mean level spacing $D_{\lambda I}$

Class-II state that mainly contribute to the fission width of the corresponding final R-matrix eigenstates

Monte Carlo route



$$\sigma_{n,f}(E_n)=\sum_{J^\pi}\{\sigma_n^{CN}(E_n,J^\pi)[\sum_{\alpha_B\in J^\pi}B_f^{\alpha_B}(E_x)W_{II}^{\alpha_B}(E_x)]W_{n,f}^{J^\pi}(E_x)\}$$

1) $\langle\langle\lambda_{II}|H_c|\lambda_I\rangle^2\rangle=\Gamma_{\lambda II(\downarrow)}\frac{D_I}{2\pi}$

2) **class-I state energies** are generated using $D_{\lambda I}$ from the **QPVR level density model**

3) **class-II state energies** are generated using $D_{\lambda II}$

4) $\Gamma_{\lambda I n}+\Gamma_{\lambda I n'},\Gamma_{\lambda II\downarrow},\Gamma_{\lambda II\uparrow},\langle\lambda_{II}|H_c|\lambda_I\rangle$ **sampled** from gaussian, $\Gamma_{\lambda I\gamma},\Gamma_{\lambda II\gamma}$ average value for each E*

5) calculation of **class-I and II admixture coefficients** and final R-matrix **eigenstates widths and energies**

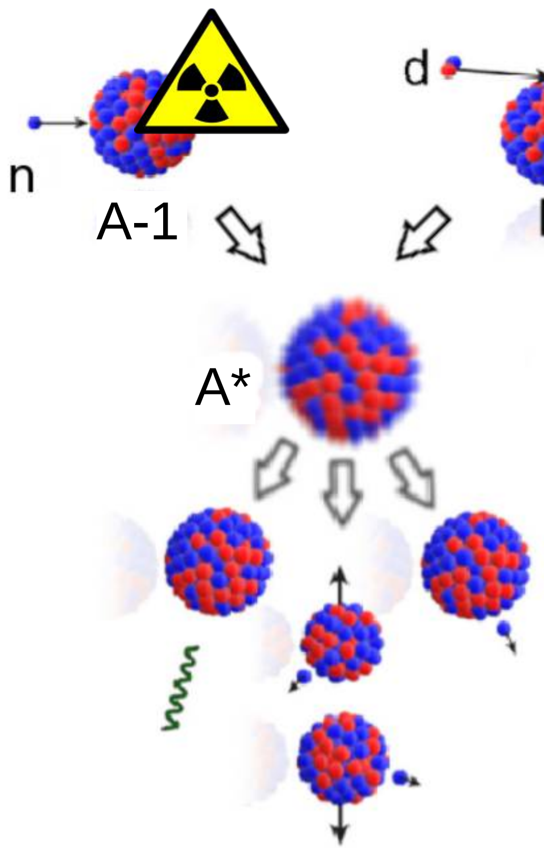
6) partial **n-induced σ are calculated** within the Single-Level Breit-Wigner approximation

Theory improvements :

surrogate reaction P

Modeling of surrogate reaction P

n-induced reaction surrogate reaction



$$\overline{\sigma_{n,c'}}(E_n)=\sigma^{CN}(E_n)*\sum_{J^\pi}[\boldsymbol{J^\pi}\,populated\,distrib\,(E_n)_{n-ind}*BR_{c'}^{J^\pi}(E_n)]$$

Deexcitation probability

$$P_{surr,c'}^{A}(E_x)=\sum_{J^\pi}[J^\pi\,populated\,distrib\,(E_x)_{surr}*BR_{c'}^{J^\pi}(E_x)]$$

Modeling of P_f in β-vibrational resonance region

Medium and giant-size resonances observed in σ(n,f) → double-hamped B_f as a function of elongation

The Hamiltonian :

$$H = H_\beta + H_{int}(\zeta;\ \beta_0) + Hc(\beta,\zeta;\ \beta_0)$$

- H_β → governing the collective elongation mode β
- $H_{int}(\zeta;\ \beta_0)$ → governing all other collective modes other than β, single-particle excitations, rotational motion
- $Hc(\beta,\zeta;\ \beta_0)$ → governing the interaction between β mode and the intrinsic excitations ζ

In the R-matrix formalism class-II states are :

$$X_{\lambda_{II}}^{(II)} = \sum_{\mu,\nu} C_{\mu\nu}^{\lambda_{II}} \chi_\mu \Phi_{\nu(\mu)}^{(II)}$$

- $\Phi_{\nu(\mu)}^{(II)}$ → Vibrational wave function
- χ_μ → intrinsic wave function

Modeling of P_f in β-vibrational resonance region

In the R-matrix formalism class-II states are :

$$X^{(II)}_{\lambda_{II}} = \sum_{\mu,\nu} C^{\lambda_{II}}_{\mu\nu} \chi_\mu \Phi^{(II)}_{\nu(\mu)}$$

Vibrational wave function

intrinsic wave function

Purely vibrational state

$$X^{(II)}_{\lambda_{II}} \approx \chi_0 \Phi^{(II)}_{\nu(0)}$$

Eigenfunctions of H_{int} for the lowest intrinsic state at saddle

Verified only if the energy of this state is very close to the second well gs energy

Input parameter database

The set of used parameters allows us to correctly reproduce the experimental $\sigma(n,f)$ and $\sigma(n,\gamma)$ for ^{236}Pu to ^{244}Pu, for E_n=few keV up to 5.5MeV

+

CS Jp distribution for chosen surrogate reaction

(V_A,V_B) and ($h\omega_A$, $h\omega_B$) are → spin independent for e-e nuclei
→ the spin dependence is estimated fitting $\sigma(n,f)$ data for E_n>100keV

Low-lyng class-I states : taken from ENSDF and expanded with additional levels to complete the rotational bands predicted by QPVR model up to ~1.1MeV E*

At higher energies : QPVR model

First simultaneous evaluation of fission probabilities and neutron-induced cross sections for the Pu fissile isotopes

O. Bouland, P. Marini

CEA, DEN, DER, SPRC, Physics Studies Laboratory, Cadarache, F-13108 Saint-Paul-lez-Durance

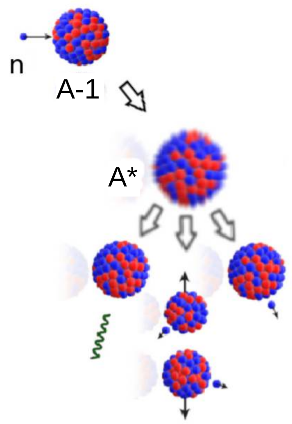
GANIL, CEA/DRF-CNRS/IN2P3, B.P. 55027, 14076 Caen Cedex 5

In memory of Olivier

Hello everyone
First of all I wish to thank the organizers for allowing me to present you this work. This is a special talk as it's the last work of Olivier Bouland before his death and it's the last work we did together. He didn't have the chance to see this work published.
I'll do my best to present you his work but I'm neither a theoretician nor an evaluator so, every improvement that it's brought from this work is thanks to Olivier, every mistake that I might make in this presentation is my own responsibility.
Despite the challenge, for me, to present you this work, I want to do it in memory of Olivier

A unique and coherent description : why ?

n-induced reaction

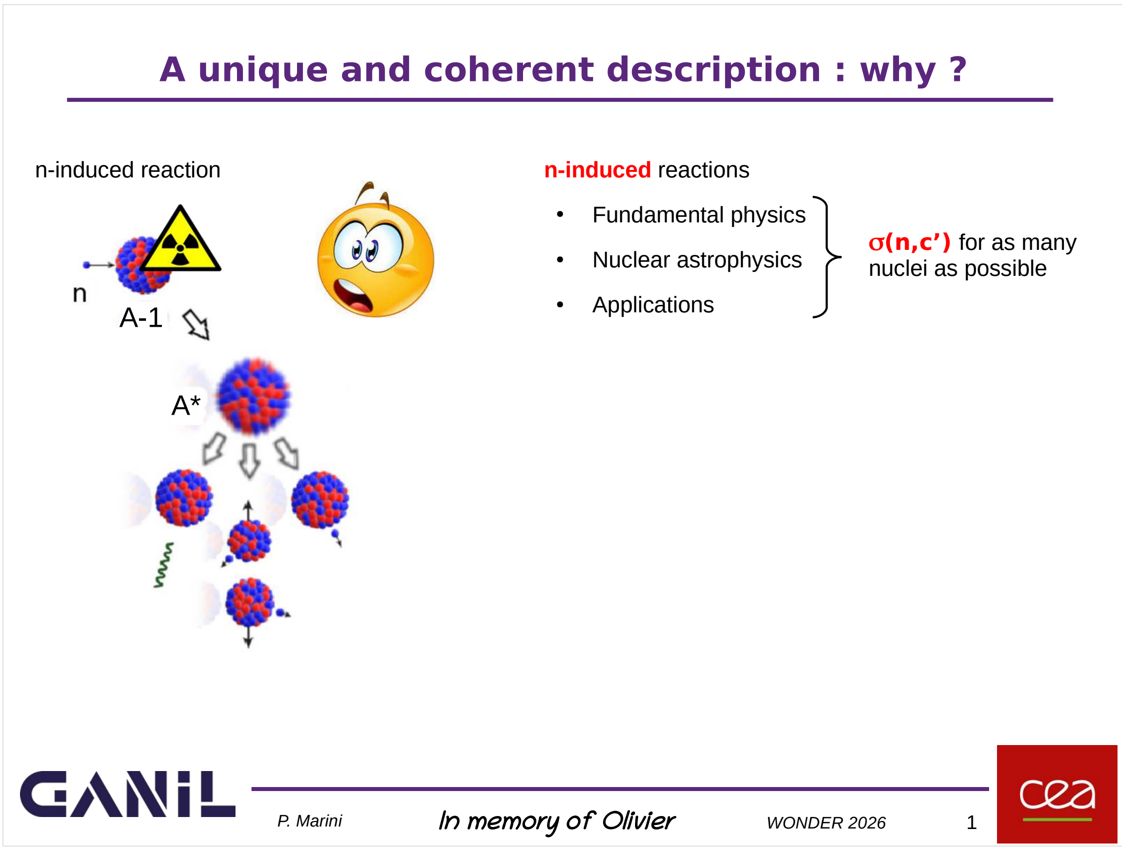


n-induced reactions

- Fundamental physics
- Nuclear astrophysics
- Applications

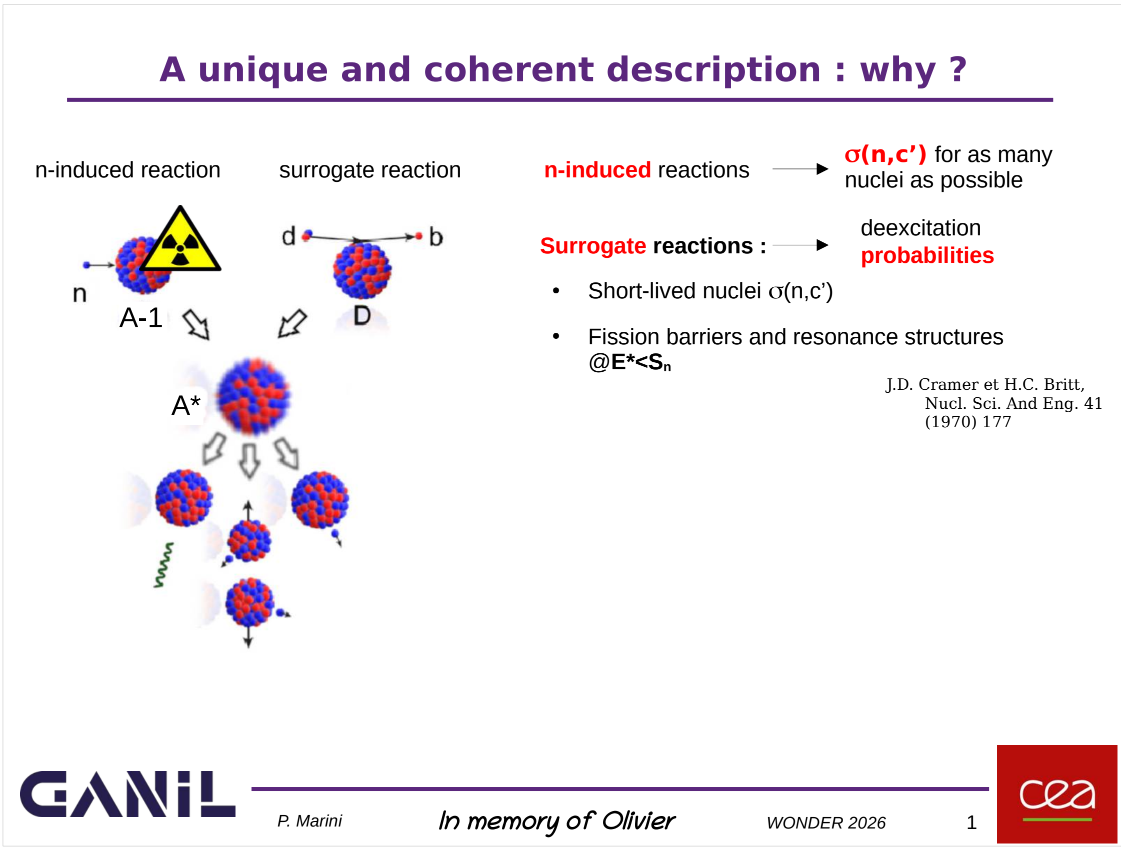
} **σ(n,c')** for as many nuclei as possible

X sections of n-induced reactions, for as many nuclei as possible, and especially for heavy targets, are highly needed in ….



X sections of n-induced reactions, for as many nuclei as possible, and especially for heavy targets, are highly needed in ….

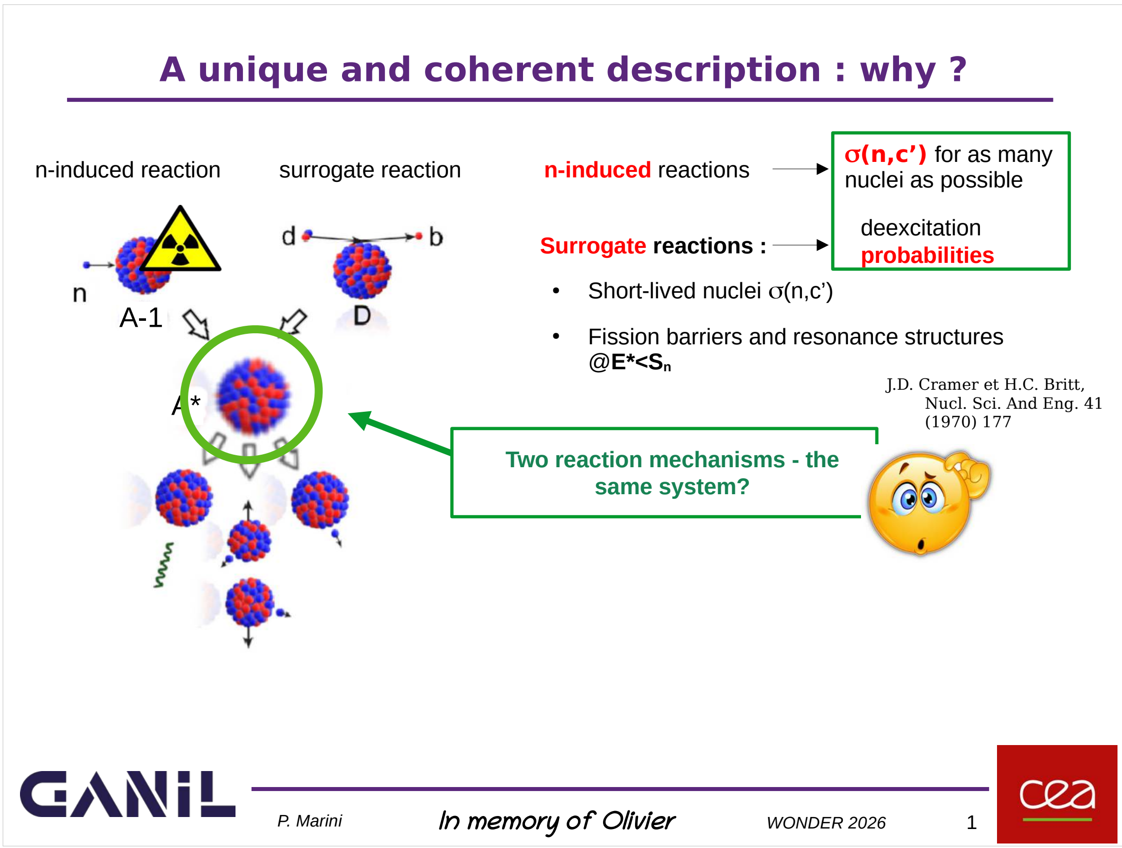
What happens is the target of interest is highly radioactive and can't be handled or its lifetime is too short for make a target out of it



X sections of n-induced reactions, for as many nuclei as possible, and especially for heavy targets, are highly needed in ….

What happens is the target of interest is highly radioactive and can't be handled or its lifetime is too short for make a target out of it

In the 70s Cramer and Britt proposed the surrogate reaction technique, which consists in producing via a transfer reaction the same CS as the one produced in n-induced reactions and measure the deexcitation probabilities of the different channels



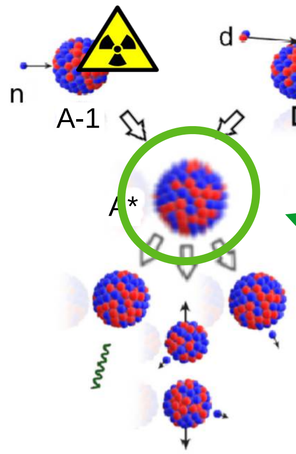
However two fundamental questions open up :
- first we don’t measure the same quantity
- the CS is produced in two different reaction mechanisms

How do we handle data coming from these two different kinds of studies?

The goal of this work was to...

A unique and coherent description : why ?

n-induced reaction surrogate reaction



n-induced reactions → **σ(n,c')** for as many nuclei as possible

Surrogate reactions : → deexcitation **probabilities**

- Short-lived nuclei σ(n,c')
- Fission barriers and resonance structures **@E*<S_n**

J.D. Cramer et H.C. Britt, Nucl. Sci. And Eng. 41 (1970) 177

Two reaction mechanisms - the same system?

Theoretical framework to **simultaneously** describe **both** reactions with a **unique set** of nuclear parameters

AVXSF-LNG code + R-matrix formalism

O. Bouland, PRC 100, 064611 (2019)

A unique and coherent description : how ?

Average CROSS Section Fission – Lynn and Next Generation

O. Bouland, PRC 100, 064611 (2019)
O. Bouland & PM, Nucl. Data Sh. 193, 105 (2024)

Ingredients :

- Hauser Feshback theory

$$\overline{\sigma_{n,c'}}(E_n) = \sigma^{CN}(E_n) * \sum_{J^\pi} [\boldsymbol{J^\pi} \textit{ populated distrib}(E_n) * BR_{c'}^{J^\pi}(E_n)]$$

The code, developped by Olivier and collabs, is based on the general HF theory, where a n-induced X section can be written as the CN X section formation, and a term which include the populated angular omentum distrib of the CS and the Br for the deexcitation in the exit channel

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- Surrogate-reaction probabilities modeling

Improvement

GANIL P. Marini *In memory of Olivier* WONDER 2026 cea

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He then included the modeling surrogate reaction probabilities. What does it mean ?

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An important point is that his code takes into account the different Jp populated distributions in n-induced and surrogate reactions

A unique and coherent description : how ?

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O. Bouland & PM, Nucl. Data Sh. 193, 105 (2024)

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- Surrogate-reaction probabilities modeling ➡ **J$^\pi$** n-induced ≠ **surrogate** reaction
- Exit channel description/competition:
  - transmission coefficients

Improvement

Concerning the description of the exit channels, their competition is described via transmission coefficients

A unique and coherent description : how ?

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O. Bouland, PRC 100, 064611 (2019)
O. Bouland & PM, Nucl. Data Sh. 193, 105 (2024)

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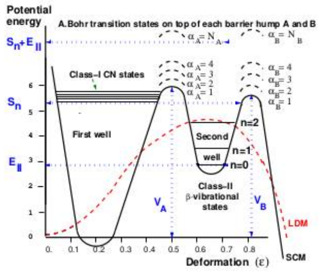
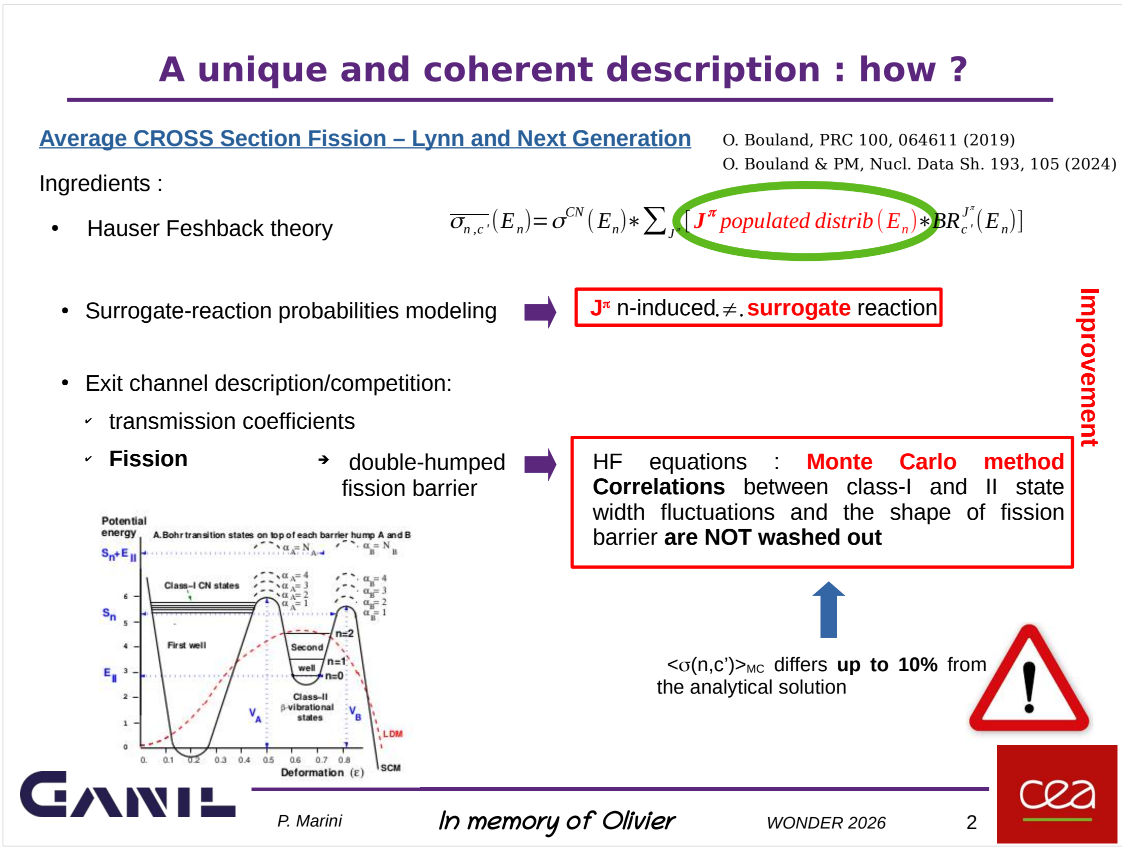
- Surrogate-reaction probabilities modeling ➡ J^π n-induced ≠ **surrogate** reaction
- Exit channel description/competition:
  - transmission coefficients
  - **Fission** → double-humped fission barrier

Improvement



Concerning the description of the exit channels, their competition is described via transmission coefficients

Fission is described including a double-humped fission barrier

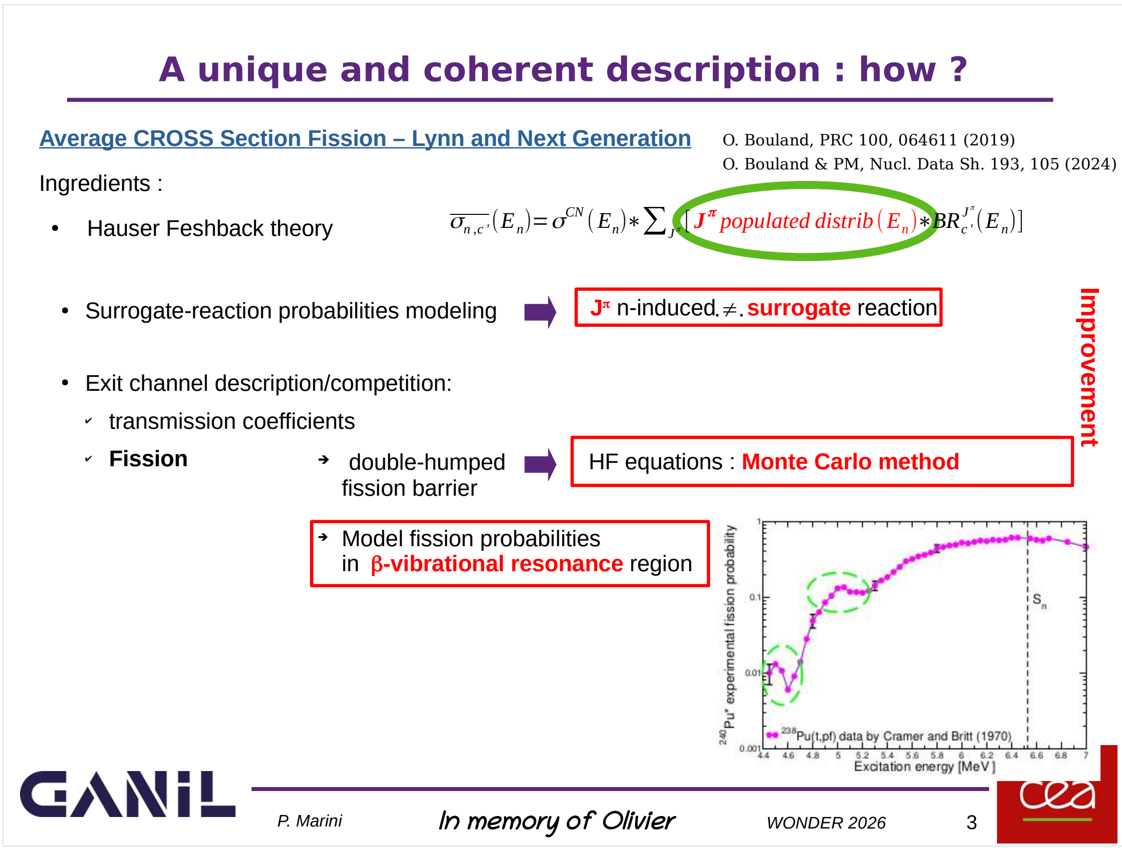


Concerning the description of the exit channels, their competition is described via transmission coefficients

Fission is described including a double-humped fission barrier

And HF equations are solved with a MC method. This is very important because,
- the analytical calculation can differ up to 10 %
- the correlation between the widths of the class-I, class-II states and the shape of the fission barrier is not washed out as in the analytical solution

This is the second main improvement implemented in his code



Moreover, as you might know, intermediate structures may show up in measured fission probabilities. He included the model of this beta-vibrational resonance region, which, we will see, plays a rôle in the calculation of the n-induced reaction X section

A unique and coherent description : how ?

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O. Bouland & PM, Nucl. Data Sh. 193, 105 (2024)

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- Surrogate-reaction probabilities modeling ➡ **J^π** n-induced.≠.**surrogate** reaction

- Exit channel description/competition: ➡ HF equations : **Monte Carlo method** **+** Model the **β-vibrational resonance** region

Improvement

- **Unique input parameters database** for n-induced and surrogate reactions

Last but not least, a unique and cohérent nuclear input parameter database is used to describe both n-induced and surrogate reactions.

A school case : $^{240}Pu^*$

Model applied to the **Pu** **fissile** isotopes [4-8MeV E_n] ⟶ $^{237-244}Pu^*$

GHM

^{239}Pu : key nucleus ⟶ high quality evaluation ⟶ **challenge** for theoretical calculation of surrogate reactions to get a good agreement

$P_f \longrightarrow \sigma(n,f)$

In addition to the improvements that i mentionned in the theory, in this work we applied the code to model n-induced X sections of the the fissile Pu isotopic chain, from 236 to 243Pu.

I'll present you the application of the code to the excited Pu240. Why ? Because it's a key nucleus for the applications and therefore high quality evalutaions and needed and are available. It's therefore a challenge for a theoretical calculation to get a good agreement between probabilities measured in surrogate reactions and n-induced cross sections

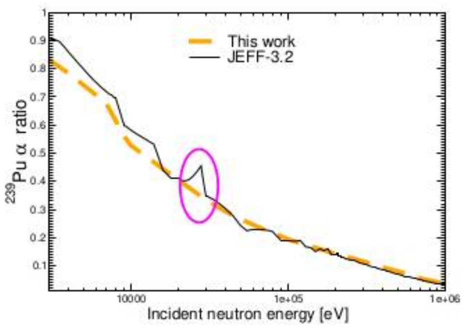
A school case : $^{240}Pu^*$

Model applied to the **Pu fissile** isotopes [4-8MeV E_n] ⟶ $^{237\text{-}244}Pu^*$

^{239}Pu : key nucleus ⟶ high quality evaluation ⟶ **challenge** for theoretical calculation of surrogate reactions to get a good agreement

$P_f \longrightarrow \sigma(n,f)$

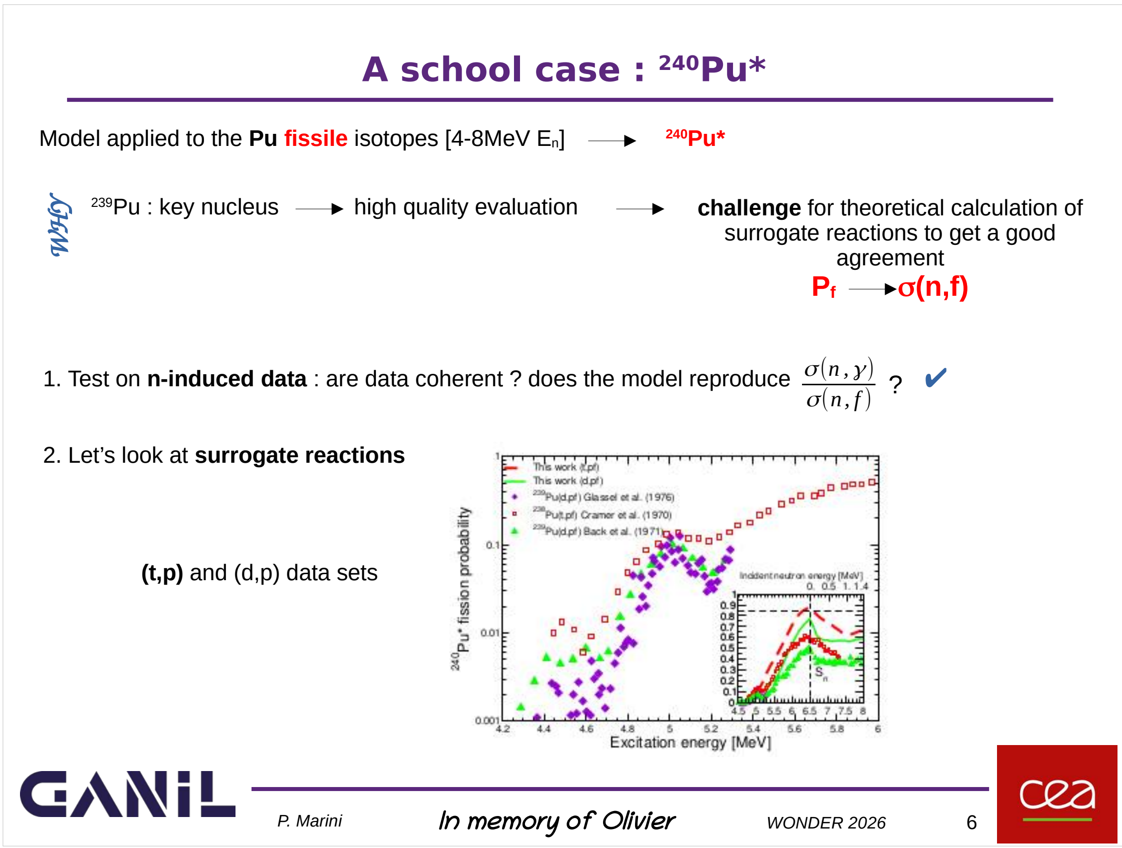
1. Test on **n-induced data** : are data coherent ? does the model reproduce $\frac{\sigma(n,\gamma)}{\sigma(n,f)}$?



$$\overline{\sigma_{n,c'}}(E_n)=\sigma^{CN}(E_n)*\sum_{J^\pi}[J^\pi distrib(E_n)*BR_{c'}^{J^\pi}(E_n)]$$

As a first step we tested the model on n-induced data and in particular on the ratio between gamma and fission X sections. This means that we get rid of the CN formation cross section in the quantity we look at.

The agreement with the JEFF evaluation is rather good, so we are confident that our starting parameters are rather good.



As newt step we look now at surrogate reactions.

Two kind of experimental data sets are available : (t,p) and (d,p) and here you have the measured fission probabilities.

We will concentrate on (t,p) reactions because it has been proved that the deuteron break-up sognificantly affect surrogate reaction technique

A school case : $^{240}Pu^*$

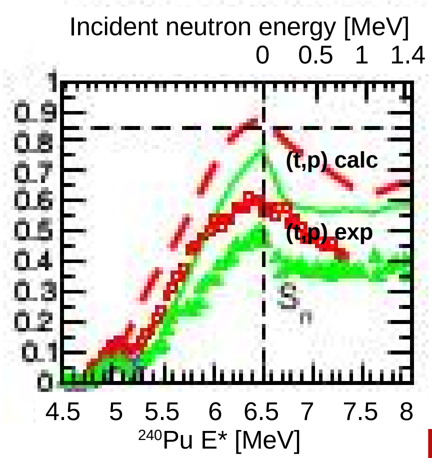
1. Test on **n-induced data** : does the model reproduce $\frac{\sigma(n,\gamma)}{\sigma(n,f)}$? ✔

2. Let's look at **surrogate reactions**

   a. Comparison of experimental and calculated **P_f at S_n**

P_f exp = **0.6±0.06** Cramer et al. (1970)

P_f calc = **0.89±??**



Do we need to renormalize experimental data of 30% ???

Is the model affected by 30% uncertainty ?

The experimental value, red symbols, and the calculated value (red line) at Sn are plotted here and differ of about 30 %

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Most **sensitive input parameters** at S_n+1eV

- ✔ V_A and V_B
- ✔ s-wave n strength function S_0
- ✔ class-I mean spacing D
- ✔ Total γ average width Γ_γ

RIPL-3
S. Bjornholm et al, Rev. Mod. Phys. 52, 725 (1980)

- ✔ Populated CS J^π distribution

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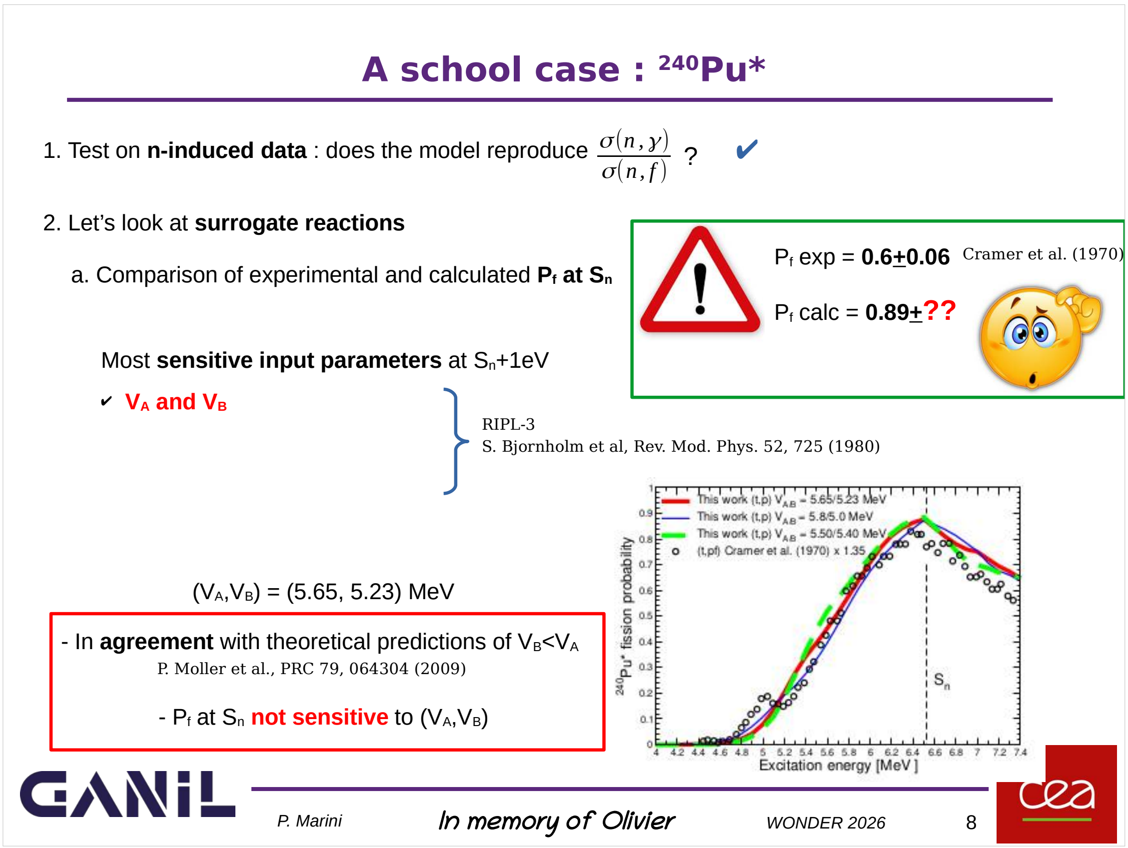

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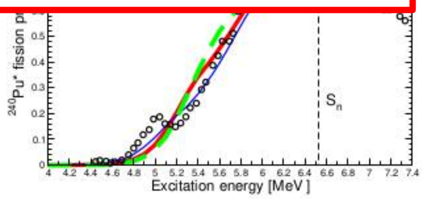
a. Com

et al. (1970)

Mos

✔ V

Fission barrier heights can be confidently extracted from **surrogate reaction data** for fissile isotopes



- In **agreement** with theoretical predictions of $V_B<V_A$
P. Moller et al., PRC 79, 064304 (2009)

- P_f at S_n **not sensitive** to (V_A,V_B)

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RIPL-3
S. Bjornholm et al, Rev. Mod. Phys. 52, 725 (1980)

Direct perturbation within reference uncertainties

Δ_{max}~ 2.1 % between calculations with REF and "our" parameters

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   - ✔ V_A, V_B, S_0, D and Γ_γ → Δ_{max}~ 2.1 %
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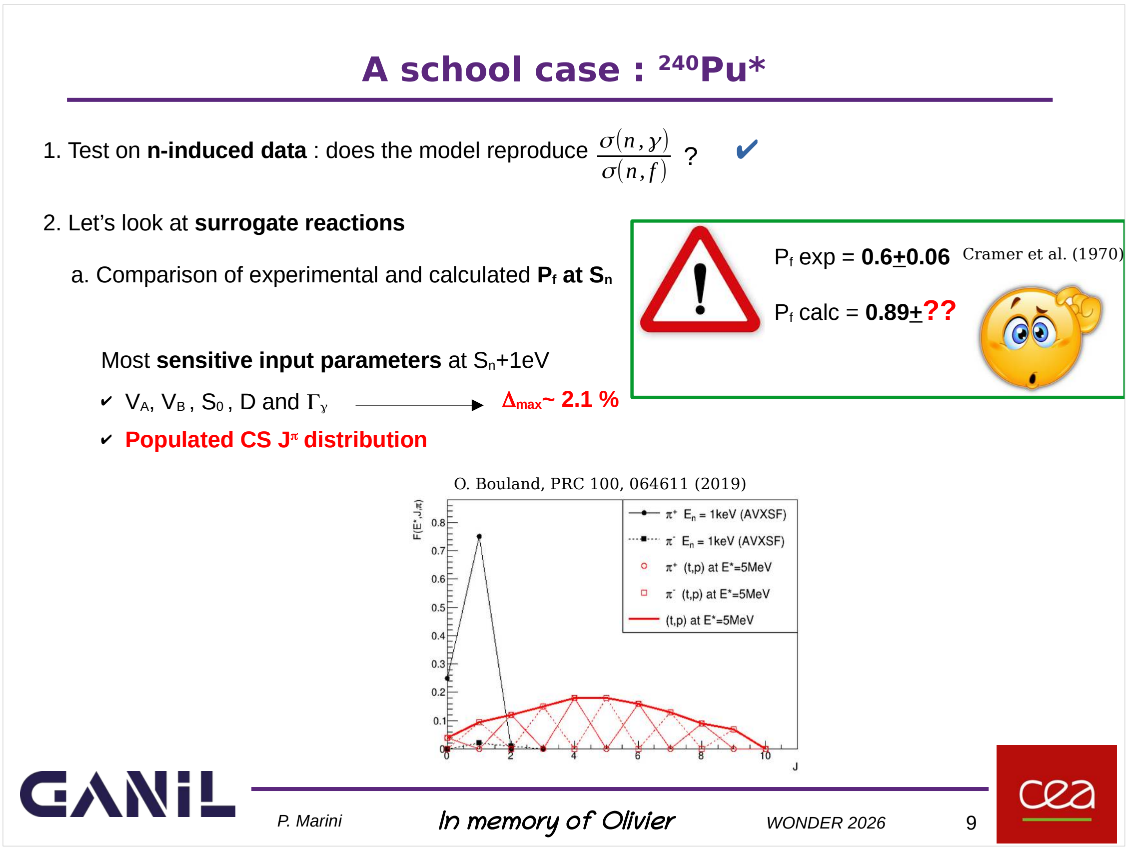

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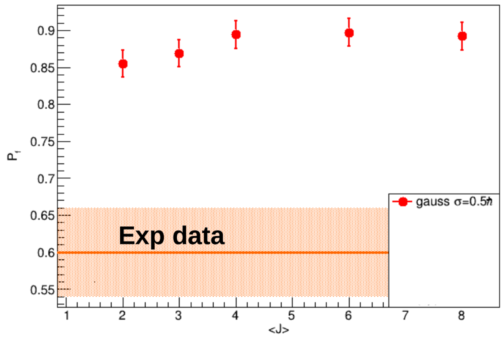
  - **Gaussian**



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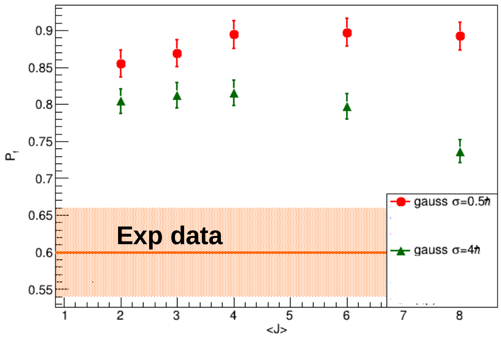

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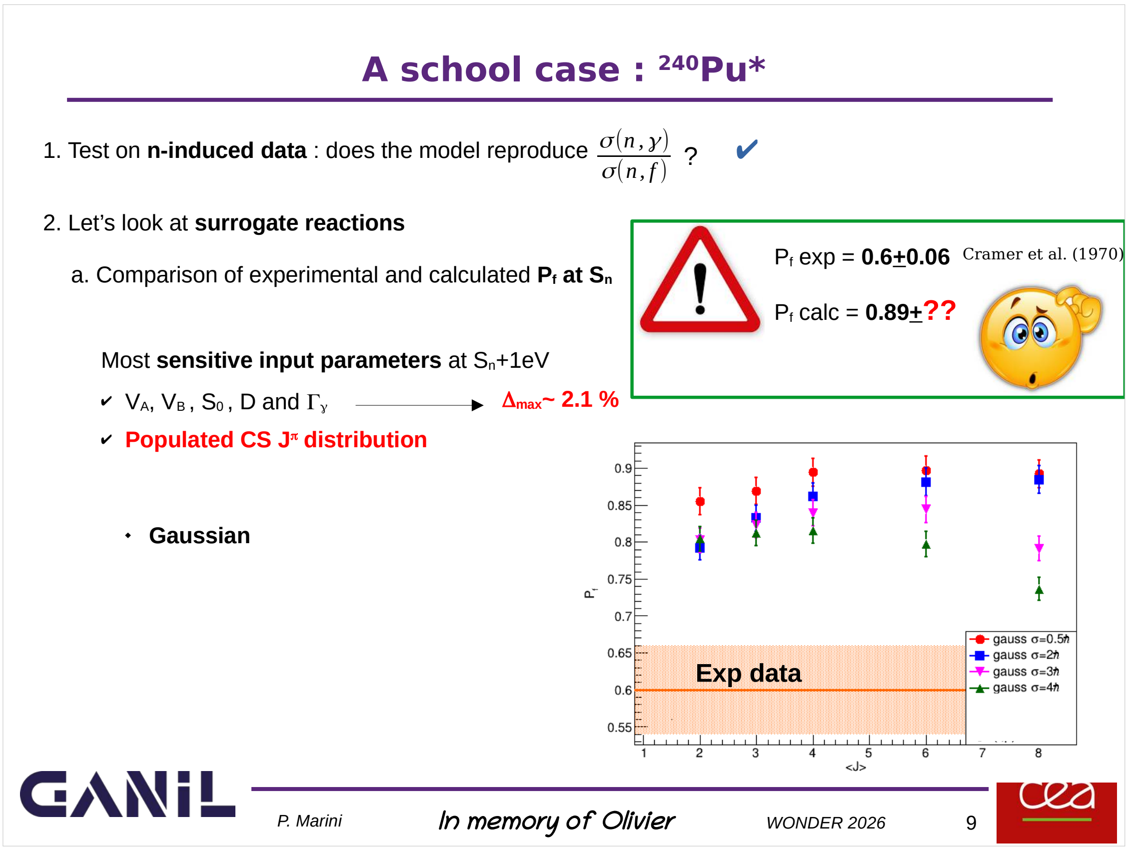

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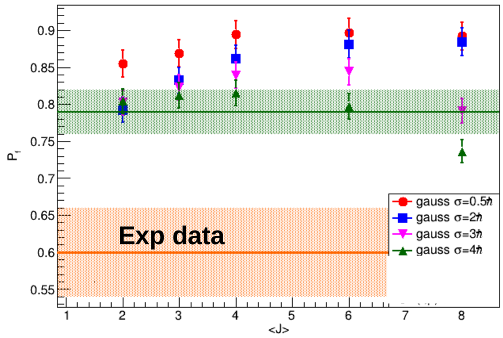
- ✔ **Populated CS J^π distribution**

  - Gaussian
  - **Gaussian but no <J> and σ assumption**



The experimental value, red symbols, and the calculated value (red line) at Sn are plotted here and differ of about 30 %

A school case : ^{240}Pu*

1. Test on **n-induced data** : does the model reproduce $\frac{\sigma(n,\gamma)}{\sigma(n,f)}$? ✔

2. Let's look at **surrogate reactions**

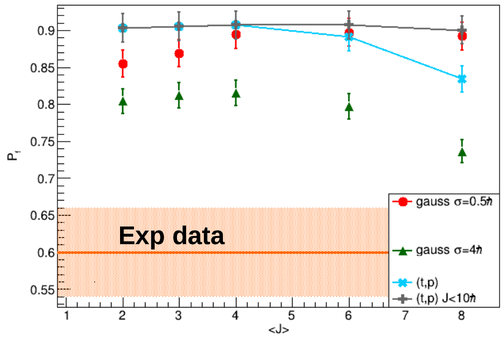
   a. Comparison of experimental and calculated **P_f at S_n**

P_f exp = **0.6±0.06** Cramer et al. (1970)

P_f calc = **0.89±??**

Most **sensitive input parameters** at S_n+1eV

- ✔ V_A, V_B, S_0, D and Γ_γ → Δ_{max}~ 2.1 %
- ✔ **Populated CS J^π distribution**
  - Gaussian
  - from Back et al. (1974) w/ and w/o cuts for J≤10h



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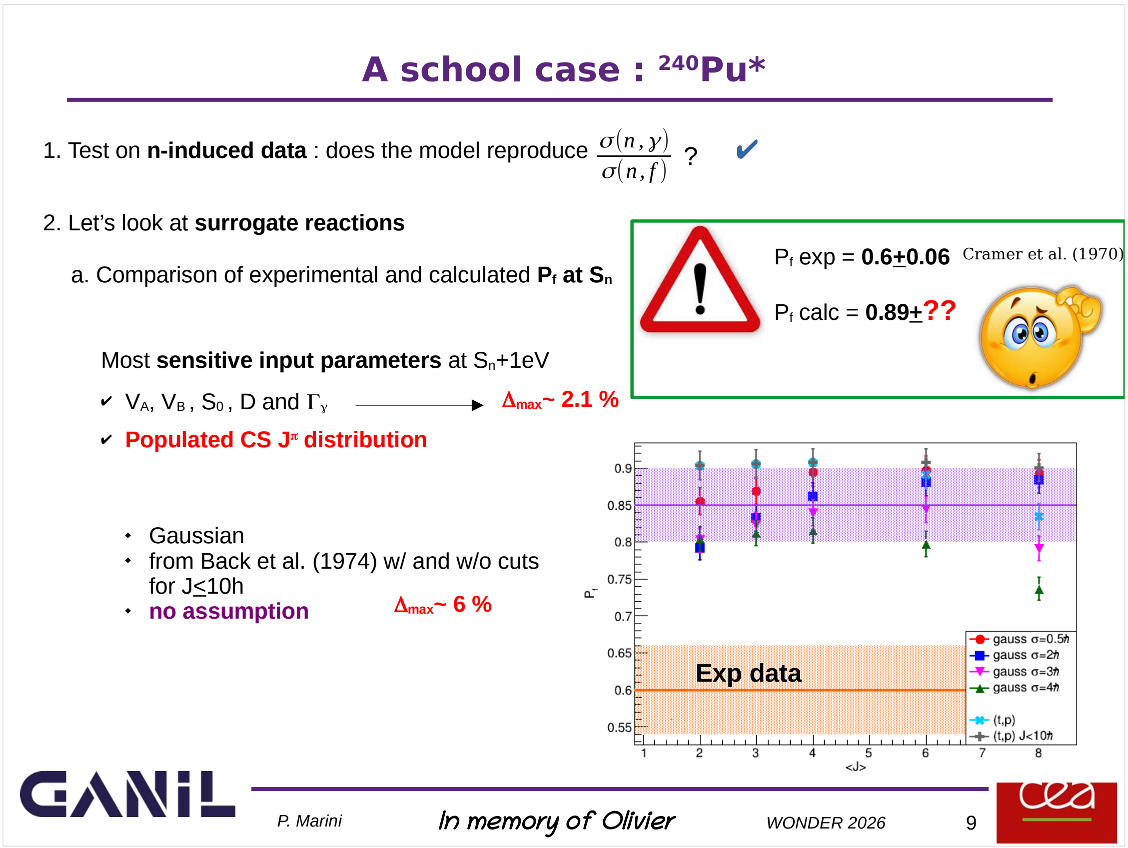

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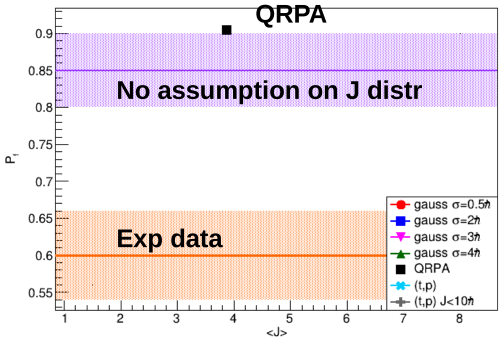
- ✔ V_A, V_B , S_0 , D and Γ_γ → Δ_{max}~ 2.1 %
- ✔ **Populated CS J^π distribution**

  - Gaussian
  - from Back et al. (1974) w/ and w/o cuts for J≤10h
  - no assumption — Δ_{max}~ 6 %

  - **QRPA calculation of J distribution** (<J>=3.9h σ=3.2h)



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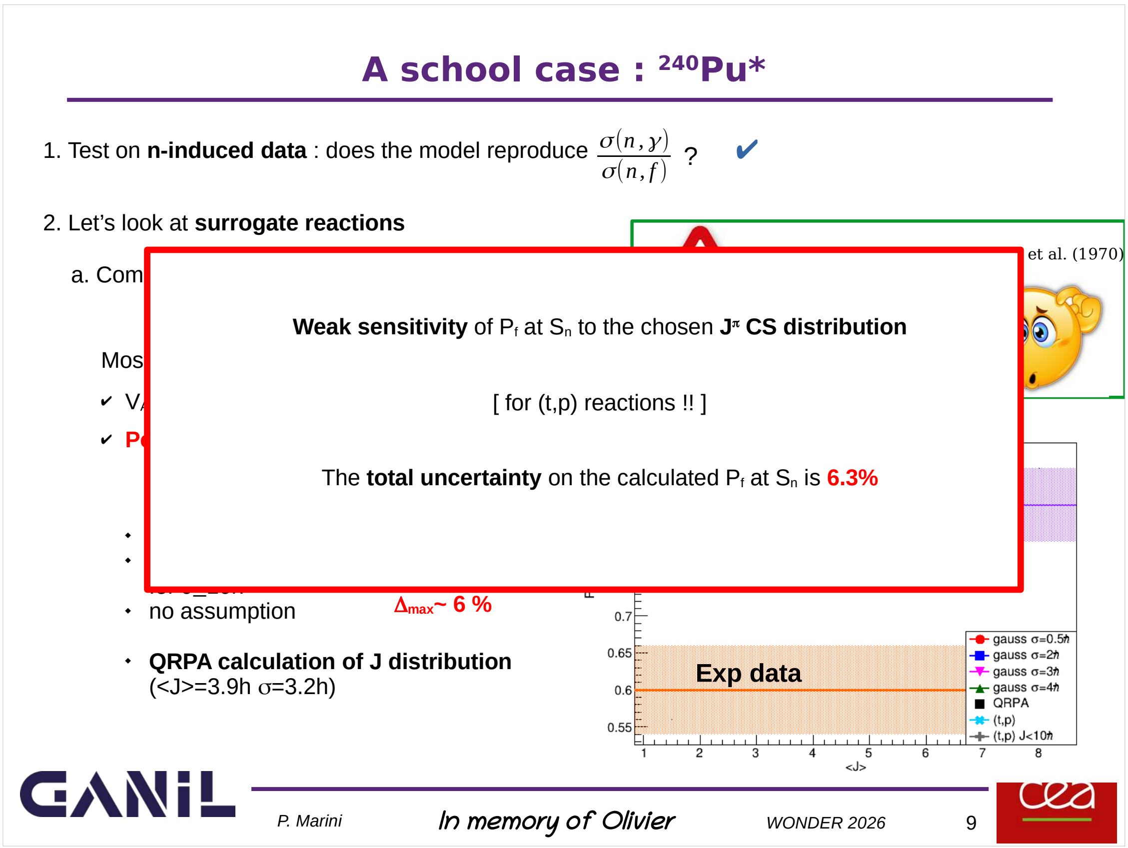

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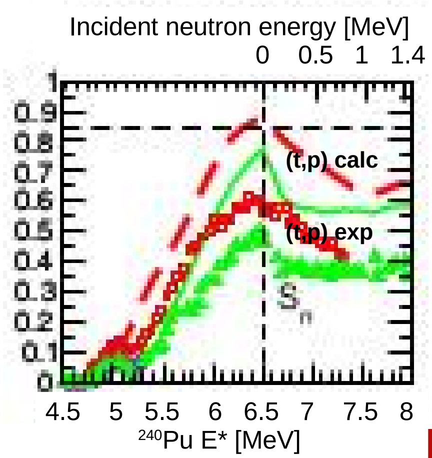
Need for a 30% **renormalization** of exp data



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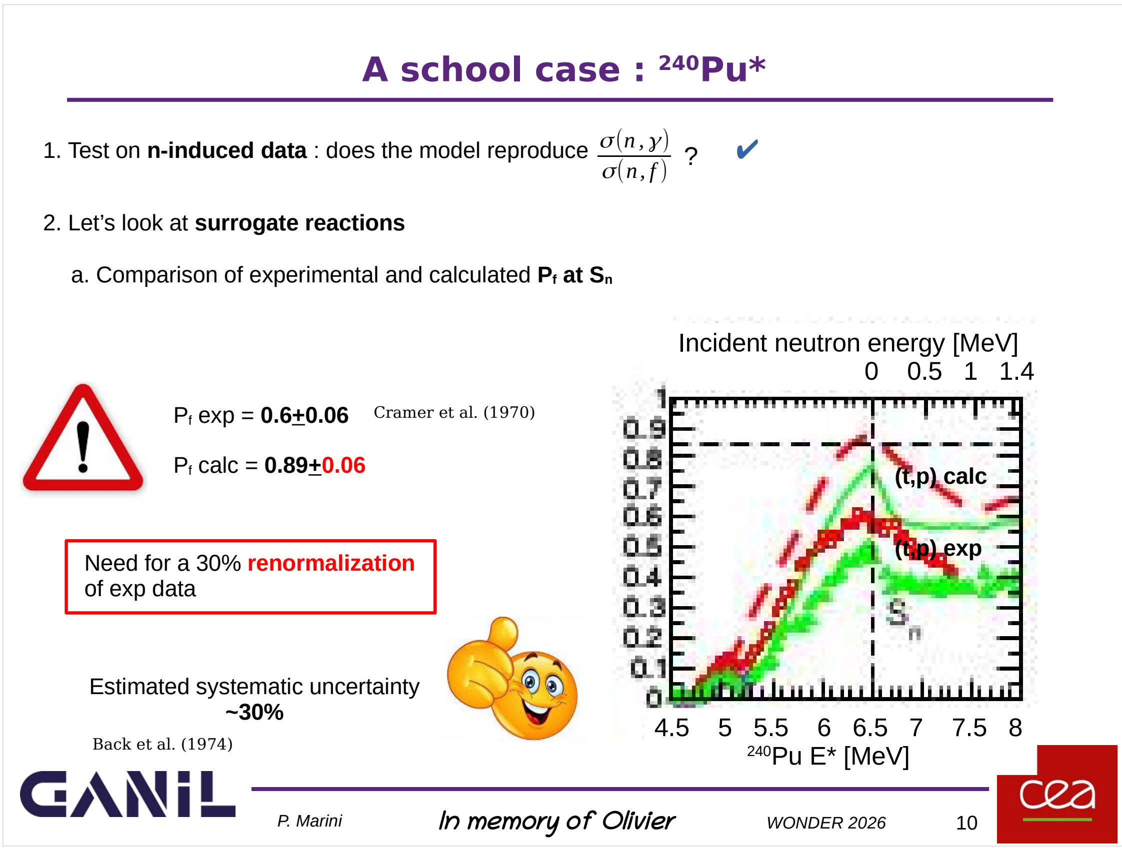


The experimental value, red symbols, and the calculated value (red line) at Sn are plotted here and differ of about 30 %

A school case : $^{240}Pu^*$

1. Test on **n-induced data** : does the model reproduce $\frac{\sigma(n,\gamma)}{\sigma(n,f)}$? ✔

2. Let's look at **surrogate reactions** +++

   a. Comparison of experimental and calculated **P_f at S_n** ➡ Need for a **renormalization** of exp data

   b. **Barrier height** estimates +++

A school case : ^{240}Pu*

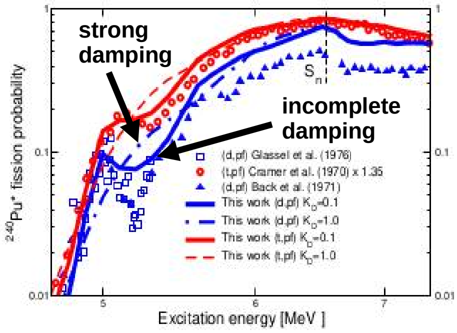
1. Test on **n-induced data** : does the model reproduce $\frac{\sigma(n,\gamma)}{\sigma(n,f)}$? ✔

2. Let's look at **surrogate reactions** **+++**

   a. Comparison of experimental and calculated **P_f at S_n** ➡ Need for a **renormalization** of exp data

   b. **Barrier height** estimates **+++**

   c. **Intermediate resonance** structures ➡ **damping strength** of β-vibrations



Does the damping strength of β-vibrations modify σ_{calc}(n,f)?

A school case : $^{240}Pu^{*}$

1. Test on **n-induced data** : does the model reproduce $\frac{\sigma(n,\gamma)}{\sigma(n,f)}$? ✔

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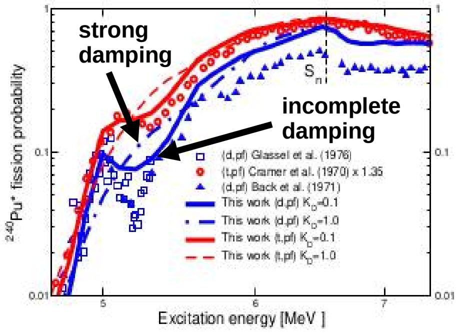
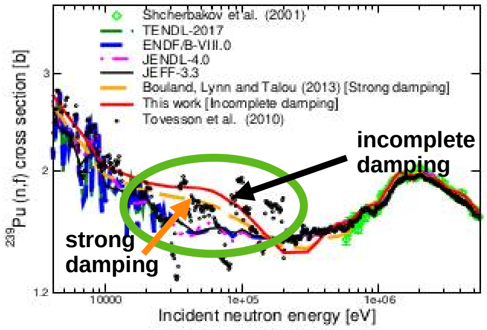




A school case : $^{240}Pu^*$

1. Test on **n-induced data** : does the model reproduce $\frac{\sigma(n,\gamma)}{\sigma(n,f)}$? ✔

2. Let's look at **surrogate reactions** +++

a. Com … exp data

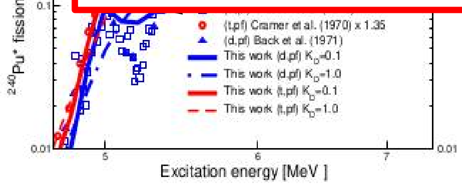
b. **Barr**

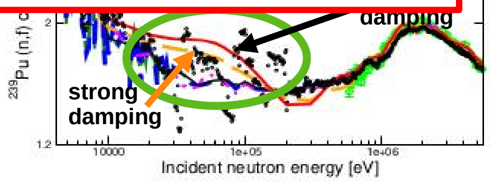
c. **Inter**

The **damping strength of β-vibration** :

- can be extracted from **surrogate** reaction data

- It's **relevant** for the **n-induced σ** calculation





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   a. Comparison of experimental and calculated **P_f at S_n** ➡ Need for a **renormalization** of exp data

   b. **Barrier height** estimates +++

   c. **Intermediate resonance** structures ➡ **damping strength** of β-vibrations +++

   d. Intermediate resonances in **individual J^π P_f** ➡ The small contribution of 1^+ P_f explains the s-wave σ(n,f)

Conclusions and perspectives

GHM

Challenge : high quality evaluations of $\sigma(n,f)$ for heavy nuclei { high target accuracy; **fissile** nuclei

Conclusions and perspectives

WHY

Challenge : high quality evaluations of σ(n,f) for heavy nuclei

- high target accuracy
- **fissile** nuclei

↑

HOW

Use **surrogate reaction** data to refine **nuclear model parameters**

Conclusions and perspectives

WHY **Challenge** : high quality evaluations of σ(n,f) for heavy nuclei { high target accuracy / **fissile** nuclei

↑

Simultaneous and **coherent** analysis of P_f and σ(n,f)

↑

HOW Use **surrogate reaction** data to refine **nuclear model parameters**

Conclusions and perspectives

WHY

Challenge : high quality evaluations of σ(n,f) for heavy nuclei — high target accuracy; **fissile** nuclei

Simultaneous and **coherent** analysis of P_f and σ(n,f)

HOW

Use **surrogate reaction** data to refine **nuclear model parameters**

- ✔ Uncertainty on calculated P_f ~6.3%
- ✔ Estimate fission barrier heights
- ✔ Estimate damping strength of β-vibrations
- ✔ Consistency test of existing surrogate and n-induced reaction data

Conclusions and perspectives

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Challenge : high quality evaluations of σ(n,f) for heavy nuclei { high target accuracy; **fissile** nuclei

Simultaneous and **coherent** analysis of P_f and σ(n,f)

HOW

Use **surrogate reaction** data to refine **nuclear model parameters**

- ✔ Uncertainty on calculated P_f ~6.3%
- ✔ Estimate fission barrier heights
- ✔ Estimate damping strength of β-vibrations
- ✔ Consistency test of existing surrogate and n-induced reaction data

FUTURE

Simultaneous analysis / measurement of **ALL deexcitation channels**

Modeling of and experimental comparison to (n,2n) data

First simultaneous evaluation of fission probabilities and neutron-induced cross sections for the Pu fissile isotopes

Thank you for your attention

In memory of Olivier

237Pu*

238Pu*

242Pu*

244Pu*

Standard HF + fission

Monte Carlo

Theory improvements

Input parameters

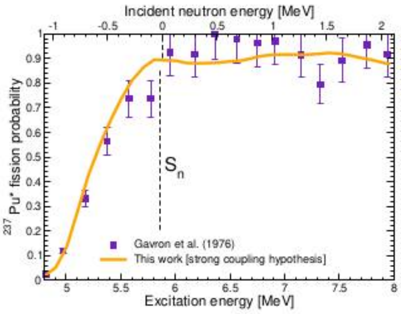
237 Pu*

The fissile Pu isotopic chain : $^{237-244}$Pu*

^{237}Pu*

$t_{1/2}$ (^{236}Pu)= 2.85y very few n-induced σ data Gerasimov et al. (1997) Gromova et al. (1990)

^{237}Np(^{3}He,t) data available Gavron et al. (1976)



- ✔ No evidence of intermediate structures ➡ Strong β-vibration damping
- ✔ (V_A,V_B) = (5.70, 5.10)MeV < S_n ➡ Fissile nucleus
- ✔ Truncated gauss distribution centered around ^{237}Pu(gs) (J=7/2)

Very **good agreement** of exp and calc P_f

The fissile Pu isotopic chain : $^{237-244}Pu^*$

$^{237}Pu^*$

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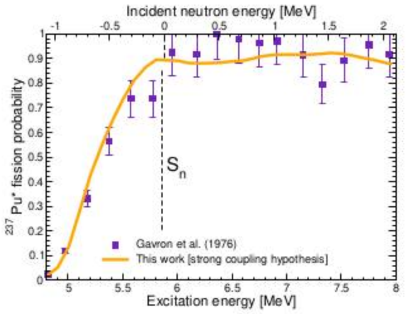

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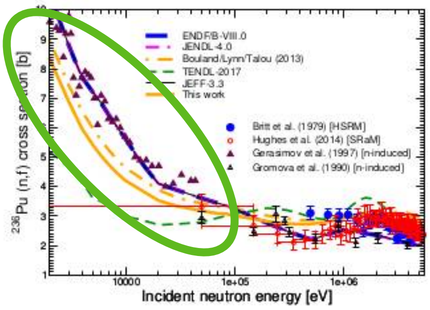


Doubts on Gerosimov's data below 50keV => **on evaluations** [but P_f dependence on J^π of (^{3}He,t) not investigated]

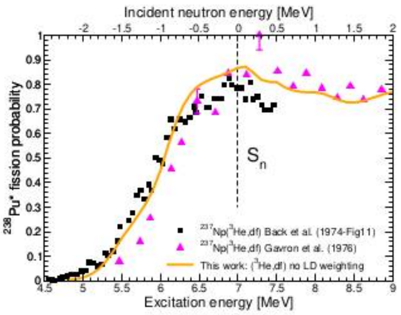
238 Pu*

The fissile Pu isotopic chain : $^{237-244}Pu^*$

$^{238}Pu^*$

$t_{1/2}$ (^{237}Pu)= 45d   no n-induced σ data

^{237}Np(^{3}He,d) data available   Back et al. (1974)
Gavron et al. (1976)



- ✔ No evidence of intermediate structures ➡ Strong b-vibration damping
- ✔ (V_A,V_B) = (5.65, 5.45)MeV < S_n ➡ Fissile nucleus
- ✔ Truncated gauss distribution centered around ^{237}Pu(gs) (J=7/2)

Very **good agreement** of exp and calc P_f

The fissile Pu isotopic chain : $^{237\text{-}244}$Pu*

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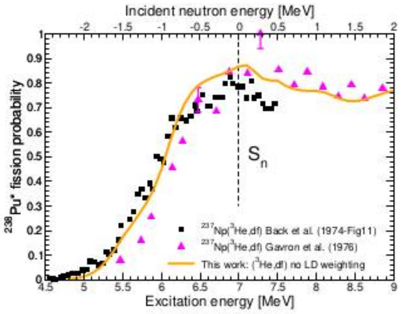
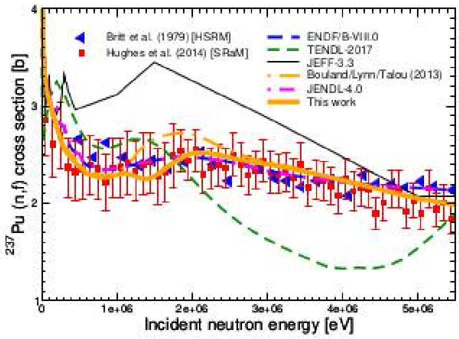




Very **good agreement** of exp and calc P_f **Not in agreement** w/ JEFF 3.3

242 Pu*

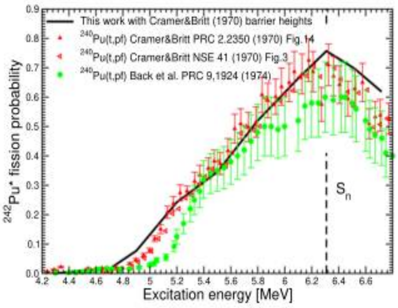
The fissile Pu isotopic chain : $^{237-244}Pu^*$

$^{242}Pu^*$

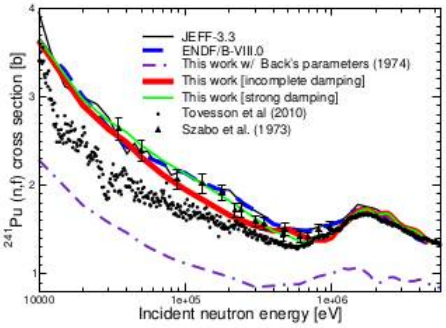
11% of total Pu mass in mixed oxide fuel

n-induced data — Tovesson et al. (2010), Szabo et al. (1973)

$^{240}Pu(t,p)$ data available — Back et al. (1974), Cramer et al (1970)



- ✔ Good agreement at Sn with Cramer at al.
- ✔ Renormalization needed for Back's data
  - ✔ (V_A,V_B) values from Back et al. do not reproduce s(n,f), while values from literature and ours do (5.30,5.30)MeV
- ✔ Doubts on Tovesson's n-induced data
  - ✔
  - ✔ In agreement with evaluations



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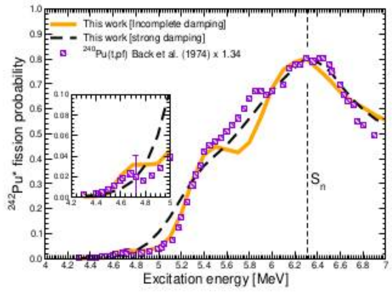

IS at 5.4MeV reproduced with incomplete damping

- ✔ Good agreement at Sn with Cramer at al.
- ✔ Renormalization needed for Back's data
  - ✔ (V_A,V_B) values from Back et al. do not reproduce s(n,f), while values from literature and ours do (5.30,5.30)MeV
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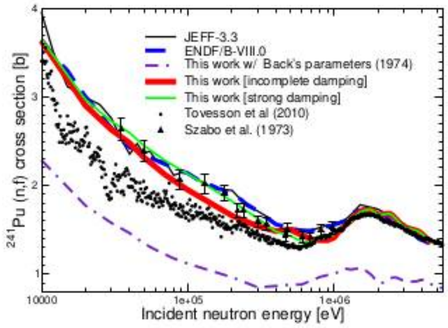


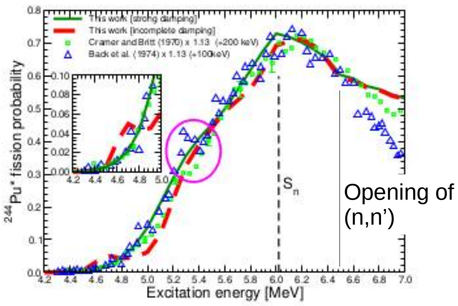
244 Pu*

The fissile Pu isotopic chain : $^{237-244}Pu^*$

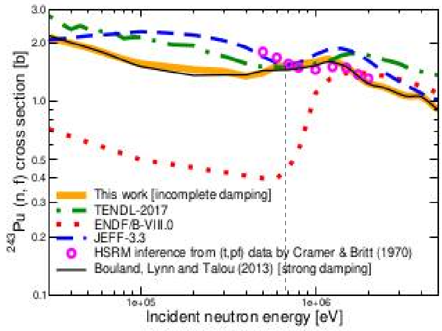
$^{244}Pu^*$

$t_{1/2}$ (^{243}Pu)= 4.95h   no n-induced σ data

$^{242}Pu(t,p)$ data available   Cramet et al. (1970)
Back et al. (1974)



- Renormalization needed (13%)
- (V_A,V_B)=(5.30,5.25)MeV in agreement with theoretical calc (V_A-V_B) but significantly different from other authors
- Too little info on IS at 5.3MeV
- s(n,f) En>700keV : good agreement
  En<700keV :
  a) absence of width fluctuation correction factor in exp data
  b) $\sigma(n,f)_{calc} < \sigma_{TENDL}$ et σ_{JEFF}
  c) $\sigma(n,f)_{calc}$ not in agreement with ENDF (choice of (V_A,V_B))?



Standard HF + fission

Standard HF theory

Average n-induced reaction cross section $\sigma_{n,c'}(E_n)=\sum_{J^\pi}[\sigma_n^{CN}(E_n,J^\pi)B_{c'}^{J^\pi}(E_x)W_{n,c'}^{J^\pi}(E_x)]$

In-out-going channel width fluctuation correction factor

N-induced CN partial formation cross section $\sigma_n^{CN}(E_n,J^\pi)=\pi\lambda g_J\sum_{s=|I-\frac{1}{2}|}^{I+\frac{1}{2}}\sum_{l=|J-s|}^{J+s}T_n^{J^\pi(ls)}(E_n)$

Incoming n transmission coefficient $T_n^{J^\pi}(E_n)=1-\exp(-2\pi S_l(E_n))$

n strength function

Heavy nuclei + low En => we can use s- and p- wave Sl extracted from the analysis of the energy-resolved resonance region and from the fit of average cross sections below 300keV

$S_l=1.044*10^{-4}$ even-l waves

$S_l=2.48*10^{-4}$ odd-l waves

Standard HF theory : exit channels

Transmission coefficients :

- n channel : $T_n^{J^\pi}(E_x) = 1 - \exp(-2\pi S_l(E_x))$

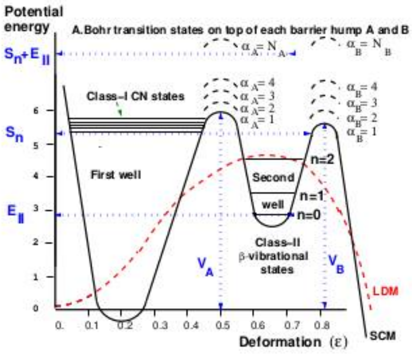
- other channels : $T_\gamma^{J^\pi} = 2\pi \frac{\langle \Gamma_\gamma^{J^\pi} \rangle}{D_{J^\pi}}$

$\langle \Gamma_\gamma^{J^\pi} \rangle$ Average capture width

D_{J^π} Average resonance spacing for a given (Jp) obtained with the combinatorial quasiparticle-vibration-rotation (QPVR) model

- fission :

Standard HF theory : fission exit channel



Total width for class-I states :
(elastic + inelastic + gamma)

$$\Gamma_{\lambda I\, tot} \approx \Gamma_{\lambda I\, n} + \Gamma_{\lambda I\, n'} + \Gamma_{\lambda I\, \gamma}$$

Total width for class-II states :

$$\Gamma_{\lambda II\, tot} \approx \Gamma_{\lambda II\downarrow} + \Gamma_{\lambda II\uparrow} + \Gamma_{\lambda II\, \gamma}$$

where the class-II fission width is

$$\langle \Gamma_{\lambda II(\uparrow)} \rangle = \frac{D_{\lambda II}}{2\pi} T_B$$

Transmission coeff through outer barrier

and the class-II coupling width is

$$\langle \Gamma_{\lambda II(\downarrow)} \rangle = \frac{D_{\lambda II}}{2\pi} T_A$$

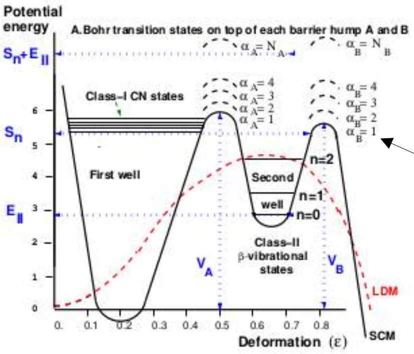
Standard HF + Aage Bohr fission theory

$$\sigma_{n,f}(E_n) = \sum_{J^\pi} \{ \sigma_n^{CN}(E_n, J^\pi) [\sum_{\alpha_B \in J^\pi} B_f^{\alpha_B}(E_x) W_{II}^{\alpha_B}(E_x)] W_{n,f}^{J^\pi}(E_x) \}$$

Class-II width fluctuation correction

Impact the calculation of $<\sigma(n,f)>$ for Pu

Standard HF theory : fission exit channel



Total width for class- II states :

$$\Gamma_{\lambda II\, tot} \approx \Gamma_{\lambda II \downarrow} + \Gamma_{\lambda II \uparrow} + \Gamma_{\lambda II\, \gamma}$$

$$\sigma_{n,f}(E_n) = \sum_{J^\pi} \{ \sigma_n^{CN}(E_n, J^\pi) [\sum_{\alpha_B \in J^\pi} B_f^{\alpha_B}(E_x) W_{II}^{\alpha_B}(E_x)] W_{n,f}^{J^\pi}(E_x) \}$$

Fission BR for a specific outer barrier transition state

$$B_f^{\alpha_B} = T_f(\alpha_B) / T_{total}$$

Depending on the E* the average formulation of B changes :

At low E* the discrete structure of class-II states impact the fission transmission coefficient T_f =>

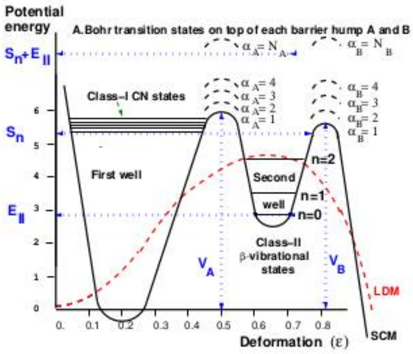
$$B_f^{\alpha_B} = f\left(\frac{T_I}{T_f}\right)$$

T_I : Damping transmission coefficient in the first well = sum of particle and gamma emission transmission coefficients

Impact the calculation of <σ(n,f)> for Pu

Monte Carlo

Monte Carlo form of HF equations



$$\sigma_{n,f}(E_n)=\sum_{J^\pi}\{\sigma_n^{CN}(E_n,J^\pi)[\sum_{\alpha_B\in J^\pi} B_f^{\alpha_B}(E_x)W_{II}^{\alpha_B}(E_x)]W_{n,f}^{J^\pi}(E_x)\}$$

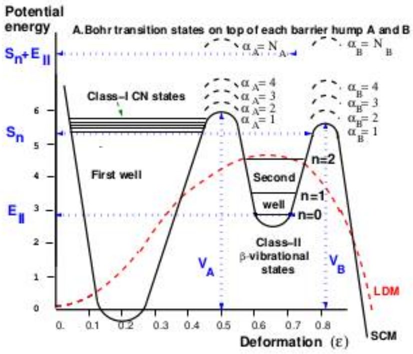
a) Analytical solution

no correlation between statistical class I and II state width fluctuations and the shape of the barrier

a) Monte Carlo algorithm

Calculate average observables accounting for statistical nuclear data fluctuations under the relevant IS

Monte Carlo route



$$\sigma_{n,f}(E_n)=\sum_{J^\pi}\{\sigma_n^{CN}(E_n,J^\pi)[\sum_{\alpha_B\in J^\pi} B_f^{\alpha_B}(E_x)W_{II}^{\alpha_B}(E_x)]W_{n,f}^{J^\pi}(E_x)\}$$

1) R-matrix average parameters for each (En,CN, residue) are calculated using :

- HF **transmission coefficients**
- mean **level spacing**

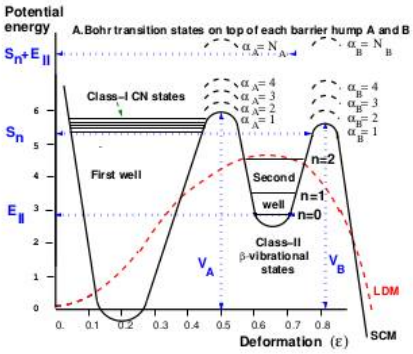
➡ $\langle\Gamma_{\lambda II(\downarrow)}\rangle$

$\langle\Gamma_{\lambda II(\downarrow)}\rangle$ used to evaluate the average of the squared coupling matrix elements

$$\langle\langle\lambda_{II}|H_c|\lambda_I\rangle^2\rangle=\Gamma_{\lambda II(\downarrow)}\frac{D_I}{2\pi}$$

They describe the **coupling** across the inner barrier **of each** class-II state, λ_{II}, to its neighboring class-I levels, $\lambda_{I\,i}$

Monte Carlo route



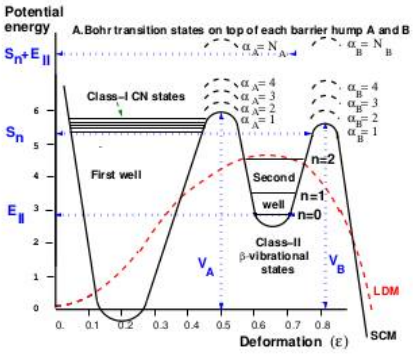
$$\sigma_{n,f}(E_n)=\sum_{J^\pi}\{\sigma_n^{CN}(E_n,J^\pi)[\sum_{\alpha_B\in J^\pi} B_f^{\alpha_B}(E_x)W_{II}^{\alpha_B}(E_x)]W_{n,f}^{J^\pi}(E_x)\}$$

1) $\langle\langle\lambda_{II}|H_c|\lambda_I\rangle^2\rangle=\Gamma_{\lambda II(\downarrow)}\dfrac{D_I}{2\pi}$

2) **class-I state energies** are generated from a Wigner distribution corrected for long-range correlations using $D_{\lambda I}$

$D_{\lambda I}$ calculated using either Gilbert and Cameron's law, or the **QPVR level density model**

Monte Carlo route



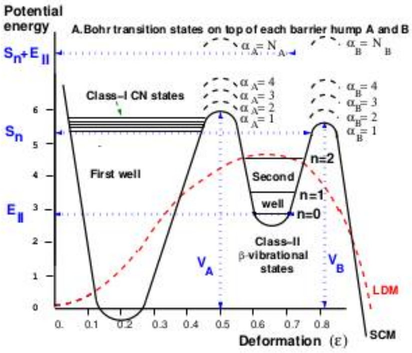
$$\sigma_{n,f}(E_n)=\sum_{J^\pi}\{\sigma_n^{CN}(E_n,J^\pi)[\sum_{\alpha_B\in J^\pi} B_f^{\alpha_B}(E_x)W_{II}^{\alpha_B}(E_x)]W_{n,f}^{J^\pi}(E_x)\}$$

1) $\langle\langle\lambda_{II}|H_c|\lambda_I\rangle^2\rangle=\Gamma_{\lambda II(\downarrow)}\frac{D_I}{2\pi}$

2) **class-I state energies** are generated using $D_{\lambda I}$ from the **QPVR level density model**

3) **class-II state energies** are generated using $D_{\lambda II}$ diagonalizing a 5x5 diagonal matrix, whose diagonal and non-diagonal elements follow a Poissonian and a Gaussian distribution, respectively

Monte Carlo route



$$\sigma_{n,f}(E_n)=\sum_{J^\pi}\{\sigma_n^{CN}(E_n,J^\pi)[\sum_{\alpha_B\in J^\pi} B_f^{\alpha_B}(E_x)W_{II}^{\alpha_B}(E_x)]W_{n,f}^{J^\pi}(E_x)\}$$

1) $\langle\langle\lambda_{II}|H_c|\lambda_I\rangle^2\rangle=\Gamma_{\lambda II(\downarrow)}\frac{D_I}{2\pi}$

2) **class-I state energies** are generated using $D_{\lambda I}$ from the **QPVR level density model**

3) **class-II state energies** are generated using $D_{\lambda II}$

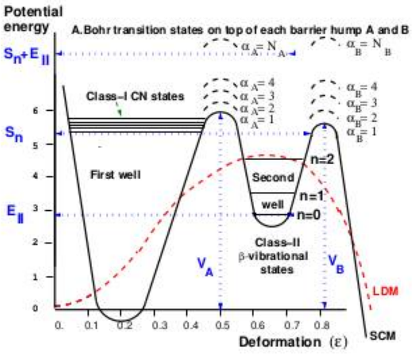
4) class-I n emission $\Gamma_{\lambda In}+\Gamma_{\lambda In'}$
class-II coupling $\Gamma_{\lambda II\downarrow}$
class-II fission $\Gamma_{\lambda II\uparrow}$
individual $\langle\lambda_{II}|H_c|\lambda_I\rangle$

width amplitudes

sampled from a gaussian distribution around their mean value $\bar{p}$ and $\sigma=\sqrt{2\bar{p}}$

$\Gamma_{\lambda I\gamma},\Gamma_{\lambda II\gamma'}$ Do not fluctuate => average value for each studied E*

Monte Carlo route



$$\sigma_{n,f}(E_n)=\sum_{J^\pi}\{\sigma_n^{CN}(E_n,J^\pi)[\sum_{\alpha_B\in J^\pi} B_f^{\alpha_B}(E_x)W_{II}^{\alpha_B}(E_x)]W_{n,f}^{J^\pi}(E_x)\}$$

1) $\langle\langle\lambda_{II}|H_c|\lambda_I\rangle^2\rangle=\Gamma_{\lambda II(\downarrow)}\frac{D_I}{2\pi}$

2) **class-I state energies** are generated using $D_{\lambda I}$ from the **QPVR level density model**

3) **class-II state energies** are generated using $D_{\lambda II}$

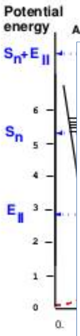
4) $\Gamma_{\lambda I n}+\Gamma_{\lambda I n'},\Gamma_{\lambda II\downarrow},\Gamma_{\lambda II\uparrow},\langle\lambda_{II}|H_c|\lambda_I\rangle$ **sampled** from gaussian, $\Gamma_{\lambda I\gamma},\Gamma_{\lambda II\gamma}$ average value for each E*

5) get the **median energy of class-II states** sampled energy → λ_{II}^{median}

$\Gamma_{\lambda II\,tot}^{median}$ compared to class-I state mean level spacing $D_{\lambda I}$

Class-II state that mainly contribute to the fission width of the corresponding final R-matrix eigenstates

Monte Carlo route



$\Gamma^{median}_{\lambda II\ tot} < 4\, D_{\lambda I}$. **Narrow class-II state hypothesis** : exact calculation of class-I and class-II admixture coefficients in the final R-matrix eigenstates performed

$\Gamma^{median}_{\lambda II\ tot} \geq 4\, D_{\lambda I}$. **Broad « median » class-II state** : its major contribution to the R-matrix eigenstates is computed from the calculated average class-I and class-II parameters and from the class-II coupling width. Second-order contribution is calculated assuming a Lorentzian pattern into the final R-matrix eigenstates

$)]W^{J^\pi}_{n,f}(E_x)\}$

$_{\lambda I}$ from the

$D_{\lambda II}$

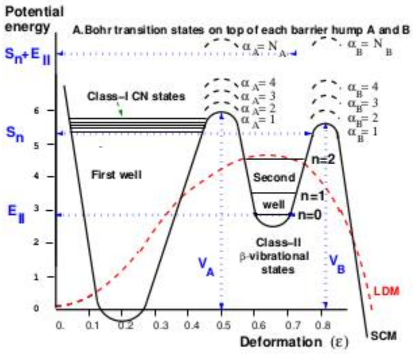
4) $\Gamma_{\lambda I}$ ... r each E*

5) get the **median energy of class-II states** sampled energy → λ^{median}_{II}

$\Gamma^{median}_{\lambda II\ tot}$. compared to class-I state mean level spacing $D_{\lambda I}$

Class-II state that mainly contribute to the fission width of the corresponding final R-matrix eigenstates

Monte Carlo route



$$\sigma_{n,f}(E_n)=\sum_{J^\pi}\{\sigma_n^{CN}(E_n,J^\pi)[\sum_{\alpha_B\in J^\pi} B_f^{\alpha_B}(E_x)W_{II}^{\alpha_B}(E_x)]W_{n,f}^{J^\pi}(E_x)\}$$

1) $\langle\langle\lambda_{II}|H_c|\lambda_I\rangle^2\rangle=\Gamma_{\lambda II(\downarrow)}\dfrac{D_I}{2\pi}$

2) **class-I state energies** are generated using $D_{\lambda I}$ from the **QPVR level density model**

3) **class-II state energies** are generated using $D_{\lambda II}$

4) $\Gamma_{\lambda I n}+\Gamma_{\lambda I n'},\Gamma_{\lambda II\downarrow},\Gamma_{\lambda II\uparrow},\langle\lambda_{II}|H_c|\lambda_I\rangle$ **sampled** from gaussian, $\Gamma_{\lambda I\gamma},\Gamma_{\lambda II\gamma}$: average value for each E*

5) calculation of **class-I and II admixture coefficients** and final R-matrix **eigenstates widths and energies**

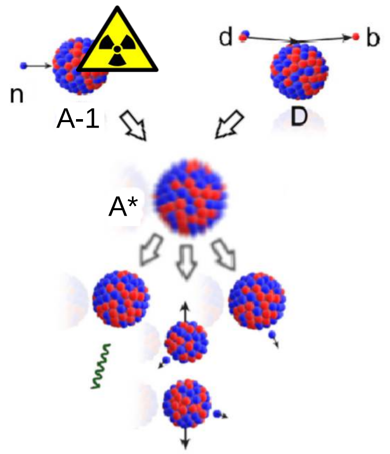
6) partial **n-induced σ are calculated** within the Single-Level Breit-Wigner approximation

Theory improvements :

surrogate reaction P

Modeling of surrogate reaction P

n-induced reaction   surrogate reaction



$$\overline{\sigma_{n,c'}}(E_n)=\sigma^{CN}(E_n)*\sum_{J^\pi}[J^\pi\,populated\,distrib(E_n)_{n-ind}*BR_{c'}^{J^\pi}(E_n)]$$

Deexcitation probability

$$P^{A^*}_{surr,c'}(E_x)=\sum_{J^\pi}[J^\pi\,populated\,distrib(E_x)_{surr}*BR_{c'}^{J^\pi}(E_x)]$$

Modeling of P_f in β-vibrational resonance region

Medium and giant-size resonances observed in σ(n,f) → double-hamped B_f as a function of elongation

The Hamiltonian :

$$H = H_\beta + H_{int}(\zeta;\ \beta_0) + H_c(\beta,\zeta;\ \beta_0)$$

- H_β: governing the collective elongation mode β
- $H_{int}(\zeta;\ \beta_0)$: governing all other collective modes other than β, single-particle excitations, rotational motion
- $H_c(\beta,\zeta;\ \beta_0)$: governing the interaction between β mode and the intrinsic excitations ζ

In the R-matrix formalism class-II states are :

$$X_{\lambda_{II}}^{(II)} = \sum_{\mu,\nu} C_{\mu\nu}^{\lambda_{II}} \chi_\mu \Phi_{\nu(\mu)}^{(II)}$$

- χ_μ: intrinsic wave function
- $\Phi_{\nu(\mu)}^{(II)}$: Vibrational wave function

Modeling of P_f in β-vibrational resonance region

In the R-matrix formalism class-II states are :

$$X_{\lambda_{II}}^{(II)} = \sum_{\mu,\nu} C_{\mu\nu}^{\lambda_{II}} \chi_\mu \Phi_{\nu(\mu)}^{(II)}$$

→ Vibrational wave function

→ intrinsic wave function

Purely vibrational state

$$X_{\lambda_{II}}^{(II)} \approx \chi_0 \Phi_{\nu(0)}^{(II)}$$

Eigenfunctions of H_{int} for the lowest intrinsic state at saddle

Verified only if the energy of this state is very close to the second well gs energy

Input parameter database

The set of used parameters allows us to correctly reproduce the experimental $\sigma(n,f)$ and $\sigma(n,\gamma)$ for ^{236}Pu to ^{244}Pu, for E_n=few keV up to 5.5MeV

+

CS Jp distribution for chosen surrogate reaction

(V_A,V_B) and ($h\omega_A$, $h\omega_B$) are → spin independent for e-e nuclei
→ the spin dependence is estimated fitting $\sigma(n,f)$ data for E_n>100keV

Low-lyng class-I states : taken from ENSDF and expanded with additional levels to complete the rotational bands predicted by QPVR model up to ~1.1MeV E*

At higher energies : QPVR model