Point-by-Point model calculation of ν(A) at incident neutron energies where multiple fission chances are involved

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Application for

n + ^{238}U at En from 1 MeV to 80 MeV

n + ^{235}U at En from thermal to 20 MeV

(and recent preliminary results up to En=50 MeV)

1. **Motivation of this work**

2. **Short description of the model**

3. **Point-by-Point (PbP) model results of ν(A) at En below the threshold of the 2-nd fission chance**
   - comparison between the ν(A) results of PbP, GEF and scaling method
   - indirect validation of ν(A) through $<\nu>_{tot} = <\nu>_{FF}$ compared with experimental data

4. **PbP results of ν(A) at En where multiple fission chances are involved**
   - ν(A) results using fission cross-section ratios (RF) of different evaluations
   - comparison between the ν(A) results of PbP, GEF and scaling method
   - indirect validation of ν(A) through $<\nu>_{tot} = <\nu>_{FF} + <\nu>_{prefiss}$ compared with experimental data
   - explanation of the vanishing of the ν(A) sawtooth shape with increasing En (i.e. excitation energy of the fissioning nucleus)

5. **Conclusions**

1. Motivation of this work

The interest in the study of neutron induced fission at En where multiple fission chances are involved is justified by the need of nuclear data for both a better understanding of the fission process and new applications (advanced systems based on fission, incineration of nuclear waste etc.)

- **Experimental Y(A,TKE) distributions at high En are required.**
- **Recent experiments were performed at Los Alamos National Laboratory for ^{238}U(n,F), ^{235}U(n,F), ^{239}Pu(n,F)**

- neutron source at LANSCE → En from 100's KeV to 100's MeV,
- Frisch-grid ionization chamber and
- the 2E analysis procedure to calculate pre- and post-neutron emission data of fragments

ν(A) are needed to re-cover the pre-neutron fragment distributions from the measured post-neutron fragment data

Experimental ν(A) data are very scarce (only for a few actinides at thermal En and at En below the 2-nd fission chance threshold). Exp. ν(A) data are completely missing at En where multiple fission chances are involved.

Hence a need to use ν(A) predicted by models

Preliminary pre-neutron Y(A,TKE) of ^{238,235}U(n,F) up to En = 20 MeV were reported at the *Int. Conf. PHYSOR, Sun Valley USA, May, 2016*)

using
ν(A) provided by:

- the scaling method
(currently used by experimentalists at low En)

- the GEF code

Significant differences between the Y(A) data obtained with these predicted ν(A) were obtained.

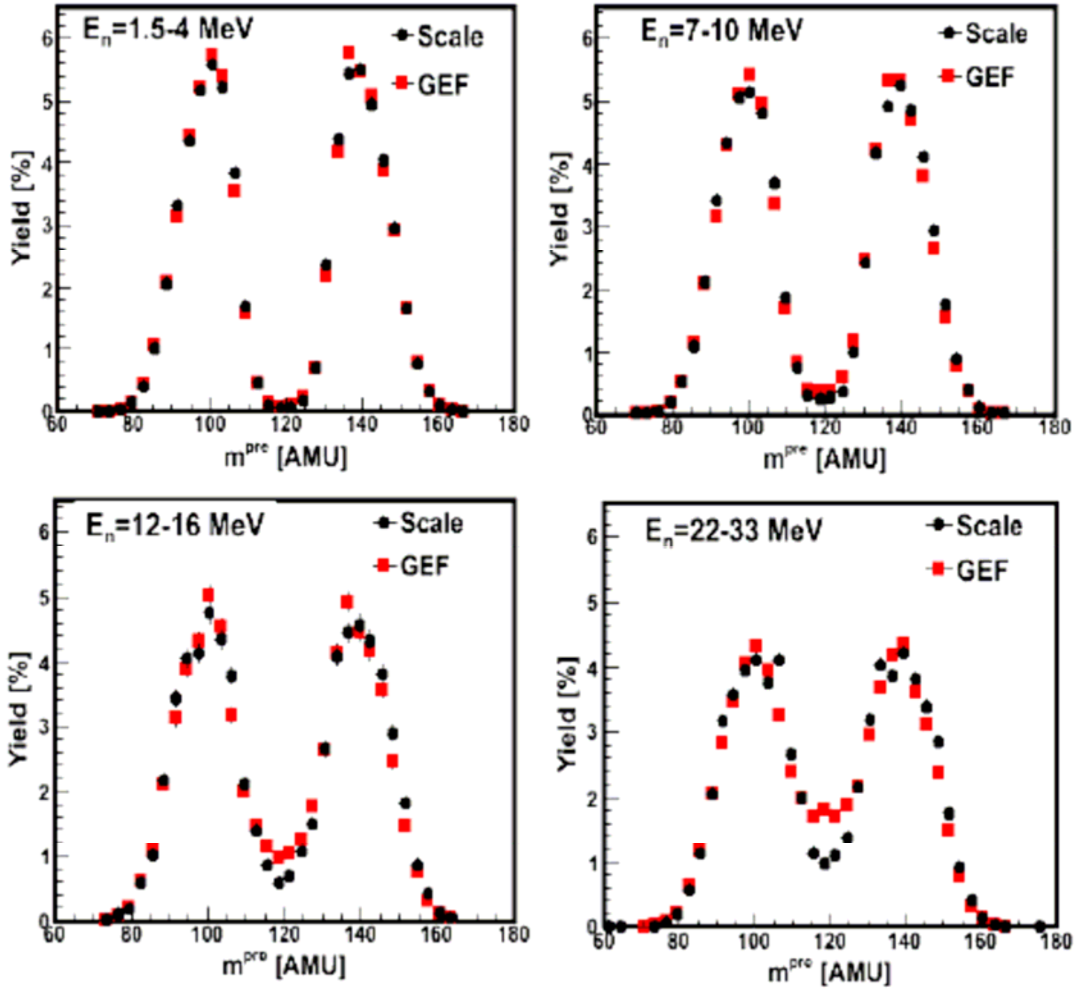


Figure 4.31: A comparison between the GEF and scaled sawtooth methods in ^{238}U when applied to the data in the 2E method. As expected, the scaled method leads to lower yield in the valley since it evaporates more neutrons in this mass region.

The Point-by-Point (PbP) model can also provide ν(A) distributions, answering to the request of ν(A) for the re-covering of pre-neutron fragment data.

A comprehensive summary about most of the models of prompt emission currently used today is given in the paper *"Prompt Fission Neutron Spectra of Actinides", Nucl.Data Sheets 131 (2016) 1-108* result of a CRP coordinated by IAEA-NDS.
Up to now the PbP model was intensively used only for SF and neutron-induced fission below the 2-nd chance fission threshold.

2. Short description of the PbP modeling at En where multiple fission chances are involved

At En above 25 – 30 MeV charged particle emission occurs and fission of secondary nucleus chains and ways must be taken into account. In the extended Los Alamos model [*A.Tudora et al., Nucl.Phys.A 740 (2004) 33*] 3 nucleus chains and 6 ways (paths) were considered. In this case we have taken into account:

***i)* the main nucleus chain (1) with neutron evaporation from the precursor of this chain (the only one taken into account at En up to about 20 – 25 MeV)**

***ii)* the "proton" way – proton emission from the nuclei of the main chain leading to the secondary nucleus chain (2)**

***iii)* the "neutron via proton" way – neutron evaporation from the precursor of the secondary nucleus chain (2)**

Other possible ways are neglected having low contributions at En up to 80 MeV.

For the reactions n + ^{238}U up to En = 80 MeV and n + ^{235}U up to En = 50 MeV the PbP calculations are done for the fissioning nuclei of

- **the main U chain → $^{239-230}$U (En = 80 MeV), $^{236-230}$U (En = 50 MeV)**
- **the secondary Pa chain → $^{238-232}$Pa (En = 80 MeV), $^{235-231}$Pa (En = 50 MeV)**

at the average excitation energies given by the following recursive formulae:

main nucleus chain

$$Ex_1^{(1)} = En + Bn_1^{(1)}$$

$$< Ex >_i^{(1)} =< Ex >_{i-1}^{(1)} - Bn_{i-1}^{(1)} - < \varepsilon_{ev} >_{i-1}^{(1)}, \quad i = 2,...N^{(1)}$$

secondary nucleus chain, "p" way

$$< Ex >_i^{(p)} =< Ex >_i^{(1)} - S_{pi}^{(1)} - < \varepsilon_{ev} >_{pi}, \quad i = 1,..., N^{(2)}$$

secondary nucleus chain "n via p" way

$$< Ex >_i^{(pn)} =< Ex >_{i-1}^{(pn)} - Sn_{i-1}^{(2)} - < \varepsilon_{ev} >_{n,i-1}^{(2)}, i = 2,..., N^{(2)}$$

$$< Ex >_1^{(pn)} =< Ex >_1^{(p)}$$

PbP model calculation for each compound nucleus undergoing fission:

- **the fragmentation range in the PbP calculations:**

for each A, 3 charge numbers Z are taken

Z being the nearest integer values above and below $Zp(A) = Z_{UCD}(A) + \Delta Z(A)$.

In [*Tudora et al., Nucl.Sci.Eng. 181 (2015) 289*] it is shown that ΔZ=|0.5| for all fragmentations does not change significantly the results. Hence, in the present work for all fragmentations ΔZ = |0.5| and p(Z,A) is taken as a Gaussian function centered on Zp(A) with rms(A) = 0.6

- **the compound nucleus c.s. of the inverse process $\sigma_c(\varepsilon)$ of all fragments optical model calculations with SCAT2 and the potential Becchetti-Greenlees.**

- **the level density parameters of fragments – super-fluid model 2 times: first at scission in the frame of the excitation energy partition (implying an iterative procedure under the condition of statistical equilibrium) and second at full acceleration.**

The obtained ν(Z,A) corresponding to each fissioning nucleus are averaged over p(Z,A) ➔ the individual $\nu_i(A)$

The **total ν(A)** at a given En:

$$\nu(A) = \sum_{k=1}^{3} \sum_{i=1}^{N(k)} RF_i^{(k)} \, \nu_i^{(k)}(A)$$

k : the fission way, i.e. the main way "n" and the secondary ways "p" and "n via p"

i : the fission chance of each way

$N^{(K)}$: number of compound nuclei of each nucleus chain / way

$\nu_i^{(k)}(A)$: the PbP result of individual ν(A) of each compound nucleus undergoing fission of the main and secondary ways

$RF_i^{(k)}$: the fission probability expressed as total and partial fission cross-section ratios $RF_i^{(k)} = \sigma_{f\,i}^{(k)} / \sigma_{f\,tot}$

A similar formula can be written for the prompt neutron multiplicity of a fragmentation (fragment pair): $\nu_{pair,i}^{(k)}(A) = \nu_i^{(k)}(A) + \nu_i^{(k)}(A_{0,i}^{(k)} - A)$

Average numbers of prompt neutrons

(Needed for the indirect validation of ν(A) results)

If Y(A) are available - the average number of prompt neutrons emitted by the fission fragments:

$$< \nu >_{FF} = \sum_{A} \nu(A) Y(A) \Big/ \sum_{A} Y(A)$$

The average number of neutrons evaporated from the compound nuclei before fission, named pre-fission neutrons:

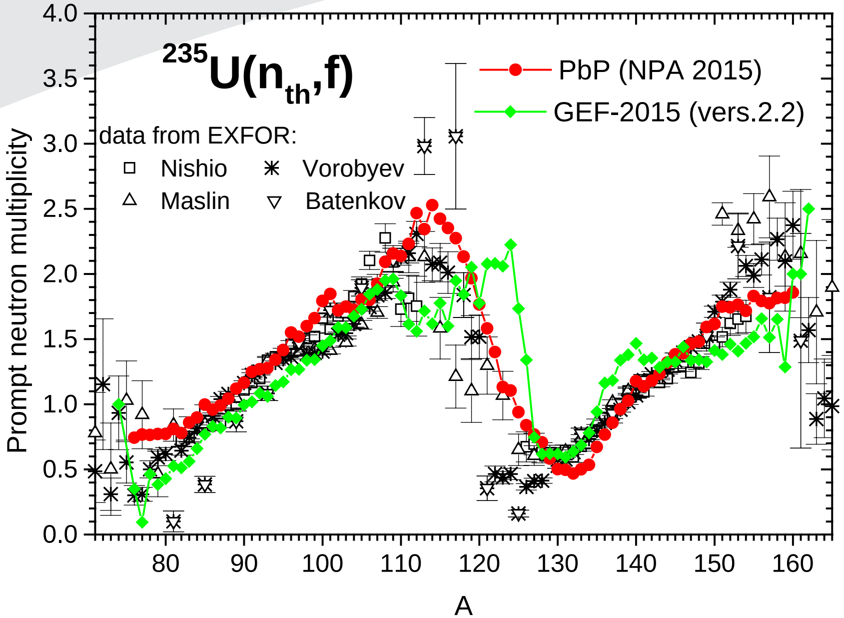
$$< \nu >_{prefiss} = \sum_{k=n,nvp} \sum_{i=1}^{N(k)} (i-1) RF_i^{(k)}$$

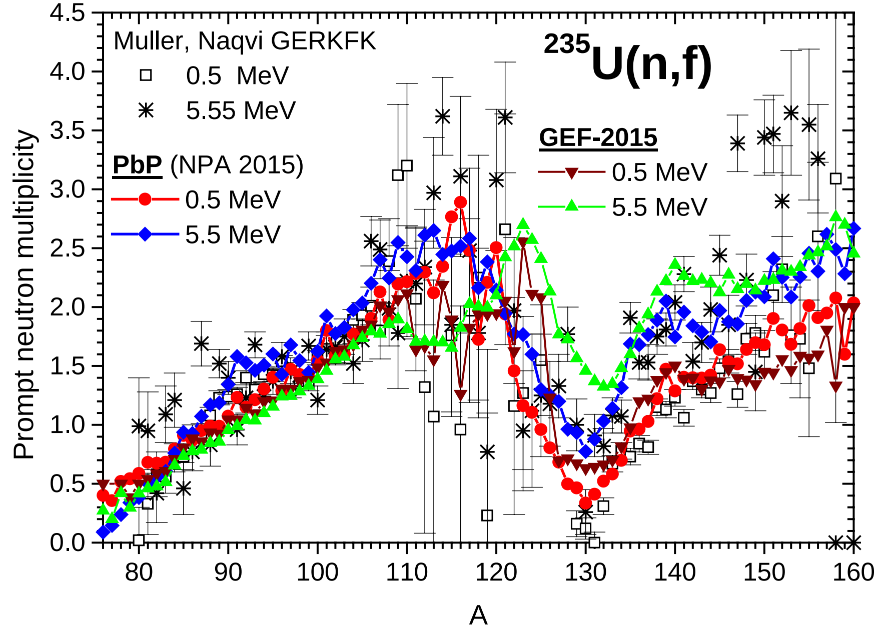
The total average number of prompt neutrons:

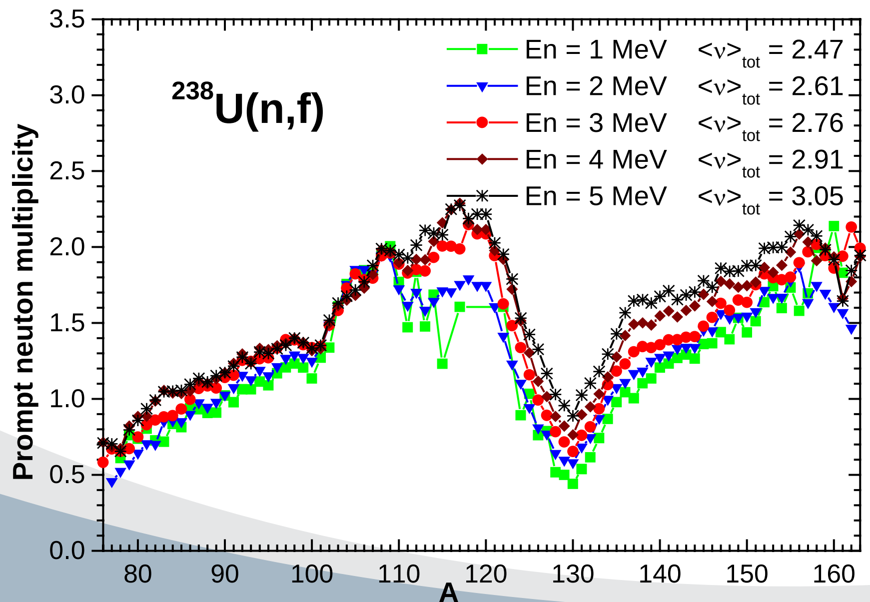
$$< \nu >_{tot} = < \nu >_{FF} + < \nu >_{prefiss}$$

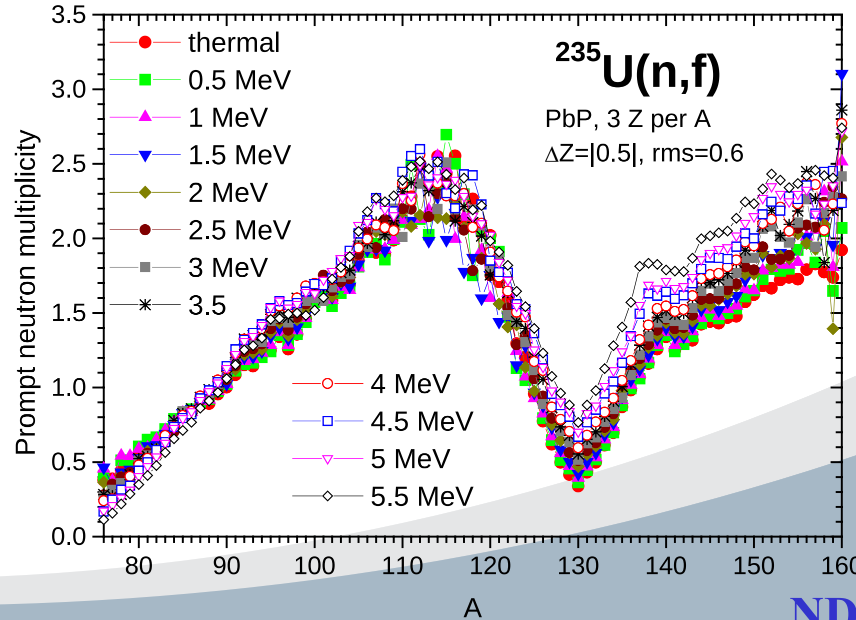
$<\nu>_{tot} = <\nu>_{FF}$ at En below the threshold of the 2-nd fission chance

3. PbP results of ν (A) at En below the 2-nd fission chance threshold

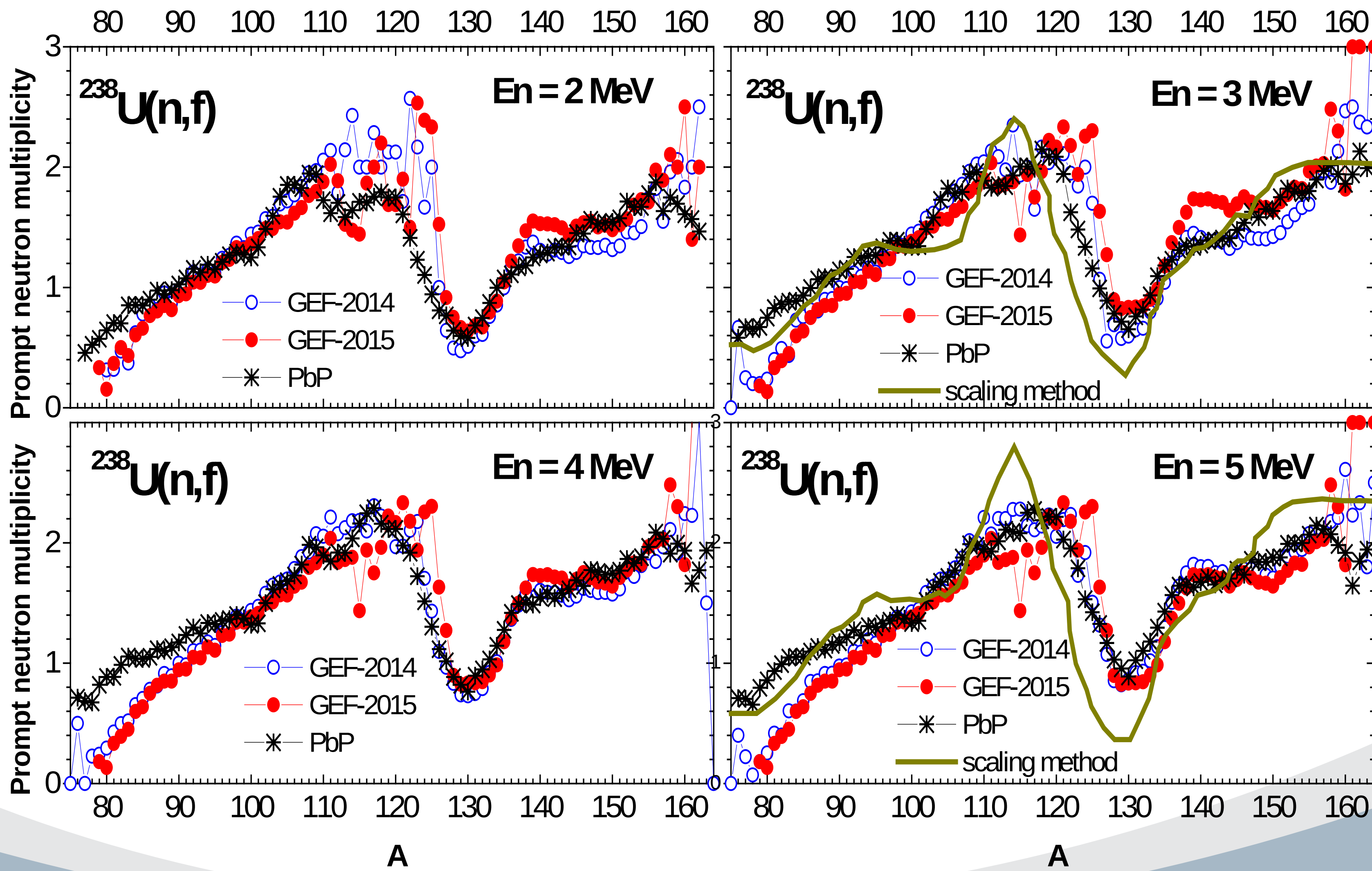




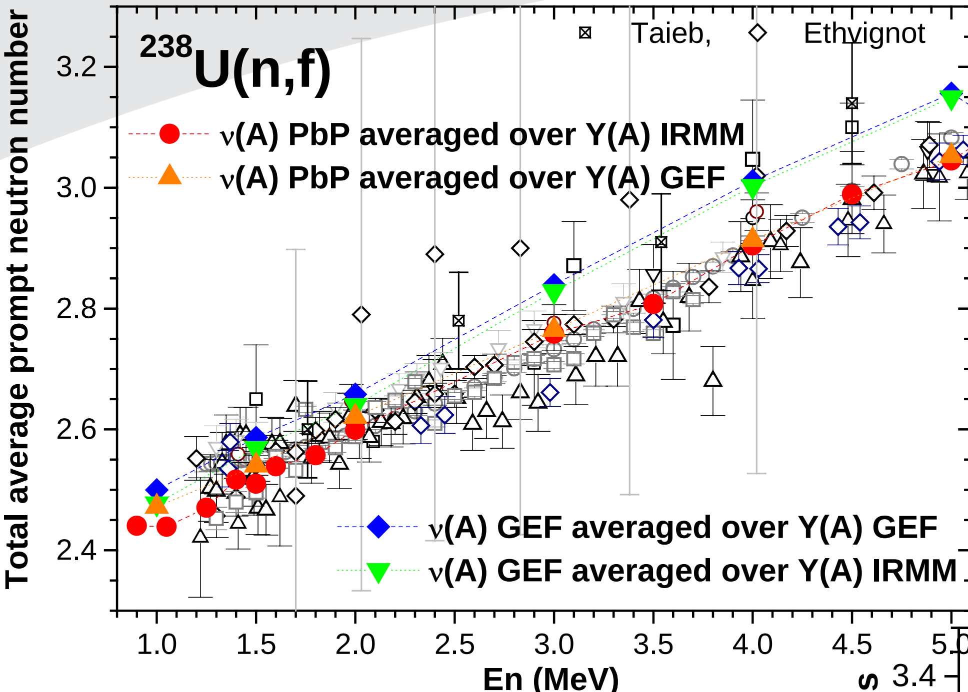




3.1 Comparison between ν(A) of PbP, GEF and scaling method

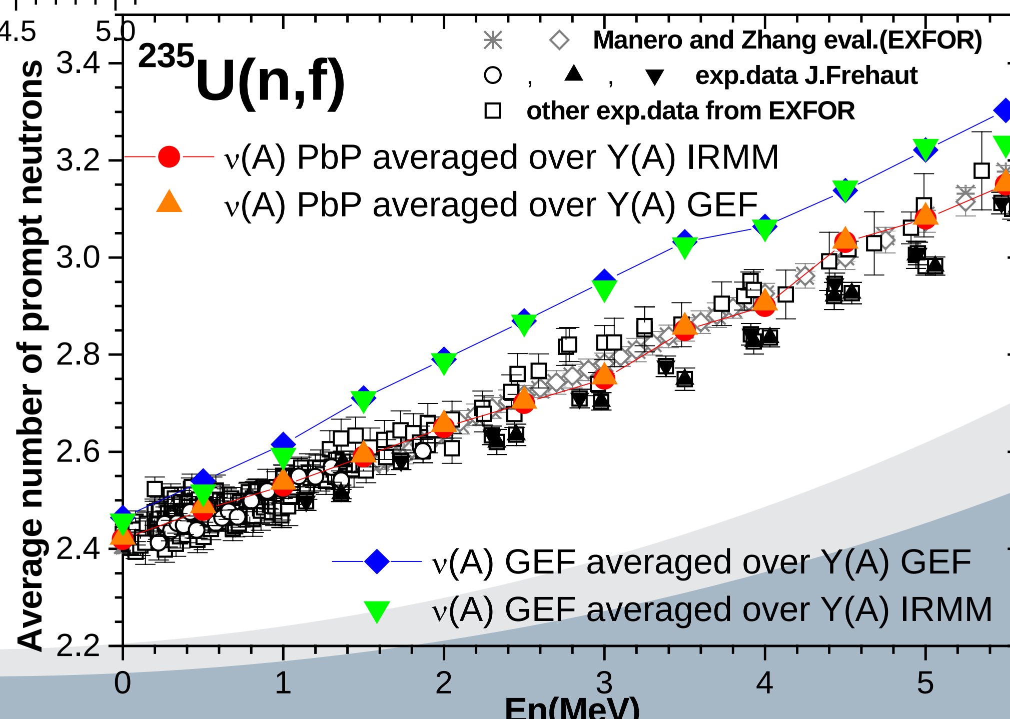


3.2 Indirect validation of ν(A) through $<\nu>_{tot}$ compared with exp.data



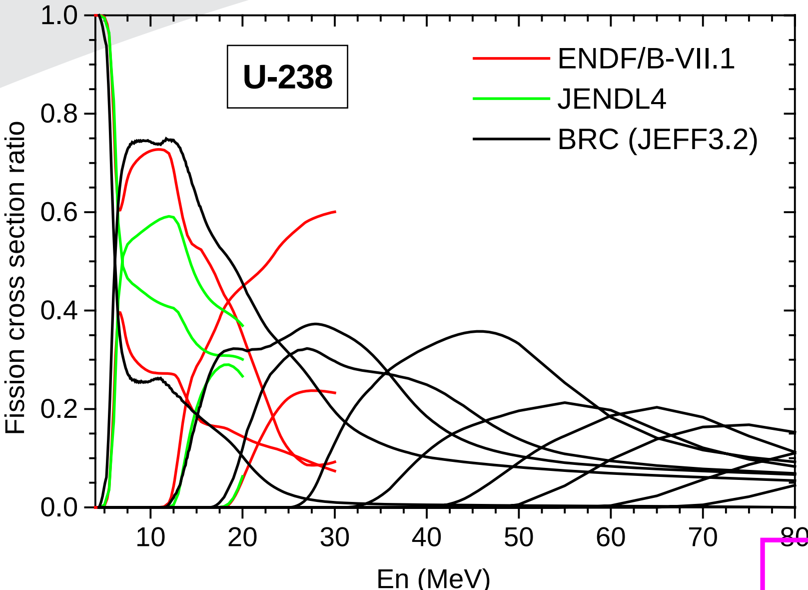
Based on the fact that $<\nu>_{tot}=<\nu>_{FF}$ is <u>strongly dependent on ν(A)</u> and has only a very <u>weak</u> <u>dependence on Y(A)</u>

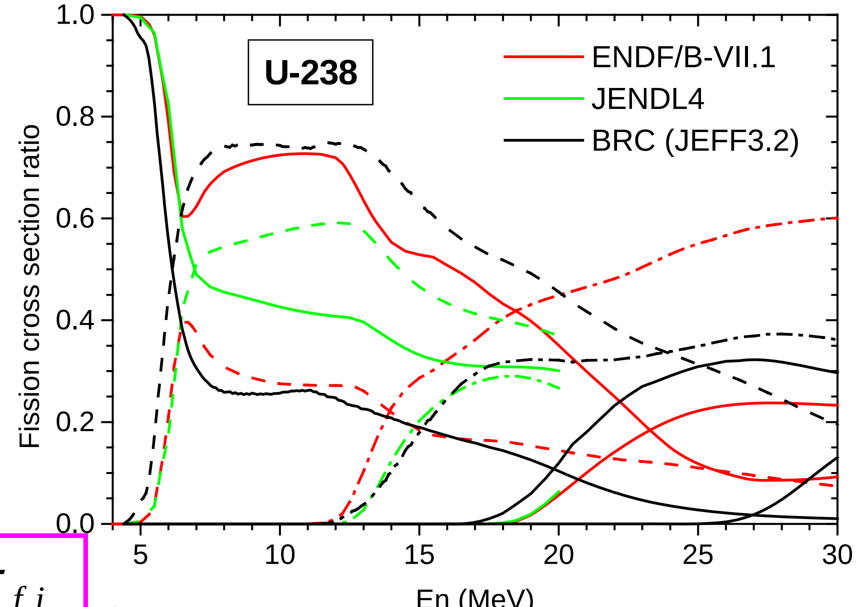
$$<\nu>_{FF}=<\nu>_{tot}=\sum_A \nu(A)Y(A)\Big/\sum_A Y(A)$$



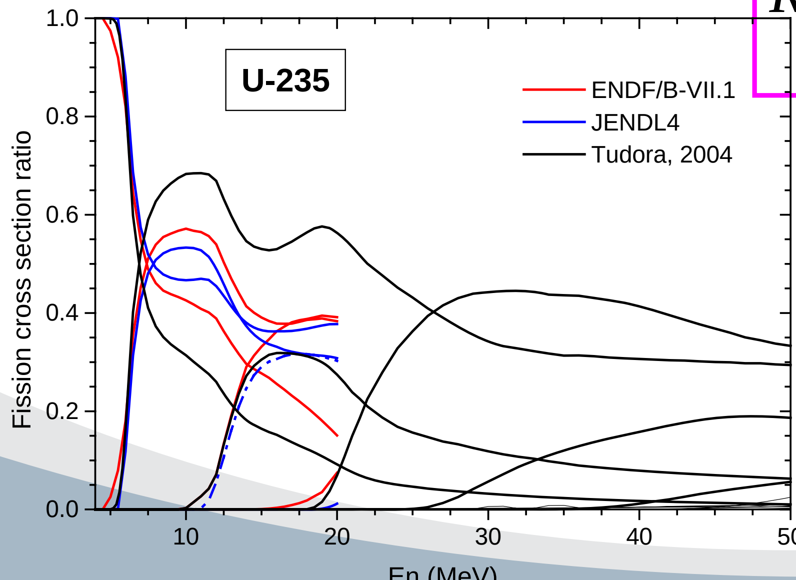
4. PbP results of ν(A) at En where multiple fission chances are involved

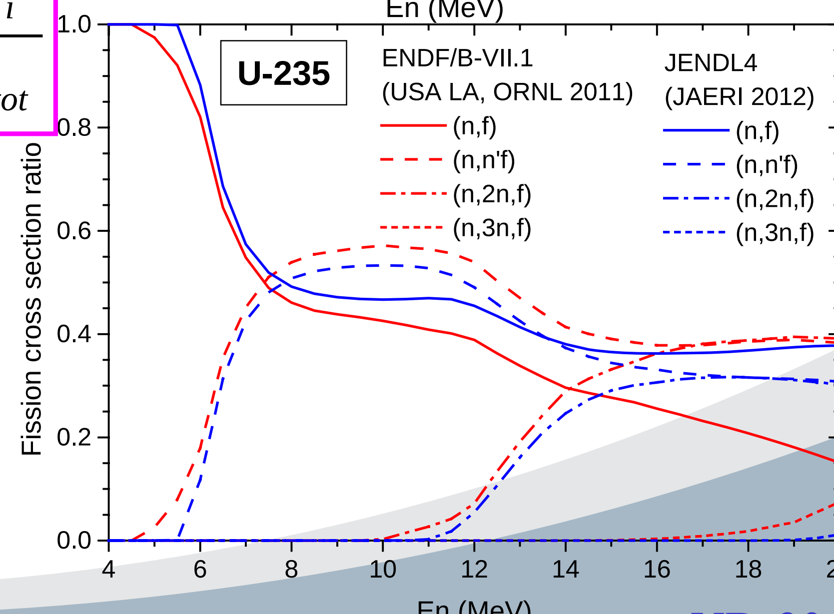
Fission cross-section ratios (RF) used to obtain the total ν(A) distribution



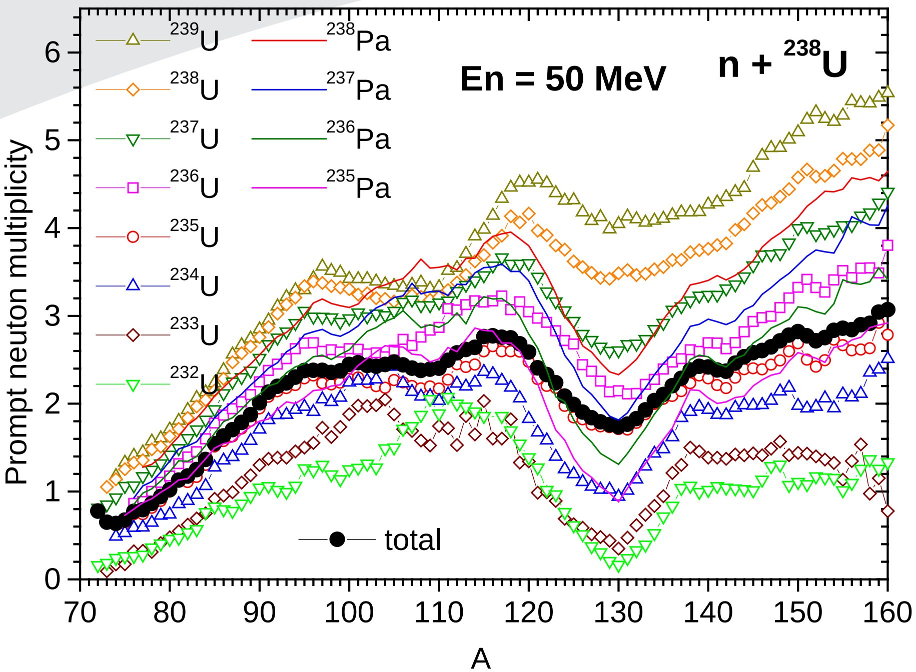


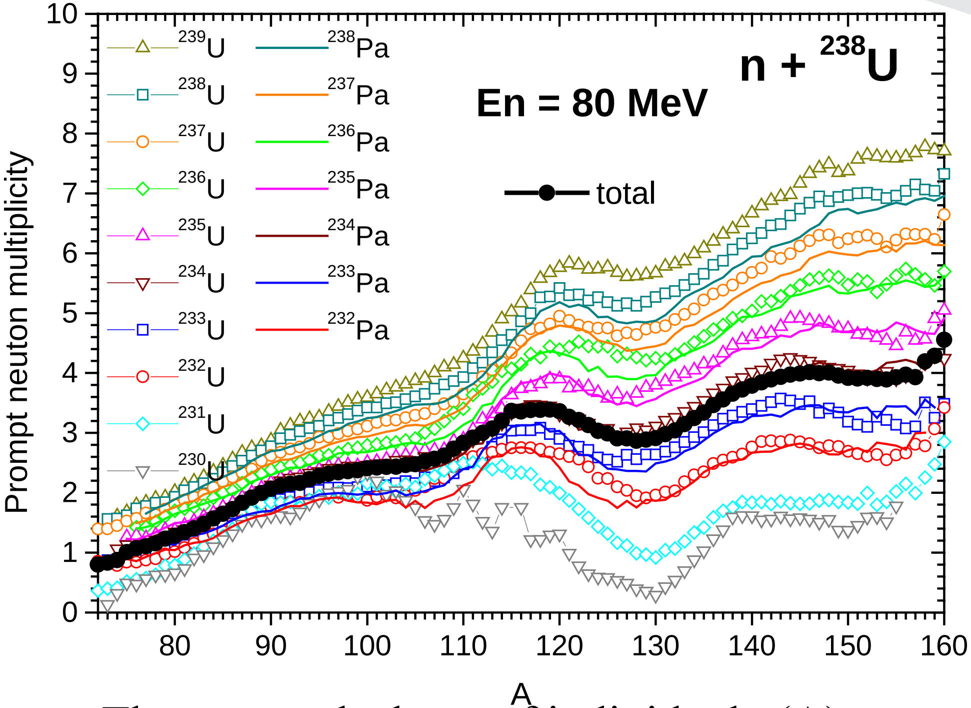
$$RF_i = \frac{\sigma_{f\,i}}{\sigma_{f\,tot}}$$

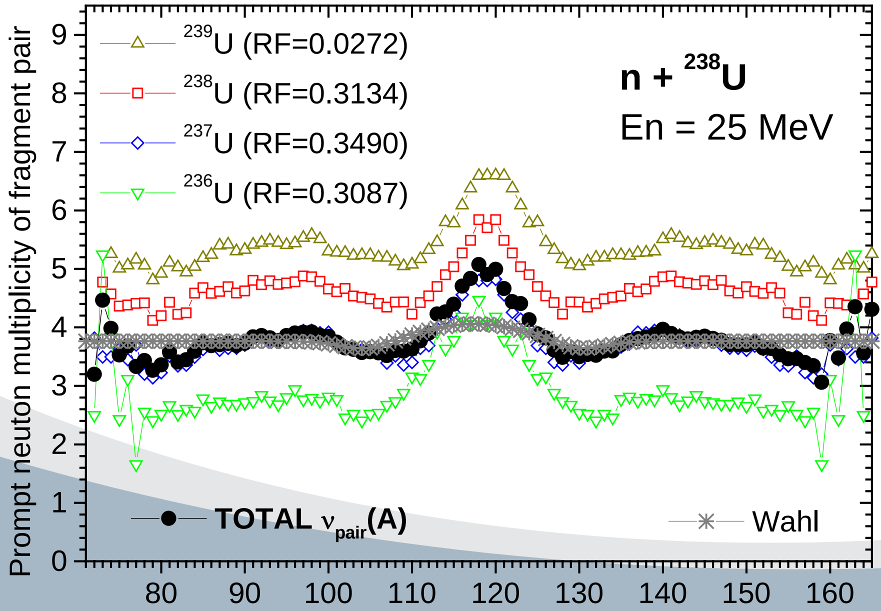




Examples of PbP results at En where multiple fission chances are involved



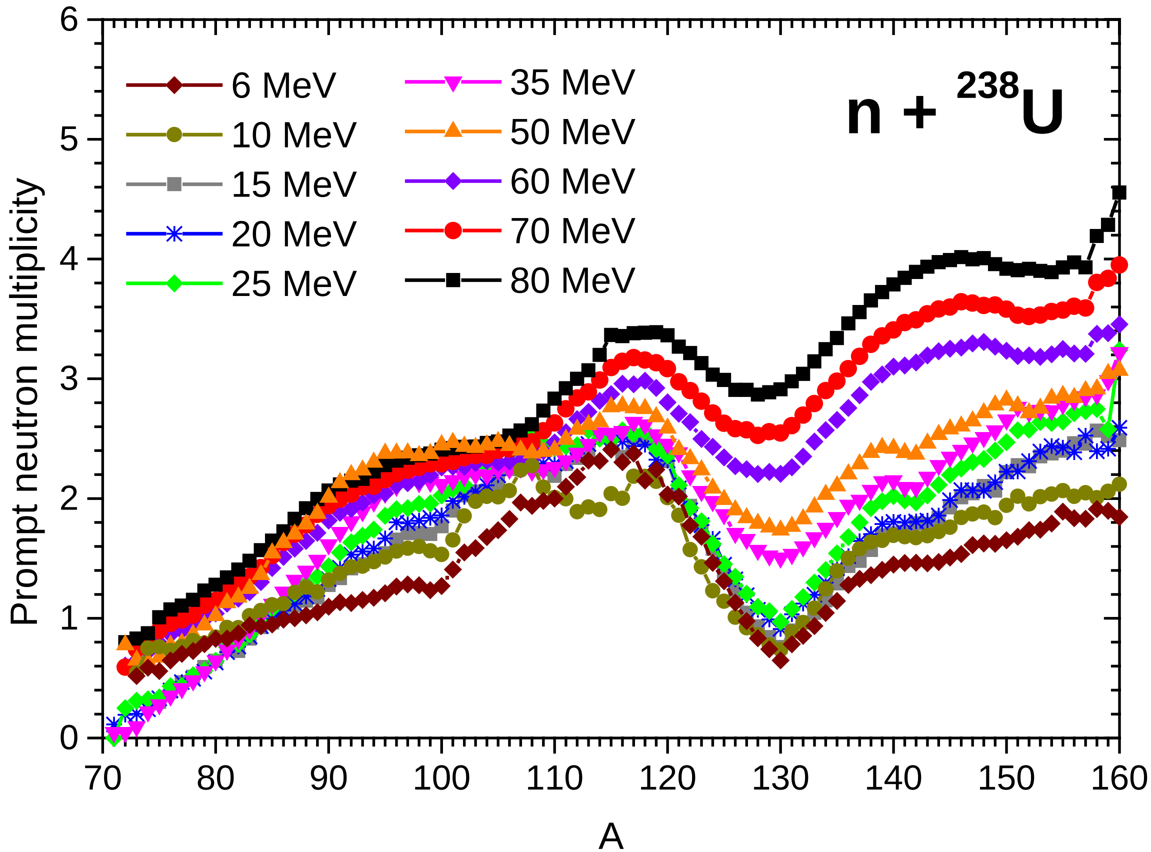




The sawtooth shape of individual ν(A) corresponding to the first few comp.nuclei of the U and Pa chains is almost vanished.

This is due to the damping of shell effects of a great part of the fragments coming from these nuclei. The excitation energies of these fragments are high enough to reach the asymptotic values of the level density parameter.

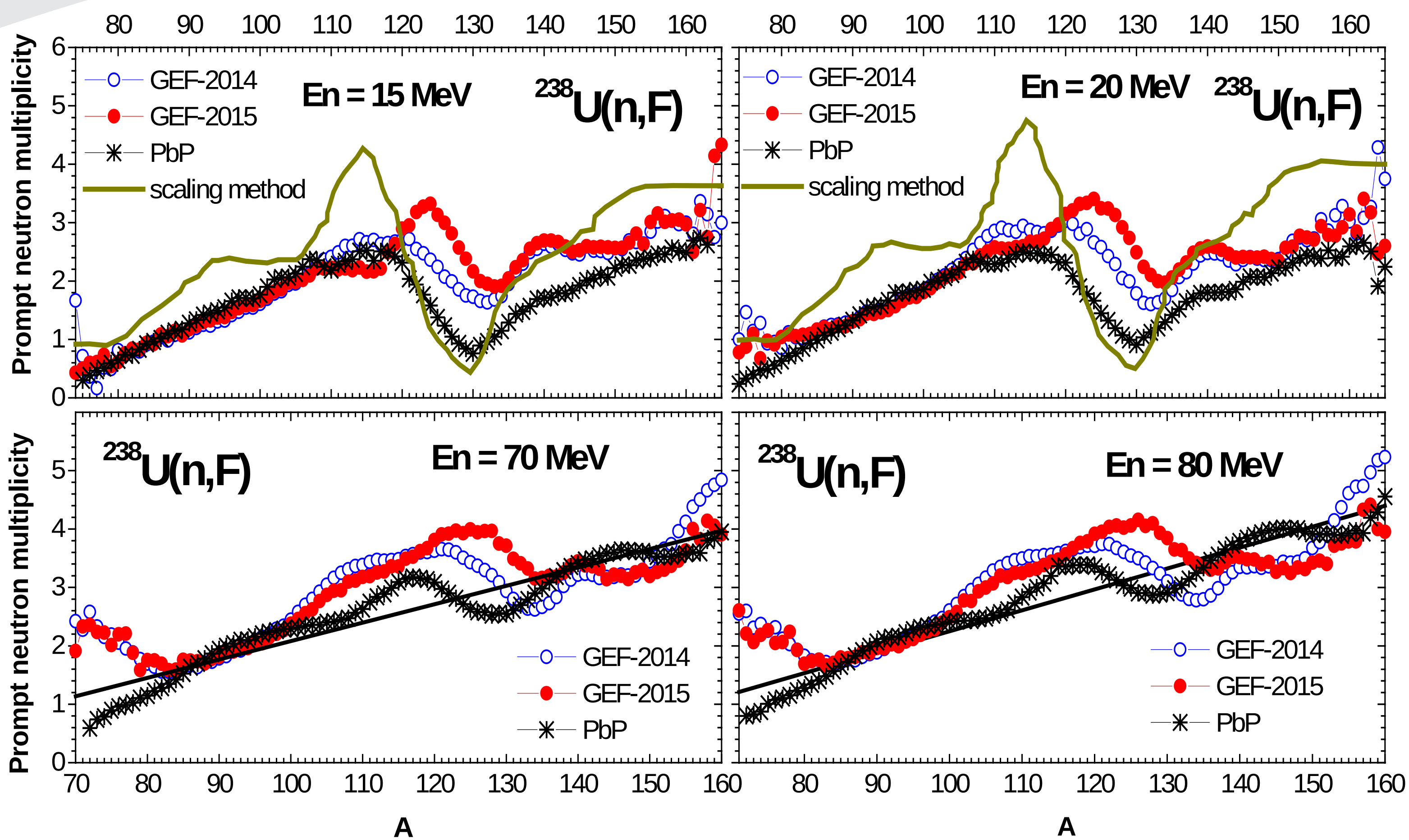
Evolution of the total ν(A) shape with increasing En



A less pronounced sawtooth shape of total ν(A) with increasing En is visible.

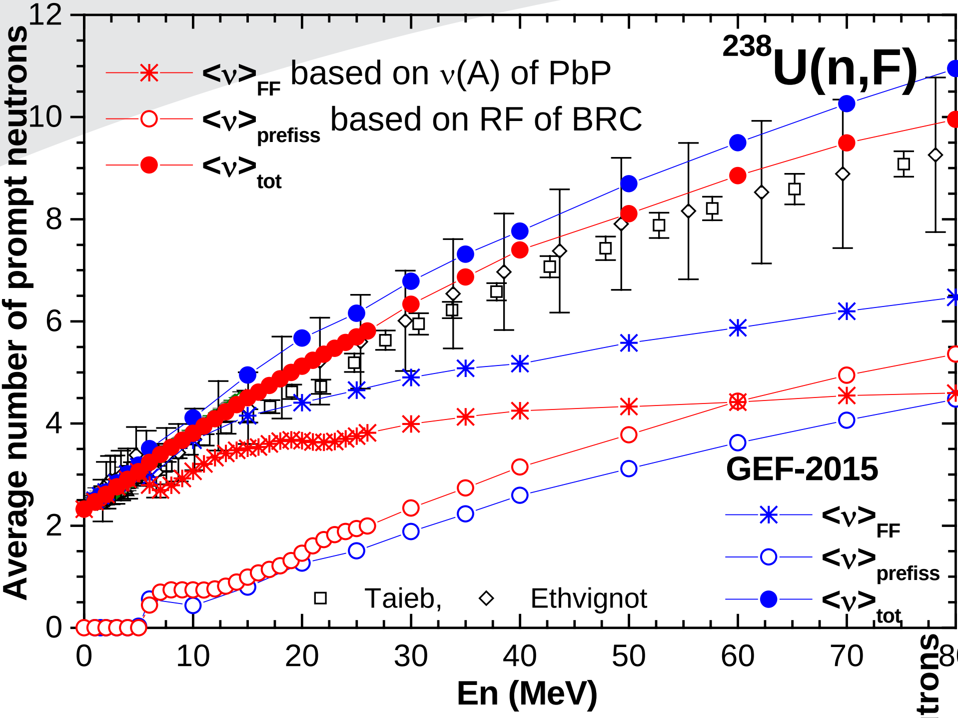
It is due to the contribution of individual ν(A) of the first compound nuclei for which the sawtooth shape is almost vanished due to the dumping of shell effects of a great part of the fragments coming from these nuclei.

4.2 Comparison between total ν(A) of PbP, GEF and scaling method



- ν(A) of the scaling method maintains a very pronounced sawtooth shape (unphysical)
- at En = 70 MeV, 80 MeV the total ν(A) of PbP exhibits only a slow oscillation in the A region of symmetric fission compared to the black line. The ν(A) results of both GEF versions clearly deviate from linearity.

4.3 Indirect validation of ν(A) through $<\nu>_{tot}$ compared with exp.data



$$<\nu>_{tot} = <\nu>_{FF} + <\nu>_{prefiss}$$

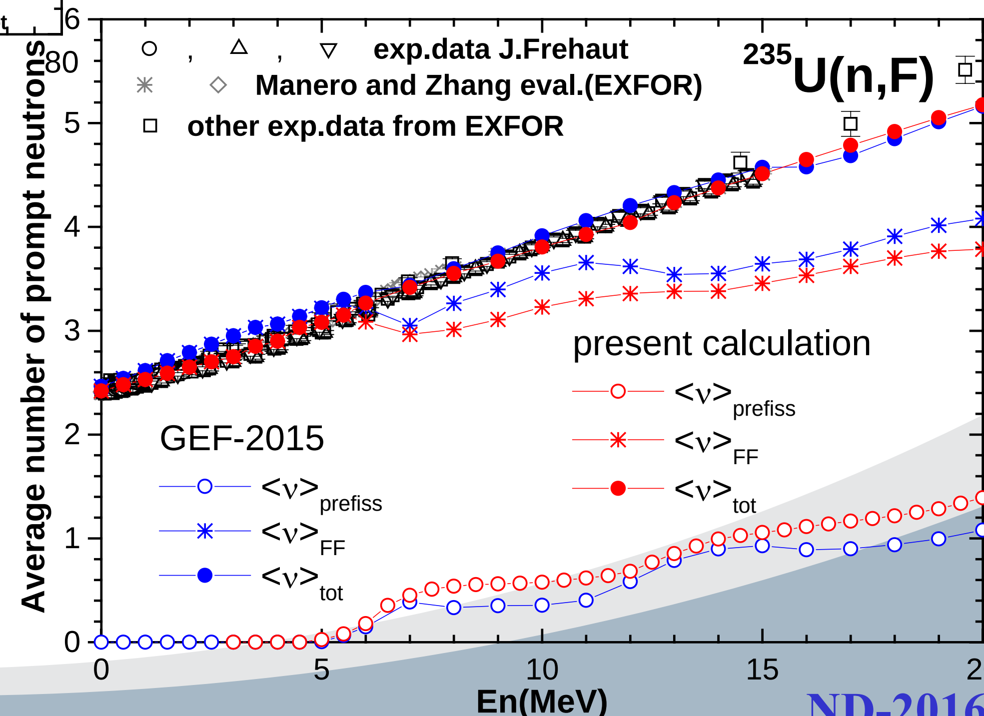
$$<\nu>_{FF} = \sum_{A} \nu(A) Y(A) \Big/ \sum_{A} Y(A)$$

$$<\nu>_{prefiss} = \sum_{k=n,nvp} \sum_{i=1}^{N(k)} (i-1)\, RF_i^{(k)}$$

Blue symbols: GEF code (vers 2015/2.2)

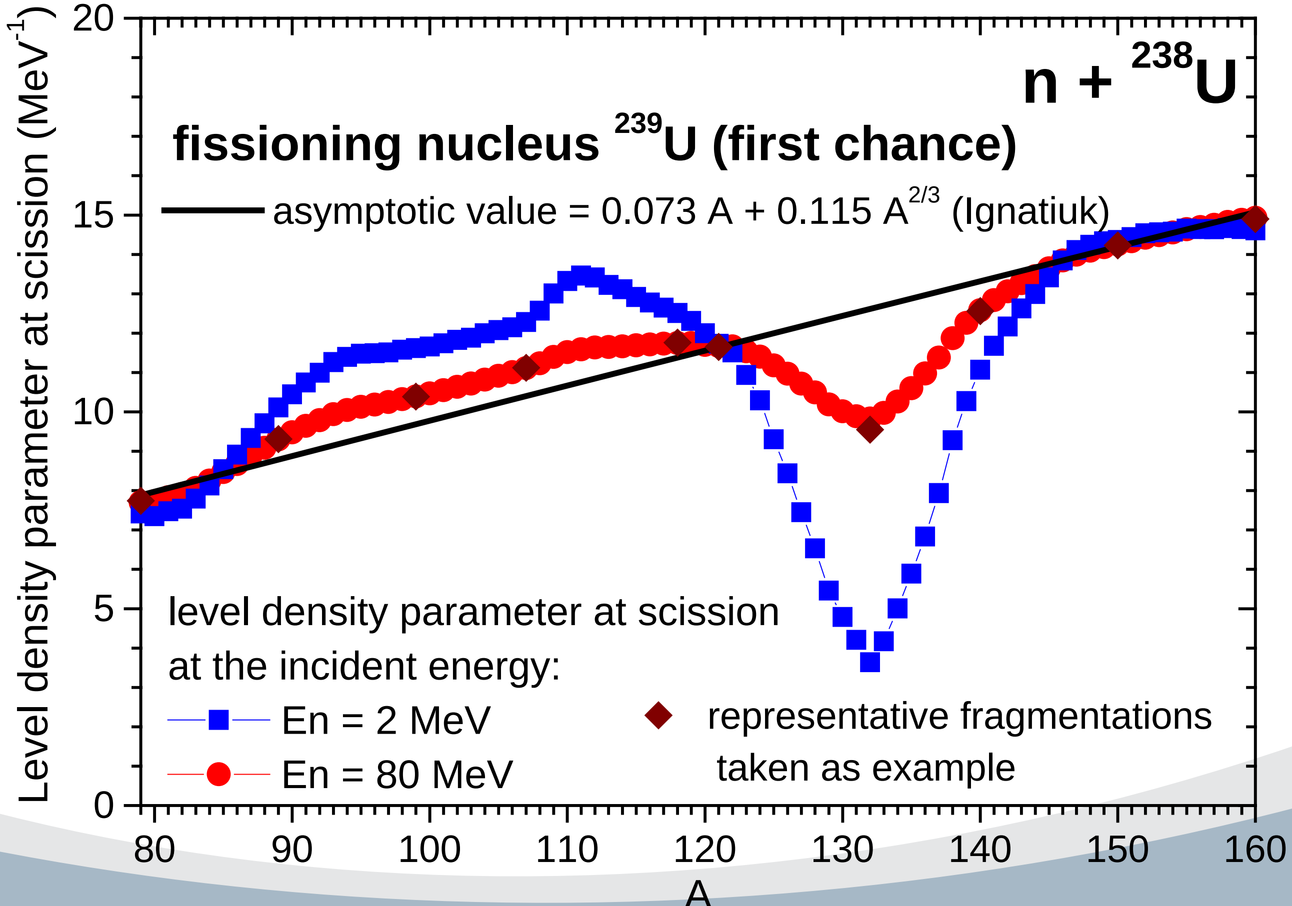
Red symbols: present results in which

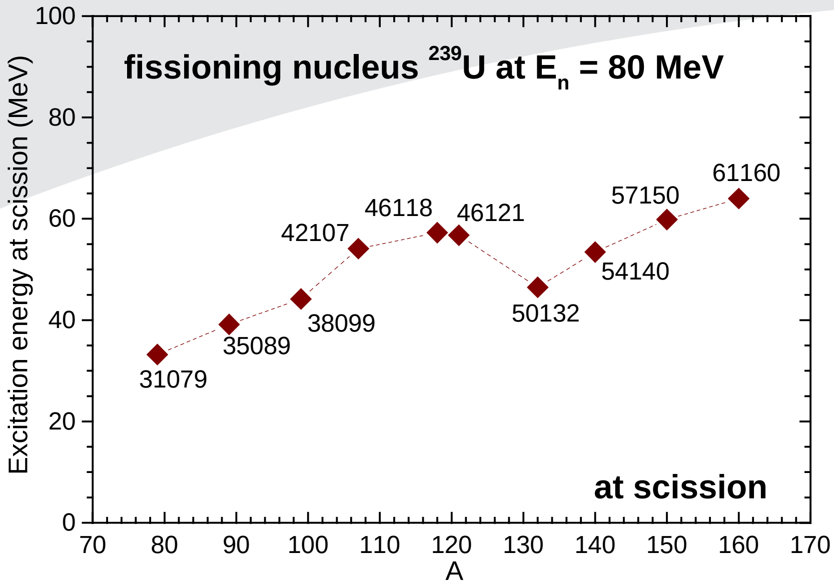
- $<\nu>_{FF}$: PbP results of ν(A) were averaged over Y(A) of GEF
- $<\nu>_{prefiss}$ based on RF of BRC (^{238}U) and ENDF/B-VII (^{235}U)

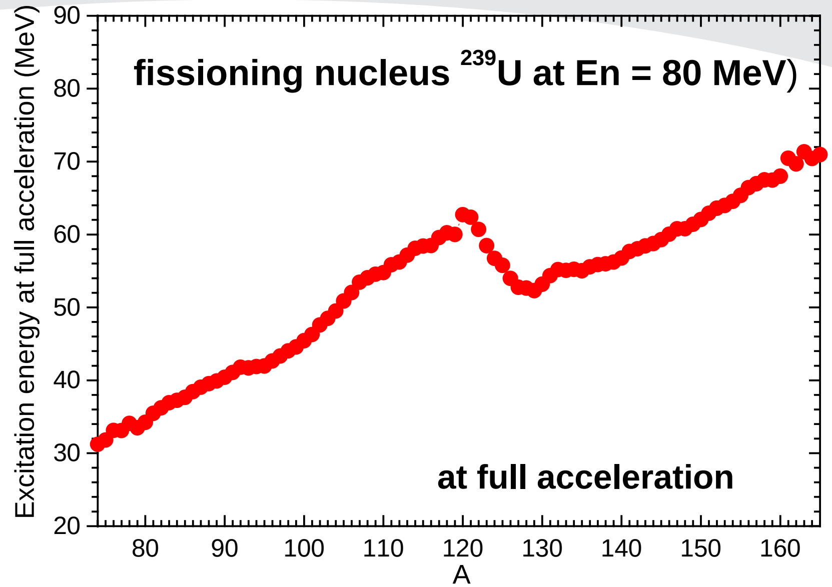


4.4 The vanishing of the sawtooth shape of individual ν(A) at high En is due to the damping of shell effects of a great part of fragments

At high En, e.g. 70 MeV, 80 MeV, the excit. energy of the first few compound nuclei of the main U chain and secondary Pa chain (which will be shared at scission) is high enough consequently for a great part of fragments the level density parameters (super-fluid model) tend to the asymptotic value.







Individual ν(A) can be taken as linear:

$$\nu(A) = \alpha A + \beta$$

Then $\nu_{pair}(A)$ is constant:

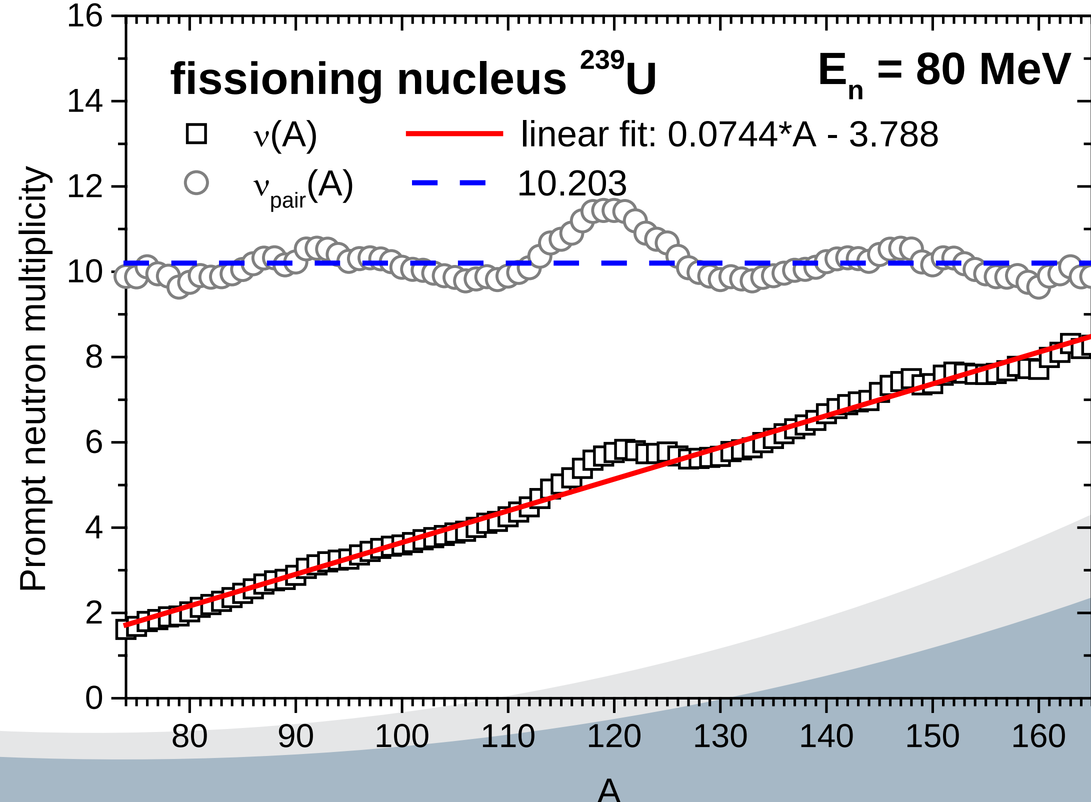
$$\nu_{pair} = \alpha A_0 + 2\beta$$

$$A_L + A_H = A_0$$

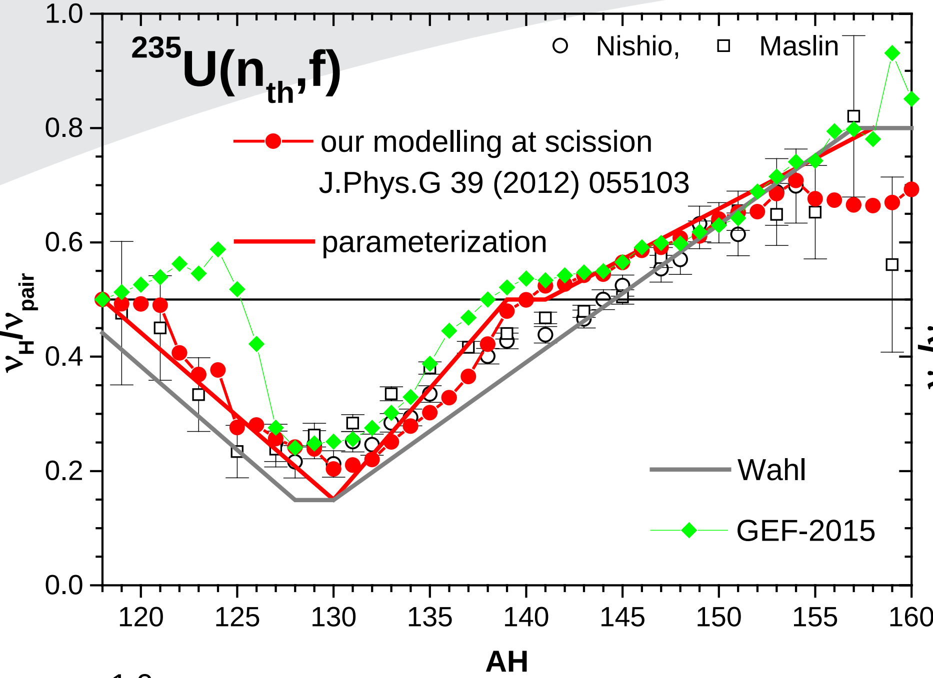
and the ratio

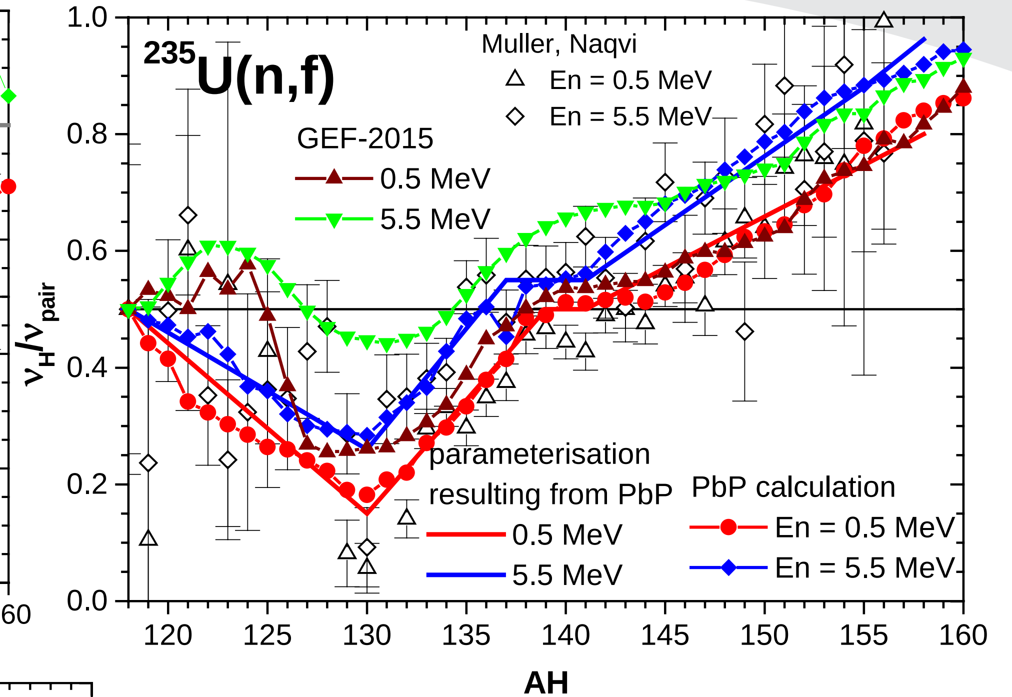
$$\nu_H / \nu_{pair}(A_H) = (\alpha / \nu_{pair}) A_H + (\beta / \nu_{pair})$$

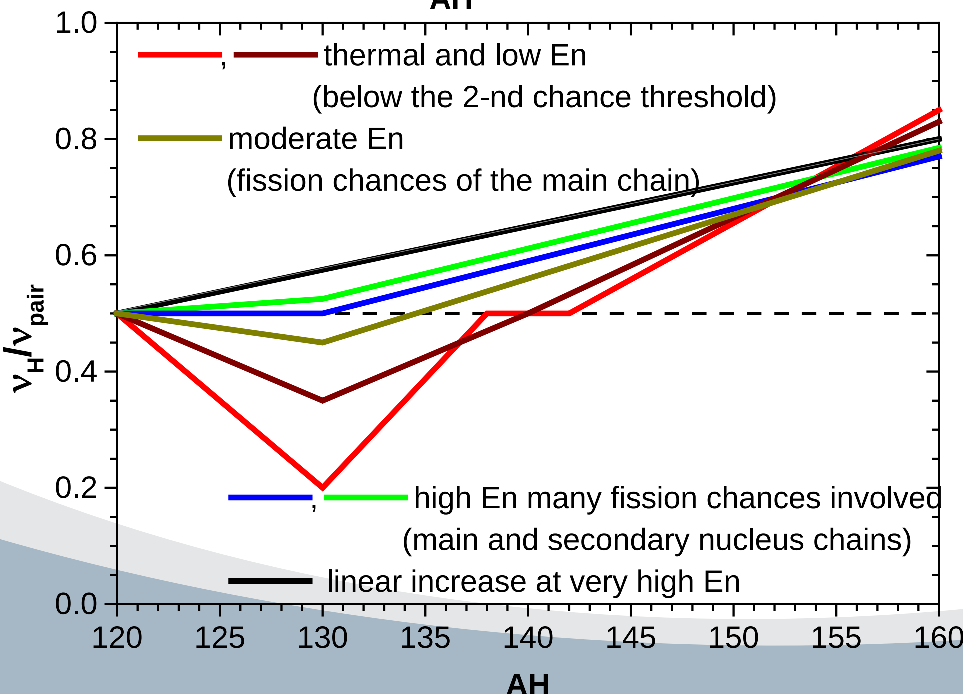
is also linear



Systematic behaviour of the ratio $\nu_H/(\nu_L+\nu_H)$ at low En







Schematic representation of the evolution of an individual ratio $\nu_H/(\nu_L+\nu_H)$ (A_H) with increasing En

(this ratio corresponds to the main compound nucleus undergoing fission)

When $\nu(A)$ is linear then this ratio is also linear:

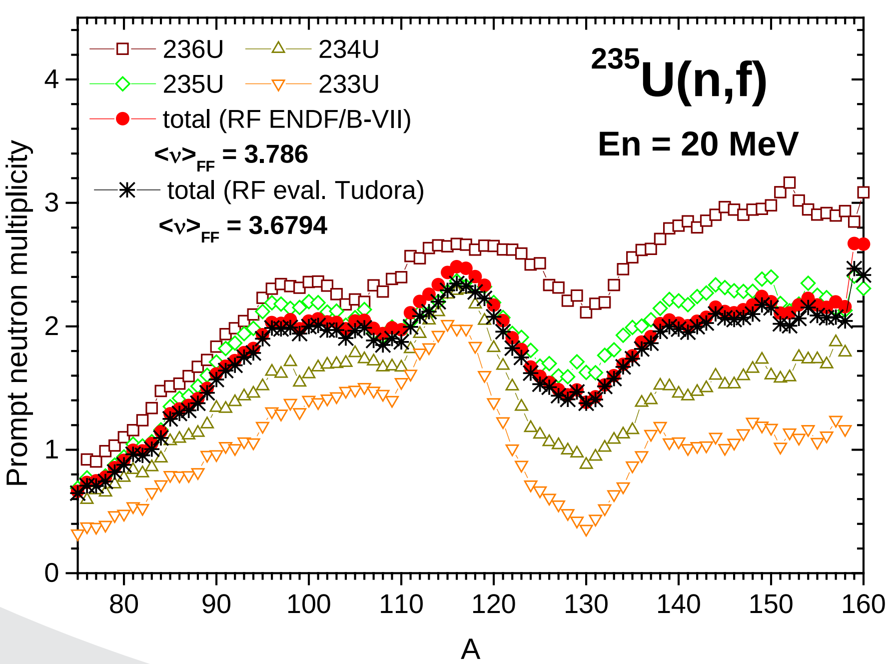
$$\nu(A) = \alpha A + \beta \qquad \nu_{pair} = \alpha A_0 + 2\beta$$

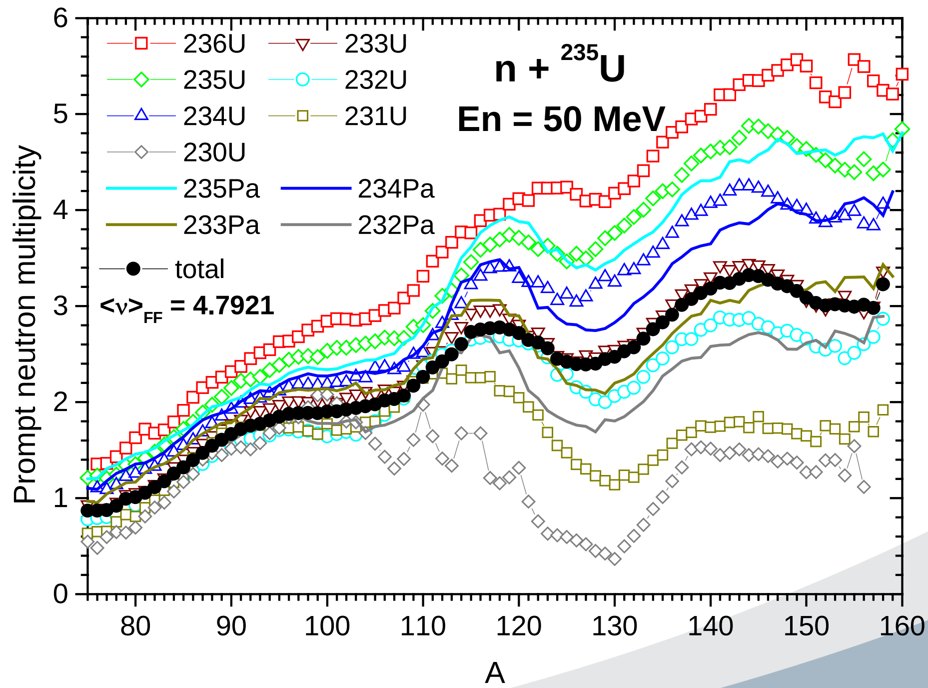
$$\nu_H / \nu_{pair}(A_H) = (\alpha/\nu_{pair}) A_H + (\beta/\nu_{pair})$$

Preliminary ν(A) results of ^{235}U(n,F) at En above 20 MeV

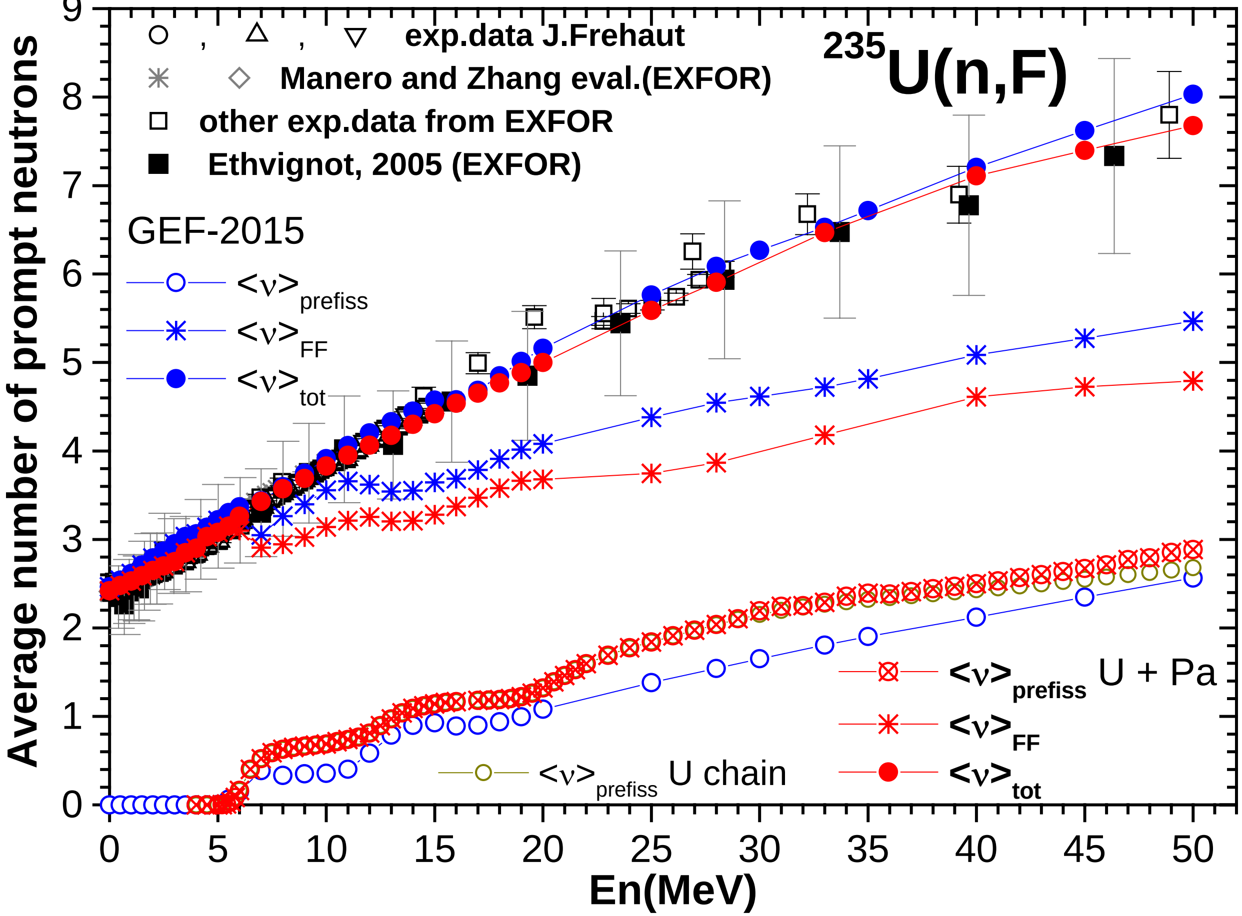
were obtained using RF of our neutron-induced cross section evaluation from 2004 up to En = 50 MeV.

Note, up to En = 20 MeV the total ν(A) results based on RF of our evaluation do not differ significantly from ν(A) based on RF of ENDF/B-VII.



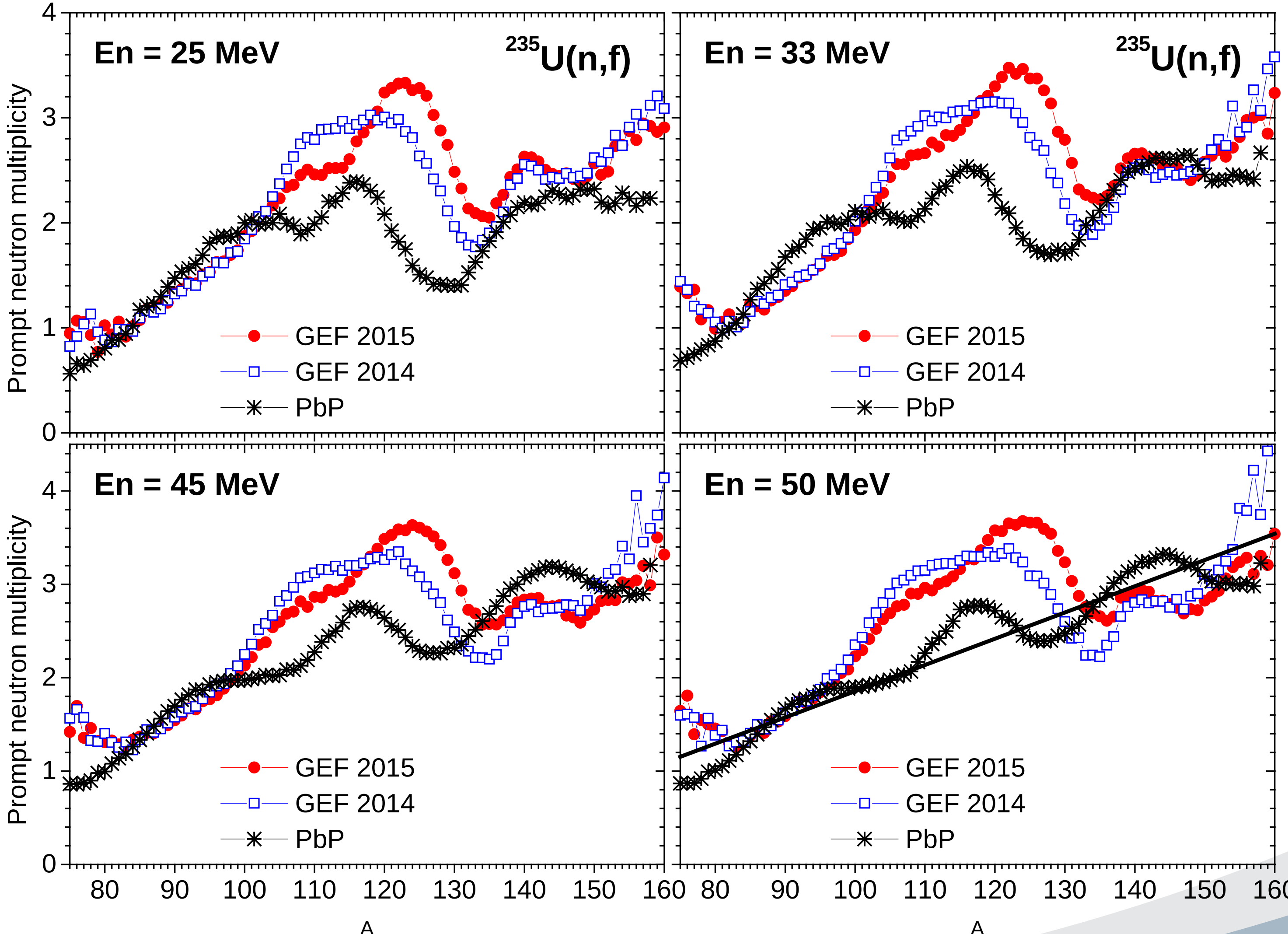


Indirect validation of predicted ν(A) by comparing $\langle\nu\rangle_{tot} = \langle\nu\rangle_{prefiss} + \langle\nu\rangle_{FF}$ with experimental data



- $\langle\nu\rangle_{tot}$ of PbP describe well the exp.data over the entire En range from thermal up to to 50 MeV.
- $\langle\nu\rangle_{tot}$ of GEF do not describe so well the data over the entire En range, it overestimates the data at En from thermal up to 5.5 MeV and at En form 11 MeV to 15 MeV. The good agreement with the data at En > 15 MeV is the result of a compensation effect: $\langle\nu\rangle_{FF}$ of GEF is higher than PbP and $\langle\nu\rangle_{prefiss}$ of GEF is lower than PbP in almost the same amount. The ν(A) results of GEF differ significantly (as shape and as magnitude) from the ones of PbP.

Comparison between ν(A) of PbP and GEF (vers.2015/2.2 and 2014/2.1)



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5. Conclusions

- ν(A) distributions are needed to obtain pre-neutron fragment distributions from the measured post-neutron fragment data. The lack of exp. ν(A) data at En where multiple fission chances are involved requires the use of ν(A) provided by model calculations.

- The PbP model can provide the individual ν(A) of the compound nuclei of the main and secondary nucleus chains that are undergoing fission at a given En. The total ν(A) is then obtained by averaging these individual ν(A) over the fission chance probabilities expressed as total and partial RF.

- The PbP calculations showed that the sawtooth shape of individual ν(A) becomes less pronounced with increasing excitation energy of the compound nucleus. At high En (70 MeV, 80 MeV) ν(A) corresponding to the first fissioning nuclei of the main and secondary nucleus chains exhibit an almost linear increase.

This is due to the complete damping of shell effects in the super-fluid expression of the level density parameter of most of the fragments.

- **An indirect validation of ν(A) is possible through the comparison of the calculated $\langle\nu\rangle_{tot}$ with existing experimental data.**

The PbP results of ν(A) averaged over available Y(A) (e.g. exp. data of JRC and Y(A) given by GEF) lead to $\langle\nu\rangle_{tot}$ in good agreement with exp. data.

- **The differences between ν(A) obtained by averaging the PbP results of individual ν(A) over RF of different evaluations (e.g. ENDF/B-VII, JENDL4, JEFF2.2) are insignificant.**

- **A comparison of present results with those of GEF revealed significant differences. Especially the ν(A) shapes at high En are different.**

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