Microscopic Level Density Treatment of Underlying Level Structure into Deformation Channels

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4th LACM-EFES-JUSTIPEN Workshop
Joint Institute for Heavy Ion Research, ORNL
March 15-17, 2010

Outline

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- Current objectives and challenges

- Treatment of Intermediate structure into fission channels
  - From classic R-matrix to deformation channels,
  - Individual states and level density construction,
  - Standard fission cross section formulations,
  - Monte Carlo R-matrix based fluctuations,
  - Input data sensibility ($\overline{D}$ distribution, V_{fi}, collectives states).

- AVXSF (Average CROSS SECTION Fission) story and modern code structure

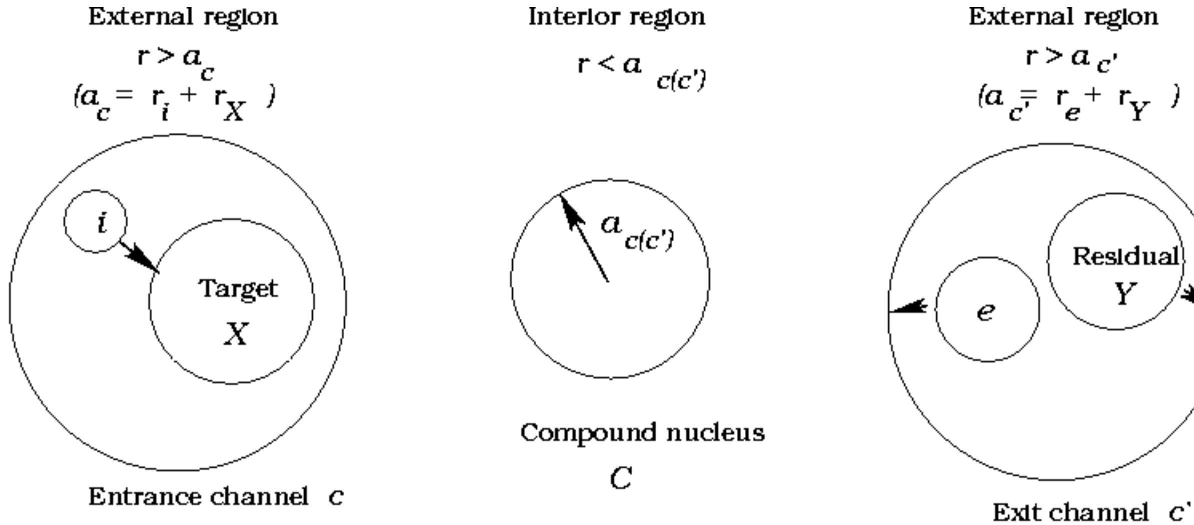
- Current and next stages – Shopping list

Current objectives and challenges

- **Improved accuracy for fission cross section calculations is needed to**
  - Better model current applications and new applications outside range of data library validation,
  - Better estimation of quantities other than cross section (fission fragments, fission spectra, etc.).
  - Reinforce our confidence in the estimation of parameter uncertainties (towards confident quality covariance data),
- **Must be achieved with better physics modeling relying on**
  - less adjusted parameters,
  - less phenomenology and,
  - less dependency on experimental fits.
- **Ongoing work (CEA/LANL framework) to create a modern and efficient tool, AVXSF (J. Eric Lynn) based, for evaluating accurate fission cross sections.**

Classic R-matrix theory in Resonance analyses

- R-matrix theory of nuclear reactions relies on:
  - an exterior region (nuclear interactions neglected): Schrödinger eq.,
  - an internal spherical region (φ_λ, E_λ unknown),



  - boundary conditions on reaction channels insure the connection.

Classic R-matrix theory in Resonance analyses (2)

- Introduces 2 major concepts
  - the reaction channel: maximum distance between the two bodies

    with,

    - entrance *c=[α, l, s, J]*; exit *c'=[α', l', s', J']*;
    - channel radii close to the saddle point

  - the R-matrix: allows the expansion of φ_λ as a linear combination of its eigenstates:

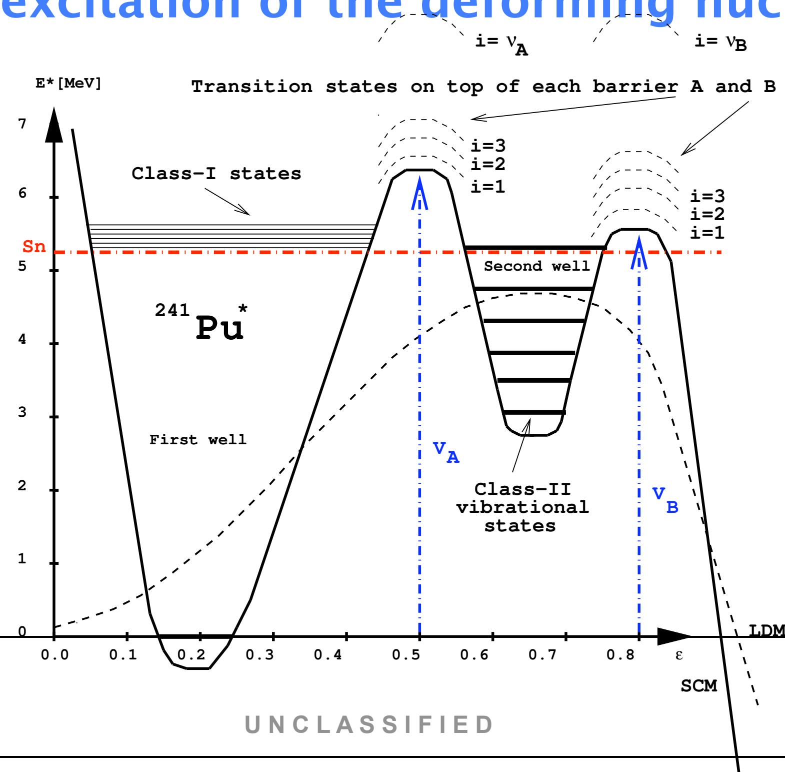
$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E},$$

Classic R-matrix theory in Resonance analyses (3)

- ❑ Original R-matrix fission channels seen as true particle reaction channels: fission products (masses, excitation states, *l*, *π*, etc.).

- ❑ Following A. Bohr theory (1956) based on fission channel at saddle point:

  “cold” deforming nucleus -> a few specific channels defined by the internal state of excitation of the deforming nucleus



Modern R-matrix theory in Resonance analyses

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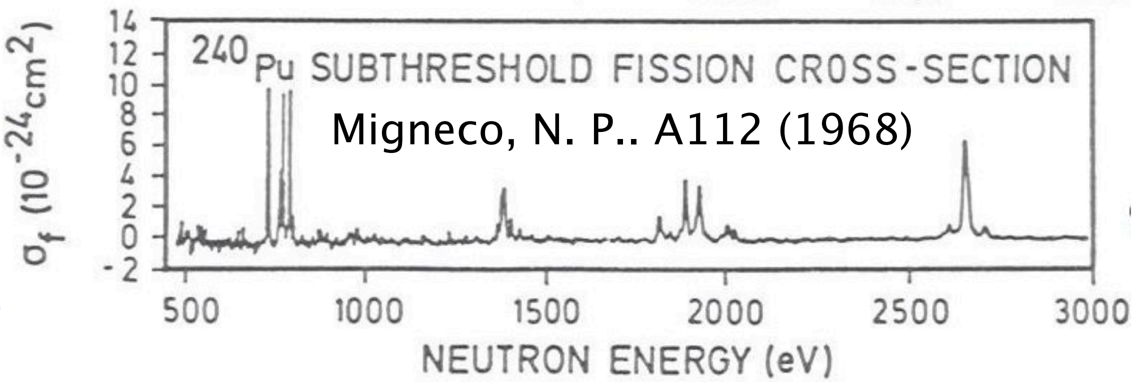
- A. Bohr's concept ("transitions states") based, modern R-matrix approximations such as Reich-Moore (1958) were developed.
  - RM hypotheses:
    - many photons channels resonance interferences cancel out:

$$A^{-1}_{\mu\lambda} \approx (E_\lambda + \Delta_{\lambda\gamma} - E - i\Gamma_{\lambda\gamma_{tot}}/2)\delta_{\mu\lambda} - \sum_{c=particle\ channels} \gamma_{\mu c} L^0_c \gamma_{\lambda c}$$

    - a few fission channels can be stipulated (2 in general)

E_λ, $\Gamma_{\lambda,n}$, $\Gamma_{\lambda,\gamma tot}$, $\Gamma_{\lambda,f1}$, $\Gamma_{\lambda,f2}$



R-matrix along the fission path

- Exp. proof of Intermediate states required the concept of deformation channel (surface shape→ η) and individual nucleon (intrinsic) coordinates (ξ) in the Schrödinger equation of the system.

$$H(\eta,\xi) = T_{\xi} + T_{\xi}(\eta) + \upsilon(\eta,\ \xi)$$

$$\equiv H_{\eta} + H_{\text{int}}(\xi,\ \eta_0) + H_c(\eta,\ \xi,\ \eta_0)$$

$\varepsilon_{\upsilon},(\eta),\ \Phi_{\upsilon}(\eta)$ ↙ ↘ $\varepsilon_{\mu}(\eta),\ \chi_{\mu}(\eta)$

- Strutinsky prescription of the deformation potential results usually in a double humped fission barrier

$$T_A(E) = \frac{1}{\left(1+\exp\left[2\pi(\upsilon_{F_A} - E)/\hbar\omega_A\right]\right)} \text{ and } T_B(E) = \frac{1}{\left(1+\exp\left[2\pi(\upsilon_{F_B} - E)/\hbar\omega_B\right]\right)}$$

with $E \rightarrow \upsilon_{F_A}$ and υ_{F_B}

Definition of *R*-matrix auxiliary states

- Expansion of the R-matrix internal states in terms of vibrational wave functions for a channel μ given such as

$$X_\lambda = \sum_{\mu,\nu} C^{\lambda}_{\mu,\nu}\, \chi_\mu\, \Phi_{\nu(\mu)}$$

↗

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

↘

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

The general R-matrix compound states are then established from the class-I and II by solving the Schrödinger equation

$$HX_\lambda = E_\lambda X_\lambda \Leftrightarrow \left(\varepsilon_\nu + \delta_\mu - E_\lambda\right) C^{\lambda}_{\mu,\nu} + \sum_{\mu',\nu'} C^{\lambda}_{\mu',\nu'} \times \left\langle \chi_\mu\, \Phi_{\nu(\mu)} \middle| H_c \middle| \chi_{\mu'}\, \Phi_{\nu'(\mu)} \right\rangle = 0$$

↘ $\Gamma_{\lambda II(c1)}$, $\Gamma_{\lambda II(f1)}$, $\Gamma_{\lambda II(c2)}$, $\Gamma_{\lambda II(f2)}$

Vibrational and intrinsic states characteristics

- **2 types of states might be present at the same excitation energy E_{exc}**
  - ✓ The vibrational states of collective nature $(500\ keV \le D_{\Phi_{\nu(\mu)}} \approx \hbar\omega \le 1200\ keV)$
  - ✓ The intrinsic states from combinations of single particle or hole states (D~100keV) (and so, $D_{II} >> D_I$)

  Note: $E_{II,\ ,g.s}$ is a least 2 MeV above $E_{I,g.s}$, less energy is available in the secondary well

- **Combined together to form band heads for rotational levels. It results in:**
  - ✓ the "Compound Nucleus" state sequences in the wells,
  - ✓ transition state sequences on top of the barriers.

$$E_N = (E_\nu + E_{\nu'} + \ldots\ldots + E_{\nu*}) + (E_{Vib} + E_{Vib'} + \ldots\ldots + E_{Vib*})$$

$$K_N = (\Omega_\nu \pm \Omega_{\nu'} \pm \ldots\ldots \pm \Omega_{\nu*}) \pm (K_{Vib} \pm K_{Vib'} \pm \ldots\ldots \pm K_{Vib*})$$

$$\pi_N = \pi_\nu \times \pi_{\nu'} \times \ldots\ldots \times \pi_{\nu*} \times \pi_{Vib} \times \pi_{Vib'} \times \ldots\ldots \times \pi_{Vib*}$$

Even-even CN vs. e-odd, odd-e and o-o

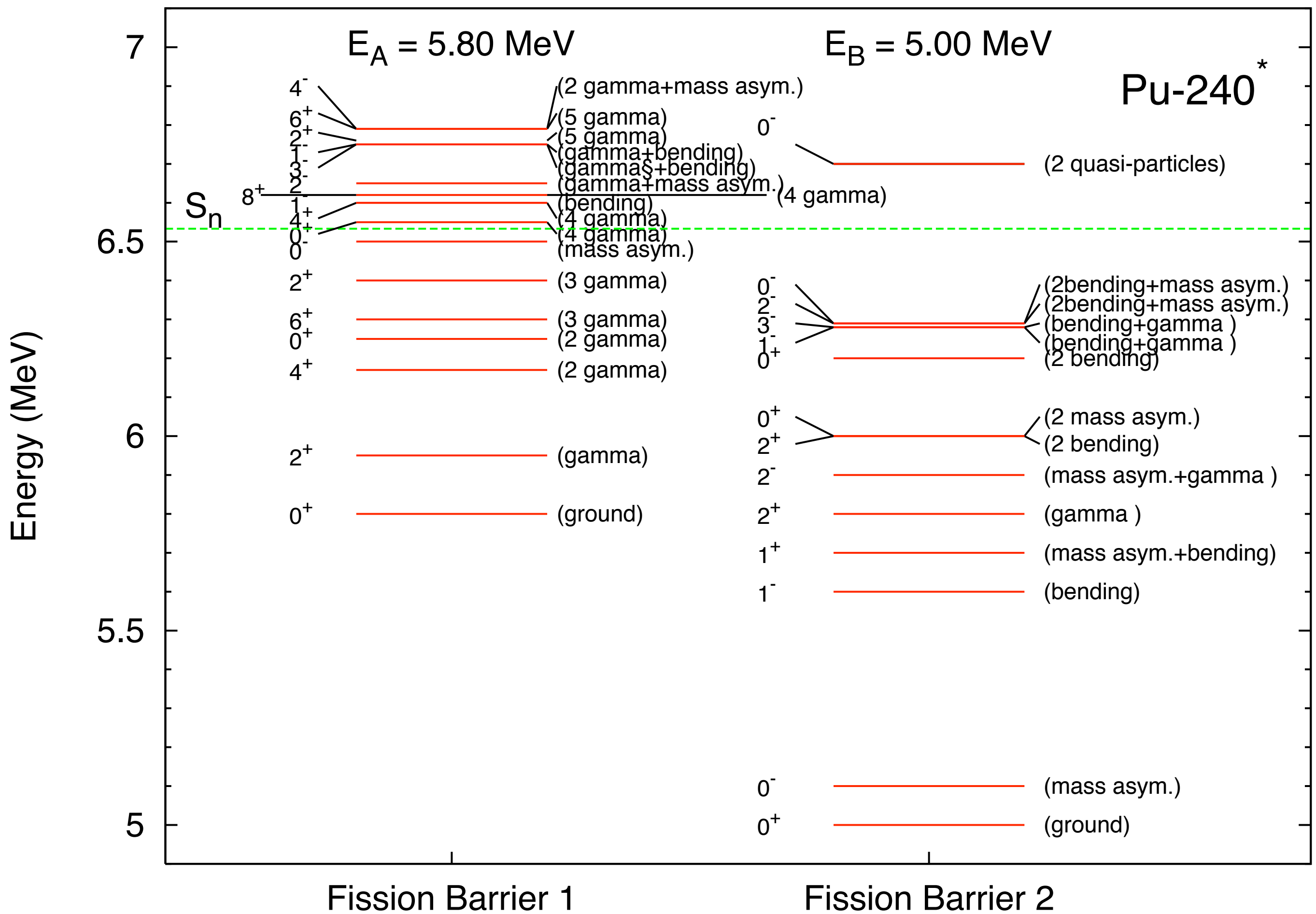
- Even-Even (^{240*}Pu): band heads (mainly vibrations β, bending, mass ass. and combinations of them) with rotational band build-up.

$$E_{rot}(J^\pi) = \frac{\hbar^2}{2\Im}\left[J(J+1) - K(K+1)\right] \text{ with } J^\pi = \begin{cases} K^\pi,\ (K+1)^\pi,\ (K+2)^\pi, \text{etc.} & \text{if } K \neq 0 \\ 0^+,\ 2^+,\ 4^+, \text{etc.} & \text{if } K = 0^+ \\ 1^-,\ 3^-,\ 5^-, \text{etc.} & \text{if } K = 0^- \end{cases}$$

- Odd (N)-Even (P) (^{241*}Pu): vibrations + independent particles (Nilson orbitals) spectrum ➔ neutron quasi-particle and vibration spectra combination; then rotational build up.

$$E_\nu^{qp}(\eta) = \sqrt{\left[\left(e_\nu^{p(n)}(\eta) - \lambda_{p(n)}(\eta)\right)^2 + \Delta_{p(n)}{}^2(\eta)\right]} \text{ with } \begin{cases} \lambda_{p(n)} \equiv \text{ Fermi energy} \\ \Delta_{p(n)} \equiv \text{ pairing energy} \\ e_\nu^{p(n)} \equiv \text{ single particle energy } (\hbar\omega_0\ unit) \end{cases}$$

Even–even excited nuclide ($^{240}Pu^*$)
Example of individual states input

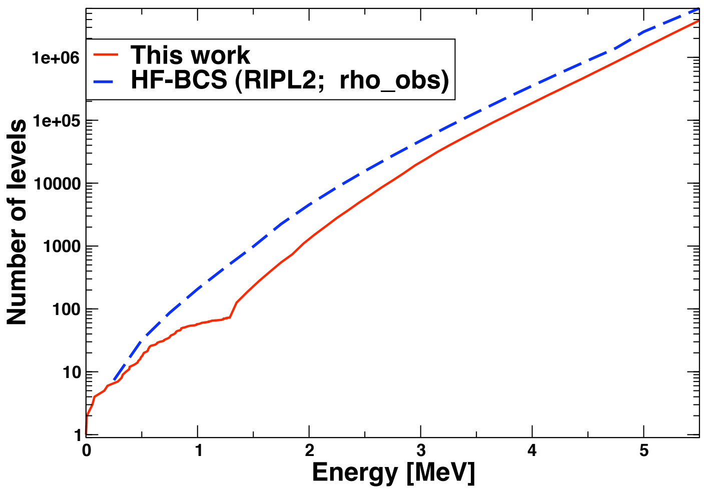


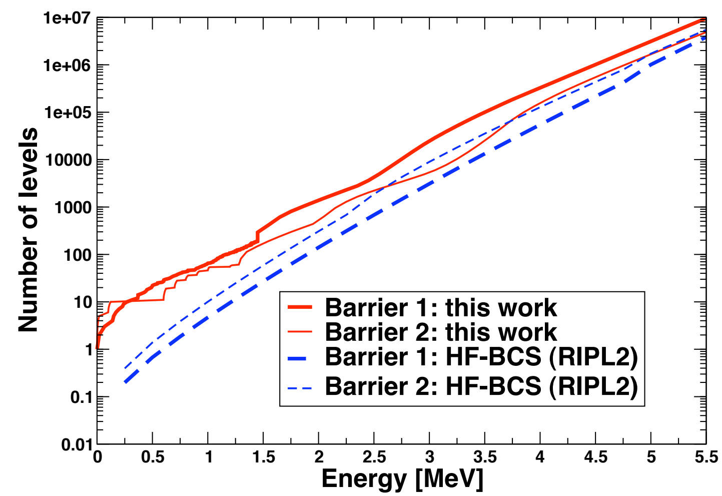
Combinatorial level density vs. Energy

- Combination of multi-quasi-particle states combinatorial + multi-vibrations and rotational band build-up,

$$U_N = E_N - \frac{1}{4}\sum_{i=n,p} \rho_{iS}\Delta_i^2(\eta) \qquad \text{'Blocking'} : \Delta'_{p(n)}(\eta) = \Delta_{p(n)} \exp\left[-q^2_{p(n),eff} \Big/ b_{p(n)} \right]$$

- Additional corrections can be made (loss of independent particle degrees of freedom to rotational and vibrational states with increasing energy).





Treatment of underlying intermediate structure (I.S) into fission channel: $^{239}Pu+n$

- Strong coupling with class-I and II fluctuation factors approximated (HF limit, $T_A \geq T_B$)

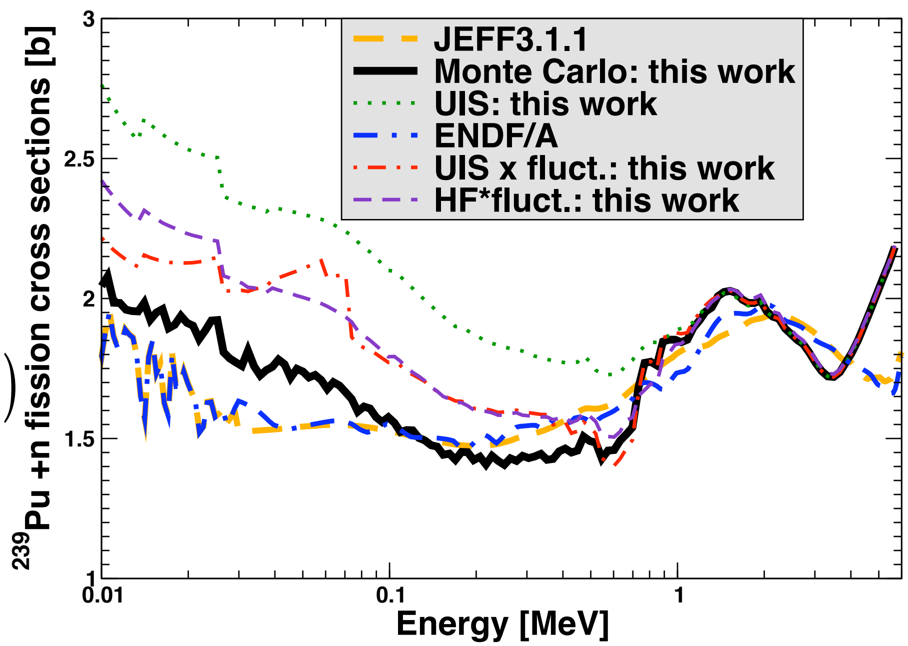
$$T_{AB}^{eff}(E_x) = \frac{T_A(E_x)T_B(E_x)}{T_A(E_x)+T_B(E_x)} \times S_{nf}^{I} \times S_{AB}^{II}$$

- Uniform spreading of the class-II state strength over the fine structure

$$\sigma_{nf}^{(un)} = \pi.\lambda bar.T_{I(n)}\left(1+b^2+2b\coth\left(\left(T_A+T_B\right)/2\right)\right)$$

- UIS $\times S_{nf}^{I} \times S_{AB}^{II}$:

Lower significantly the average fission cross section



- Full MC calculation of the fluctuation factors based on R-matrix theory in deformation space channel exhibiting microscopic level densities characteristics

Realistic MC calculations of intermediate structure and statistical fluctuations combined effects.

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- **The sampling procedure for each incident neutron energy involves**
  - ✓ A unique set of 500 class-I energies sampled from a generalized Wigner distribution with long range correlations

$$p(s)ds = K_\nu s^\nu \exp\left[-C_\nu s^2/\pi^2\right]ds$$

  - ✓ Average of the fluctuating fission cross section over N samplings of the class-I (except energies) &II level parameters and of the associated coupling Hamiltonian.

$$\left\langle \sigma_{n,f}^{HF\ with\ fluct}(E)\right\rangle = \pi \frac{\lambda_n^2}{4\pi^2} g_n \frac{1}{N} \frac{1}{\left\langle \Delta E\right\rangle_N} \sum_{S=1}^{N} \left(\sum_{c'}^{\substack{number\ of\\ fission\\ channels}} \left(\frac{\Gamma_n(E)\Gamma_{f,c'}(E)}{\Gamma_{tot}(E)} \right)_{channel} \right)_S$$

  - ✓ The fluctuating fission cross section is then renormalized to the correct total cross section magnitude.

$$\left\langle \sigma_{n,f}^{HF-UPF\ with\ fluct}(E)\right\rangle = \left\langle \sigma_{n,f}^{HF\ with\ fluct}(E)\right\rangle \frac{\left\langle \sigma_{n,tot}^{HF-UPF}(E)\right\rangle}{\left\langle \sigma_{n,tot}^{HF\ with\ fluct.}(E)\right\rangle}$$

Zoom on class-I & II fission resonance parameters sampling (2)

- Determination of E_λ and X_λ $(HX_\lambda = E_\lambda X_\lambda)$
  - ✓ Case $\Gamma_{\lambda II}(f) << D_{II}$ and $\Gamma_{\lambda II}(f) <<$ few D_I

$$C_{\lambda(\lambda_I)} = -\frac{\langle H^2(\lambda_I \lambda_{II})\rangle}{E_{\lambda_I} - E_\lambda} C_{\lambda(\lambda_{II})} \text{ and } C^2_{\lambda(\lambda_{II})} = \left[\sum_{\lambda_I} \frac{\left|H(\lambda_I \lambda_{II})\right|^2}{\left(E_{\lambda_I} - E_\lambda\right)} + 1\right]^{-1}$$

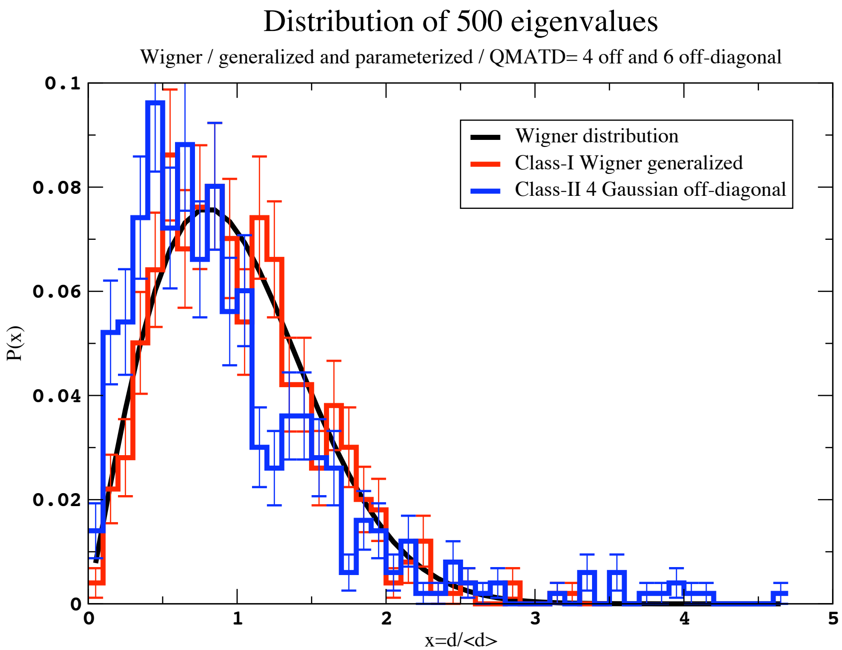
  - ✓ Finally, in narrow resonance approximation

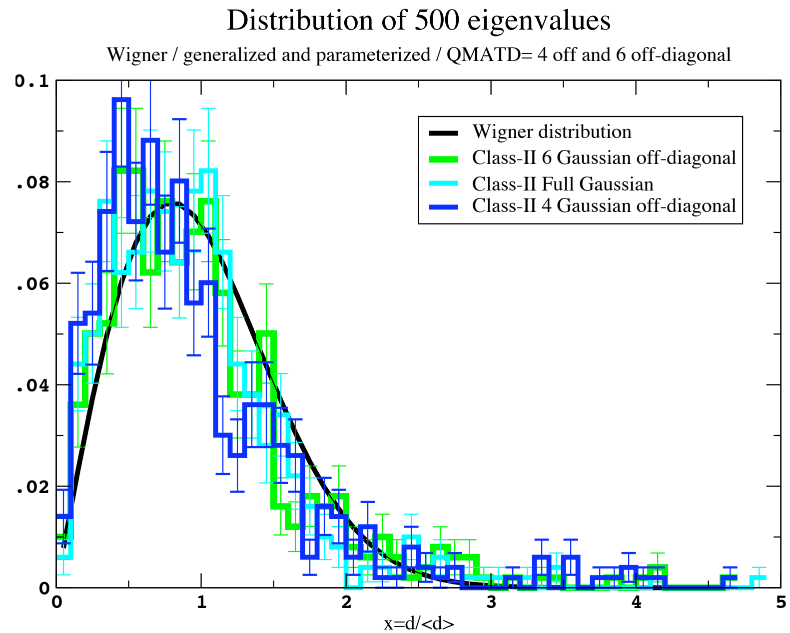
$$\Gamma_\lambda(f) = \sum_{\beta=1}^{\nu_{outer}} C^2_{\lambda(\lambda_{II})} \Gamma_{\lambda_{II},\beta}(f)$$

Input data sensibility:
Class-I vs. class-II states spacing distributions

Class-I: quantum chaos properties

Class-II: departure from chaos properties – **How far from chaos?**



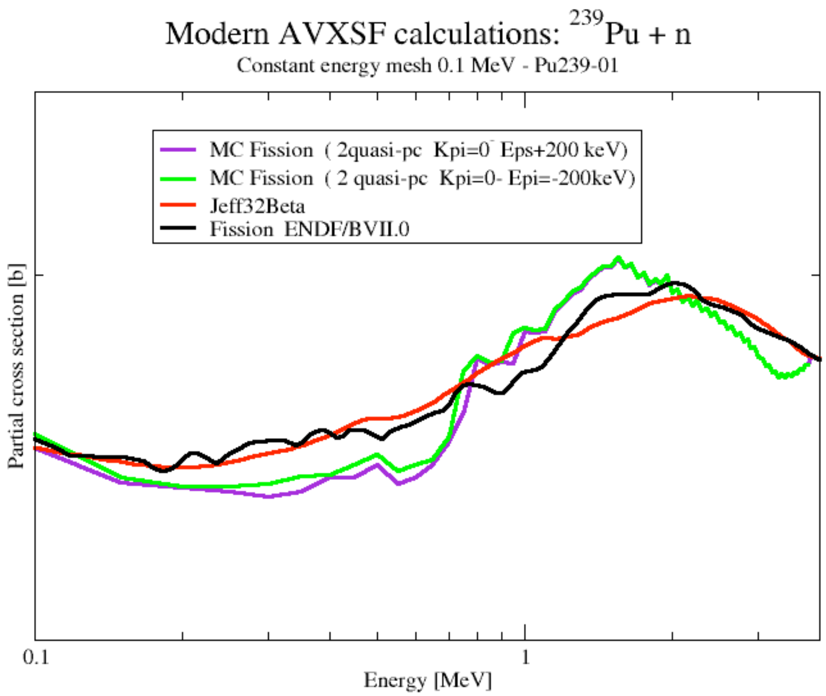


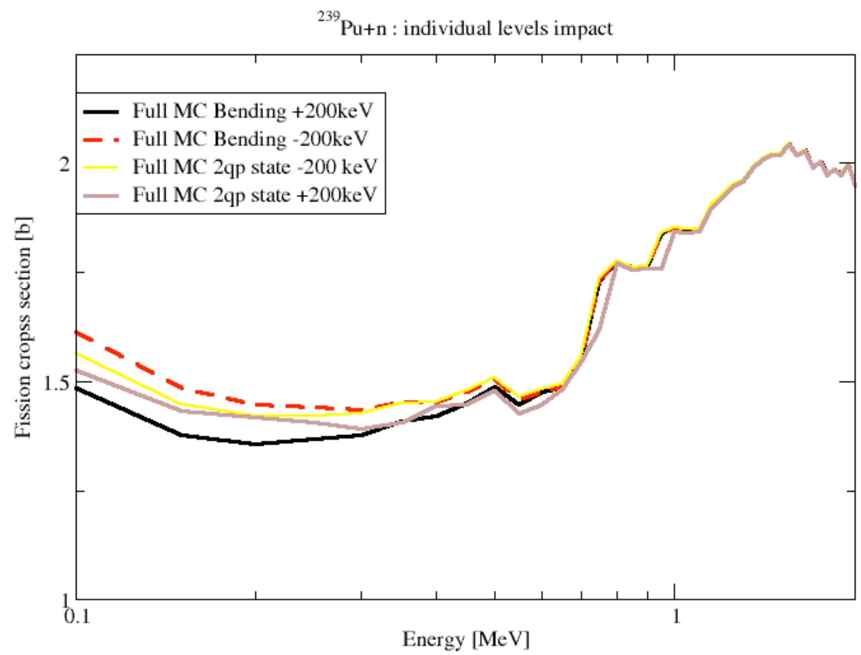
Distribution type	Wigner	Class-I	Class-II 4-off G	Class-II 6-off G	Class-II Full G
Mean	1.0	1.006	0.9435	1.001	0.954
Variance	1.273	1.298	1.406	1.467	1.299

Input data sensibility: individual s.p. and collective states energies

- **Level density sensibility:** impact of ±200 keV uncertainty
Inelastic (E_n>1.3MeV), inner barrier (E_n>0.7MeV) , outer barrier (E_n>0)

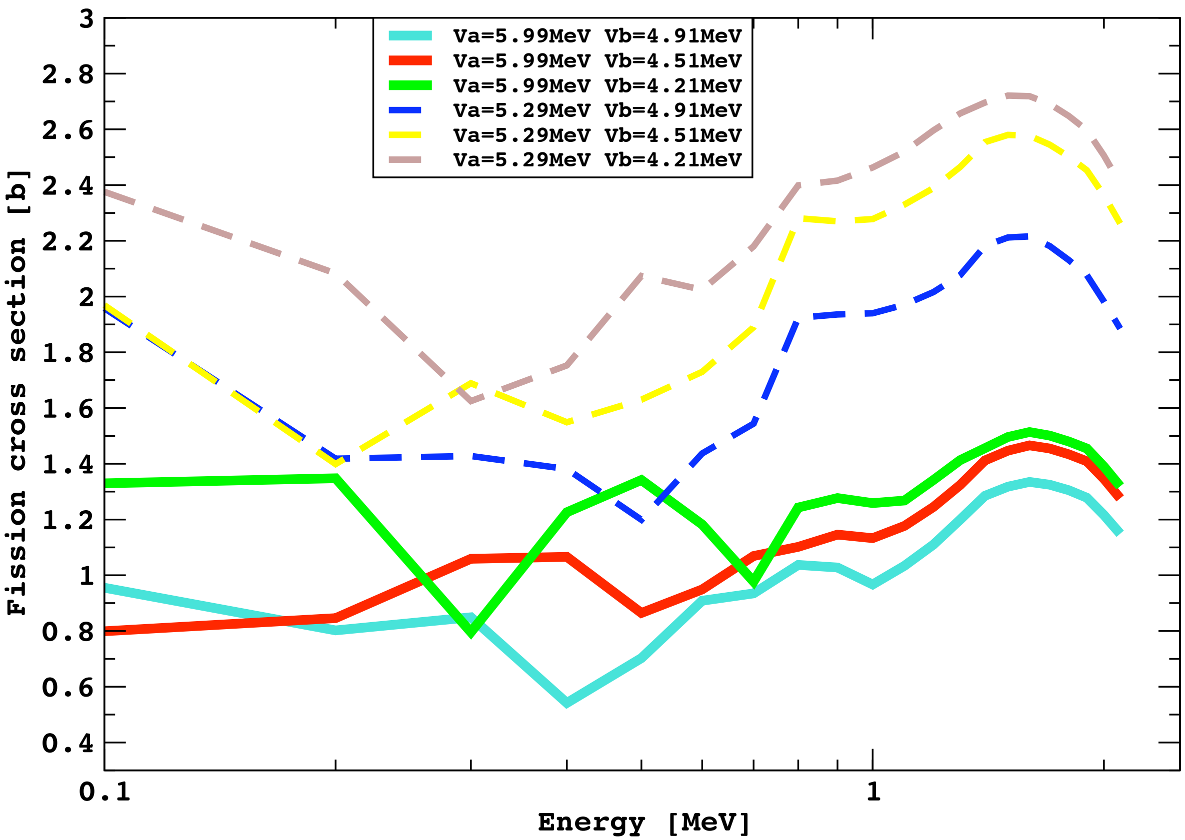
- **Accurate Intermediate Structure calculation is somehow less critical except for a few Kπ values (e.g: 0^-, 0.7MeV, m.asym; 2^-, 0.7MeV, bending; 0^-, 1.4MeV, 2qp, etc.)**





Input data sensibility: barrier height values

^{239}Pu neutron induced fission cross section vs barrier heights
(with MonteCarlo fluctuations and based on Moller s.p. 2009)



- Quoted uncertainties on barriers heights ±0.7 to ±1 MeV

Barrier and level density values are strongly correlated

AVSXF story (1970 –): J. Eric Lynn

- **URR fission cross section representation over the ages;**

1960-1970: Class-II observed and explained (Strutinsky, Michaudon, Paya, Lynn, Weigmann, etc.)

1960| - - - - - - 1970 - - - - - - 1980- - - - - - 1990- - - - - - 2000- - - - - - 2010 →

1970	1980	2000	2010
AVXSF-1,	GNASH	GNASH(BRC)	McGNASH
	EMPIRE	STATIS	CONRAD
	SAMMY,FITACS	SAMMY-FITACS	AVXSF-15
		TALYS	EMPIRE2.19

- **Weaknesses;**
  - Neutron entrance channel transmission coefficient,
  - Programming (language, structure), portability, robustness.

Modern AVXSF code structure

- **Modern AVXSF code structure (2008-)** [CEA-LANL **collaboration framework**]

  - AVXSF being re-written in modern Fortran 95 and architecture under XCODE platform and SUBVERSION management,
  - Series of test cases to insure Quality Insurance,
  - Towards a single consistent input data set per nuclide consistent for a suite of isotopes,
  - Need to be coupled with modern O.M. c.c. calculations,
  - S.p. orbitals energies and level densities libraries foreseen.

Present status and tasks in progress

- More accurate calculations of Intermediate Structure average cross sections are NOW available using MC calculations based on microscopic R-matrix theory with underlying I.S

    - ✓ This effect is significant relatively to current approximate prescriptions (up to 20%),

    - ✓ The effect of the SLBW approximation between class-II states is being quantified (Reich-Moore implemented),

    - ✓ The impact of the type of class-II distribution (departure from chaos) is being studied,

    - ✓ Monte Carlo convergence is being checked.

- Homogenization/consistency of input data is seeked for the complete suite of Pu isotopes relying on single set of data, more theoretical background (macro-micro or micro) and recent experimental data (LANSCE support).

Shopping list

More information is desired on

- In general on class-II states distributions,
- Collective, single-particle states and level densities,

$$(e_{\nu}^{p(n)}, \lambda_{p(n)}, \Delta_{p(n)}, \hbar^2/2\Im\ , ...)$$

- Barrier parameters (heights, curvatures) and validity of the one dimension projection and inverted parabola approximation,

  ➔ One dimension (possibly curvilinear axis) numerical barrier.

- Branching ratios between different fission modes,
- Realistic uncertainties on those quantities.

Thank you for your kind attention