An analytic approach to probability tables for the unresolved resonance region?

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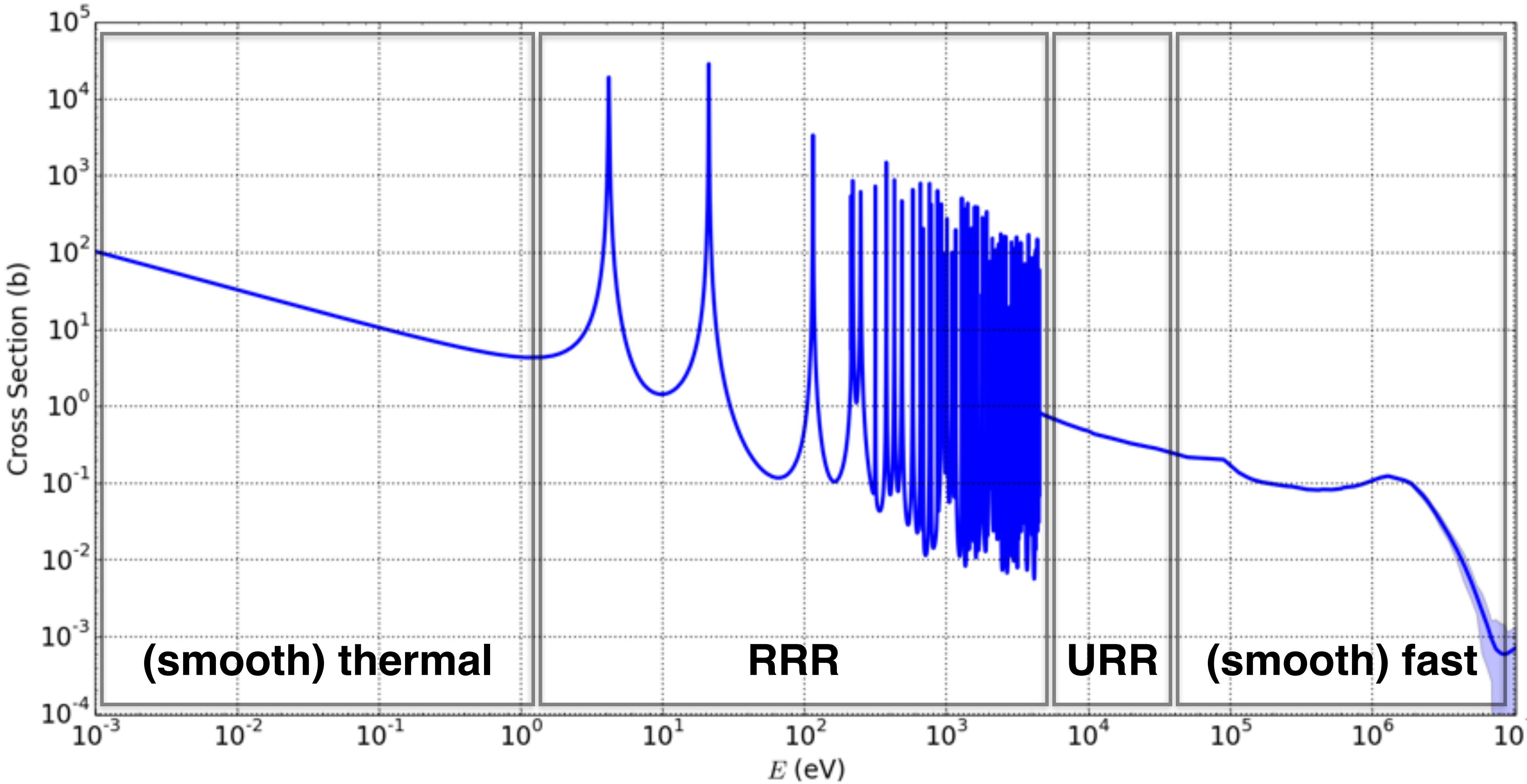
In ENDF libraries, the matching between RRR, URR and Fast has always been problematic



In ENDF, the RRR, URR and Fast regions are described with wildly different approaches

- **RRR uses various R-matrix approximations**
  - SLBW, MLBW, Reich-Moore and full R-matrix in Wigner-Eisenbud formulation
  - Stored as set of $\{E_R, \Gamma_{R\gamma}, \Gamma_{Rn}, \ldots\}$
- **URR formulated with R-matrix, but energy-averaged over resonances**
  - SLBW only, weak coupling limit in ENDF (want to fix that if possible)
  - Stored as $\{\langle D(E)\rangle, \langle\Gamma_\gamma(E)\rangle, \boldsymbol{\nu}_\gamma, \langle\Gamma_n(E)\rangle, \boldsymbol{\nu}_{n}, \ldots\}$
  - Meant to be used for average cross section & "probability tables"
- **Fast region derived from Hauser-Feshbach theory with WFC**
  - Only average cross sections (& distributions) stored, after things like WFC applied
  - WFC is phenomenological adaption of SLBW result

Conventional wisdom

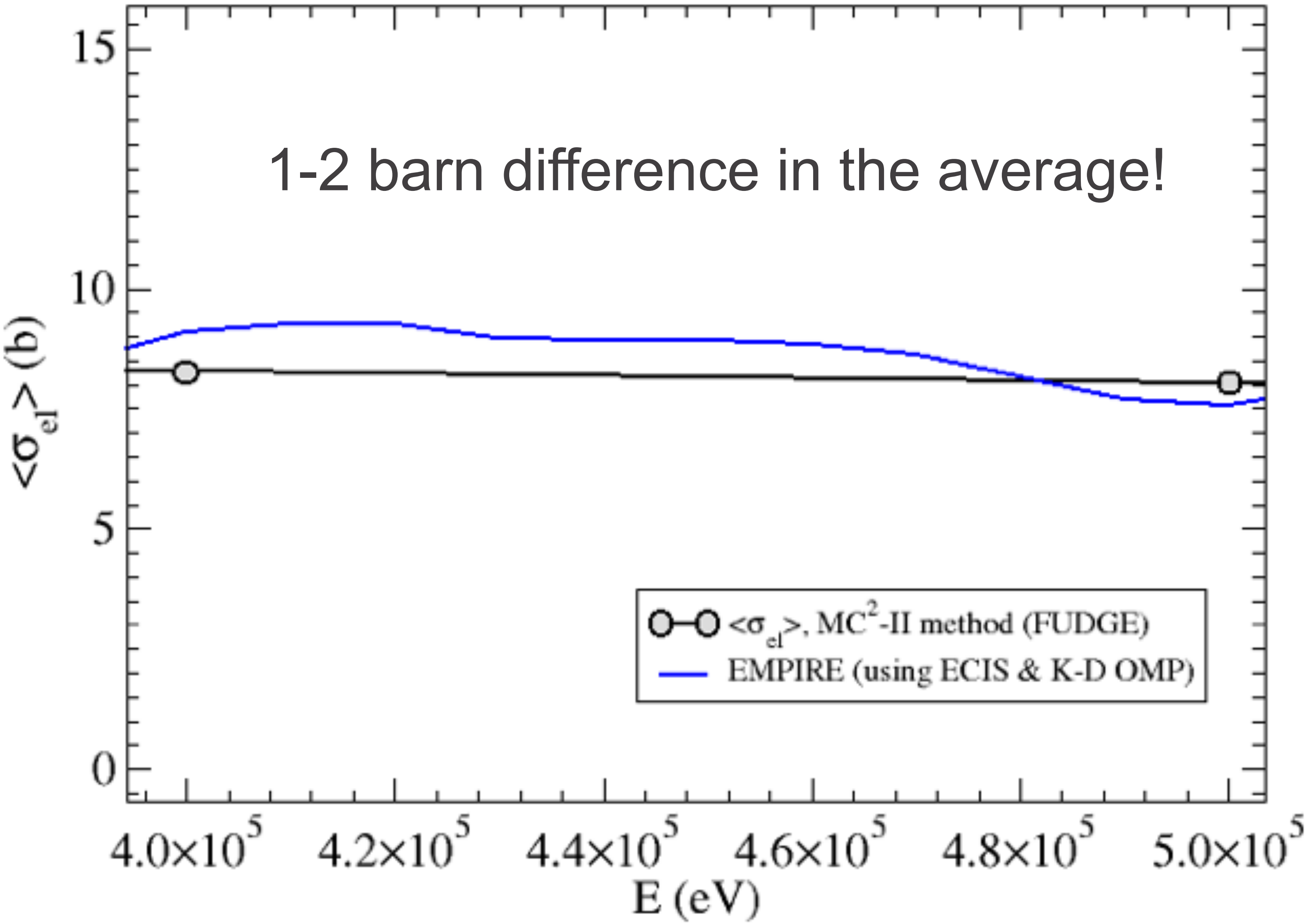
- The energy average URR cross section should equal the output from a Hauser-Feshbach code, at least approximately

$$\left\langle \sigma_{el}^{URR} \right\rangle \approx \left\langle \sigma_{el}^{HF} \right\rangle$$

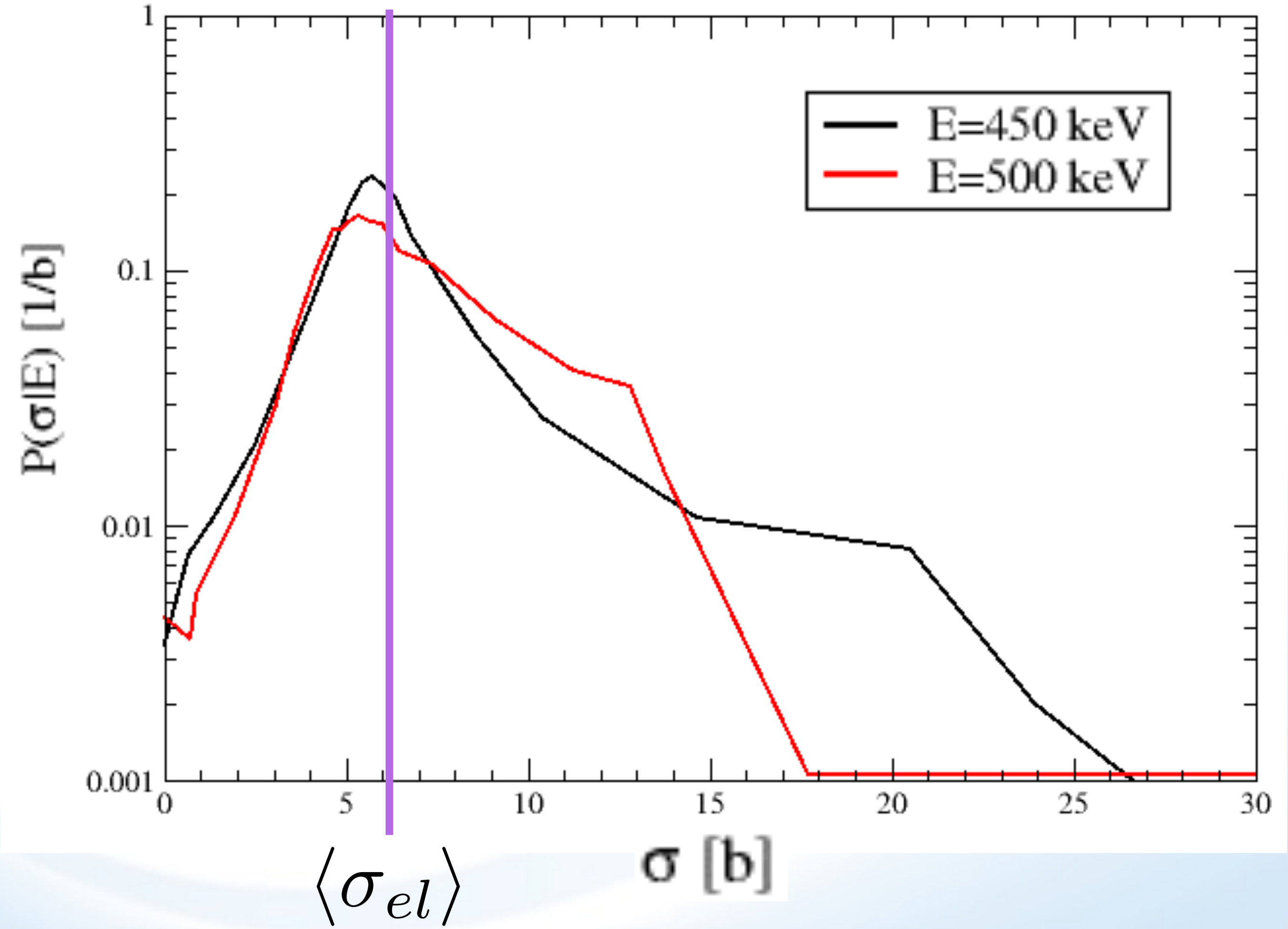
- so I did an experiment…

(I could look at other channels too, but I'm testing with 90Zr which only has elastic scattering and capture)

^{90}Zr(n,el) in URR



In the URR, cross section fluctuates wildly so need cross section probability distribution, P(σ|E)



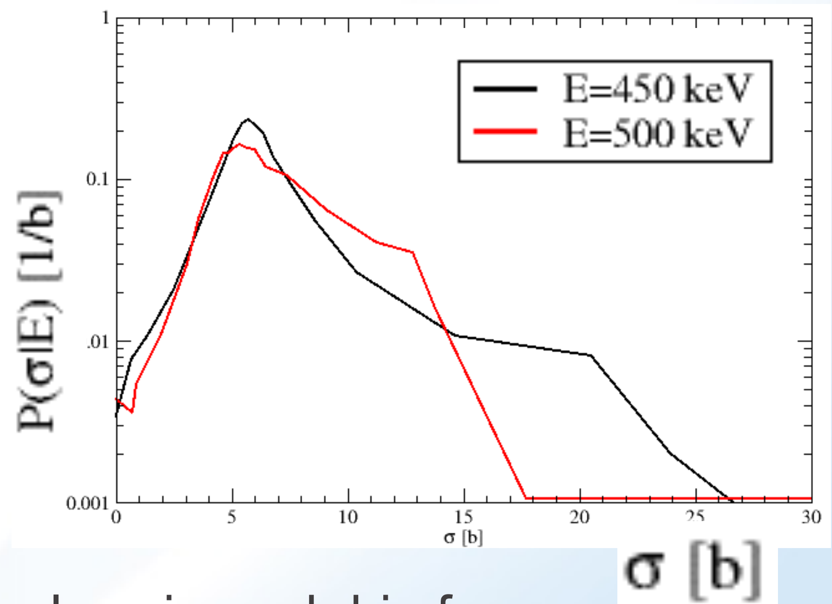
90Zr(n,el) calculation from NJOY2012

In the URR, cross section fluctuates wildly so need cross section probability distribution, P(σ|E)

Brute force used in processing

- Monte-Carlo realizations of resonances (of various quality)
- Compute cross section for each realization (usu. SLBW)
- Group cross sections in fine bins
- Then either
  - Make histogram of cross section values in each bin from realizations (e.g. NJOY, AMPX)
  - Match moments of cross sections (e.g. CALENDF)

90Zr(n,el) calculation from NJOY2012



But… is there a better way? Could we compute $P(\sigma_x|E)$ analytically?

The Idea:

- **Assume $P(\sigma_x|E)$ is approximately log normal or maybe chi^2 or Poisson**
  - looks like Gaussian PDF
  - but with constraint that $\sigma_x>0$
- **Compute $\langle\sigma_x\rangle$ and $cov(\sigma_x,\sigma_y)=\langle\sigma_x\sigma_y\rangle-\langle\sigma_x\rangle\langle\sigma_y\rangle$ using WFC-like approach**
- **Convert to form appropriate for our assumed PDF**

Both URR & HF w/ WFC use same basic theory, but key differences

URR

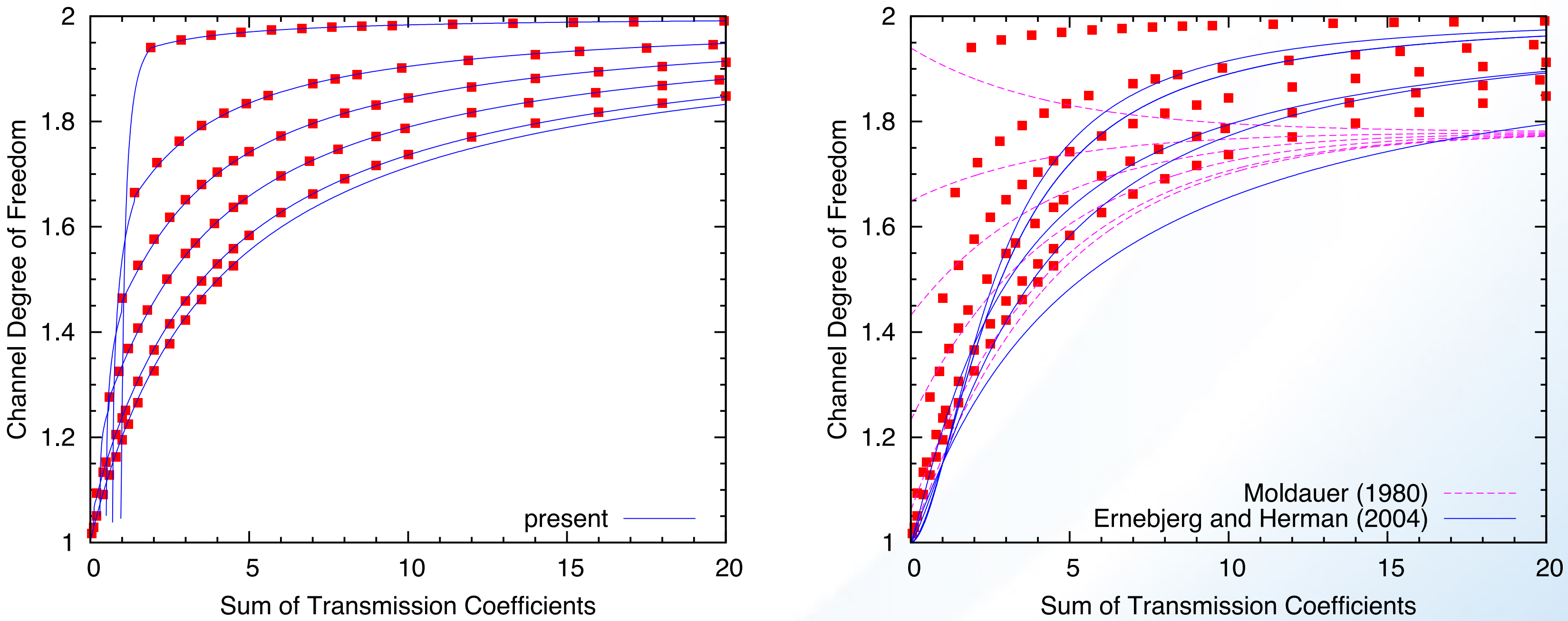
1. Energy average SLBW
2. Assume weak coupling so have narrow isolated resonances
3. Ensemble average over SLBW widths using Porter-Thomas
4. **DOF given in ENDF file by evaluator**
5. Implement with MC^2-II algorithm

HF with Moldauer WFC

1. Energy average SLBW
2. Assume weak coupling so have narrow isolated resonances
3. Ensemble average over SLBW widths using Porter-Thomas
4. **Phenomenological DOF in terms of Tc's: can correct for weak coupling approximation**

Kawano-Talou systematics for DOF helps WFC work in strong coupling limit

Channel Degree Freedom as Functions of $\sum T$



Each curve and symbols correspond to the case of $T_a = 0.95$, 0.7, 0.5, 0.3, 0.1, and 0.01 from the top to the bottom.

Moldauer's asymptotic value is 1.78, not 2.0.

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Moral: they can be made to agree

Let's review the WFC derivation for the compound nuclear cross section

1. Energy average the SLBW cross section:

$$\langle \sigma_{cc'} \rangle = \frac{1}{\Delta E} \int_{E-\Delta E/2}^{E+\Delta E/2} dE' \sigma_{cc'}(E')$$

2. Assuming narrow isolated resonances, extend integral

$$\langle \sigma_{cc'} \rangle \approx \frac{4\pi g_c}{\Delta E k_c^2} \sum_{\mu} \frac{\Gamma_{c\mu}\Gamma_{c'\mu}}{4} \times \int_{-\infty}^{\infty} dE' \frac{1}{(E - E_0)^2 + \Gamma_{\mu}^2/4}$$

$$\approx \frac{2\pi g_c}{D_c k_c^2} \sum_{\mu} \frac{\Gamma_{c\mu}\Gamma_{c'\mu}}{\Gamma_{\mu}}$$

this is straightforward pole integration

… conclude derivation

3. Now do ensemble average

$$\sum_{\mu}\frac{\Gamma_{c\mu}\Gamma_{c'\mu}}{\Gamma_{\mu}} = \int_0^{\infty} d\Gamma_c\ \wp^{PT}\left(\frac{\Gamma_c}{\overline{\overline{\Gamma}}_c}\middle|\nu_c\right) \times \int_0^{\infty} d\Gamma_{c'}\ \wp^{PT}\left(\frac{\Gamma_{c'}}{\overline{\overline{\Gamma}}_{c'}}\middle|\nu_{c'}\right) \times \prod_{c''\neq c,c'}\int_0^{\infty} d\Gamma_{c''}\ \wp^{PT}\left(\frac{\Gamma_{c''}}{\overline{\overline{\Gamma}}_{c''}}\middle|\nu_{c''}\right)\frac{\Gamma_c\Gamma_{c'}}{\Gamma}$$

get usual cross section with WFC

$$\langle\sigma_{cc'}\rangle = \frac{2\pi g_c}{k_c^2 D_c}\frac{\overline{\Gamma}_c\overline{\Gamma}_{c'}}{\overline{\Gamma}}\left(1+\delta_{cc'}\frac{2}{\nu_c}\right) \times \int_0^{\infty} dt \prod_{c''}\left(1+\frac{2t\overline{\Gamma}_{c''}}{\nu_{c''}}\right)^{-(\delta_{cc''}+\delta_{c'c''}+\nu_{c''}/2)}$$

Let's do the compound nuclear cross section correlation the same way

- This time, the energy average gives us

$$\langle \sigma_{cc'} \sigma_{c'c''} \rangle \approx \frac{\pi/4}{\Delta E} \left(\frac{4\pi g_c}{k_c^2} \right) \left(\frac{4\pi g_{c''}}{k_{c''}^2} \right)$$

$$\sum_{\mu\nu} \left(\frac{\Gamma_{c\mu}\Gamma_{c'\mu}}{\Gamma_\mu} \right) \left(\frac{\Gamma_{c''\nu}\Gamma_{c'''\nu}}{\Gamma_\nu} \right)$$

$$\times \left\{ \frac{(\Gamma_\mu + \Gamma_\nu)/2}{(E_\mu - E_\nu)^2 + (\Gamma_\mu + \Gamma_\nu)^2/4} \right\}$$

$$\approx \frac{\pi/4}{\Delta E} \left(\frac{4\pi g_c}{k_c^2} \right) \left(\frac{4\pi g_{c''}}{k_{c''}^2} \right)$$

$$\times \sum_\mu \frac{\Gamma_{c\mu}\Gamma_{c'\mu}\Gamma_{c''\mu}\Gamma_{c'''\mu}}{\Gamma_\mu^3}$$

since $|E_\mu - E_\nu| \gg \Gamma_\mu, \Gamma_\nu$

…continuing

- and the ensemble average gives us

$$\langle \sigma_{cc'}\sigma_{c'c''}\rangle \approx \frac{\pi/4}{\Delta E}\left(\frac{4\pi g_c}{k_c^2}\right)\left(\frac{4\pi g_{c''}}{k_{c''}^2}\right)$$

$$\times \frac{\overline{\Gamma}_c\overline{\Gamma}_{c'}\overline{\Gamma}_{c''}\overline{\Gamma}_{c'''}}{\overline{\Gamma}^3}\left(1+\frac{2\delta_{cc'}}{\nu_c}\right)\left(1+\frac{2\delta_{c''c'''}}{\nu_{c''}}\right)$$

$$\times \int_0^\infty dx\frac{x^2}{2}\prod_f\left(1+\frac{2\overline{\Gamma}_f}{\nu_f\overline{\overline{\Gamma}}}x\right)^{-\Delta}$$

$$\Delta = \delta_{cf}+\delta_{c'f}+\delta_{c''f}+\delta_{c'''f}+\nu_f/2$$

interesting… looks a lot like the WFC

Define WFC & WFC-like factors

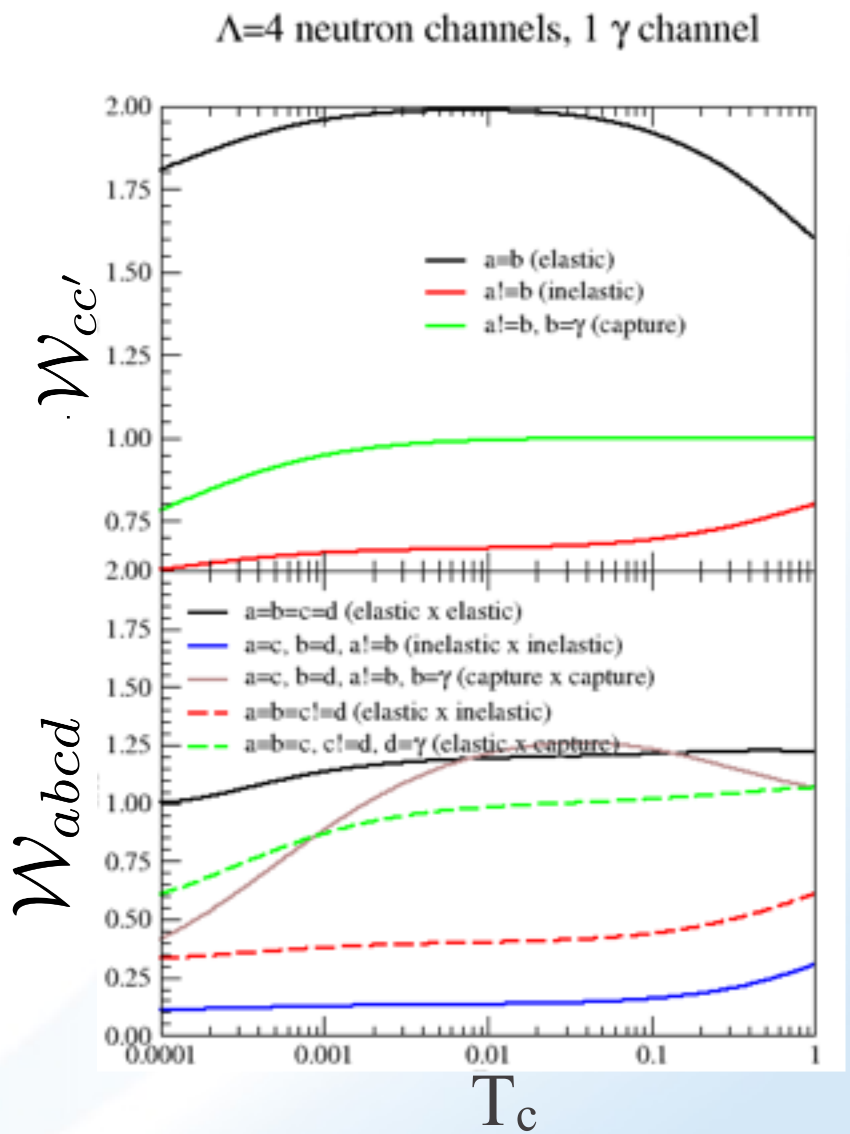
- Collecting the WFC & WFC-like integrals, we can write

$$\langle \sigma_{cc'} \rangle = \frac{g_c}{k_c^2} \frac{T_c T_{c'}}{\sum_{c''} T_{c''}} \mathcal{W}_{cc'}$$

$$\langle \sigma_{ab} \sigma_{cd} \rangle = \frac{\pi \Delta E}{\Gamma} \frac{\mathcal{W}_{abcd}}{\mathcal{W}_{ab} \mathcal{W}_{cd}} \langle \sigma_{ab} \rangle \langle \sigma_{cd} \rangle$$

$$= \frac{2\pi^2}{T} \frac{\mathcal{W}_{abcd}}{\mathcal{W}_{ab} \mathcal{W}_{cd}} \langle \sigma_{ab} \rangle \langle \sigma_{cd} \rangle$$

- Test calc with 4 n channels, same width, 1 g channel
- Kawano-Talou systematics for nu

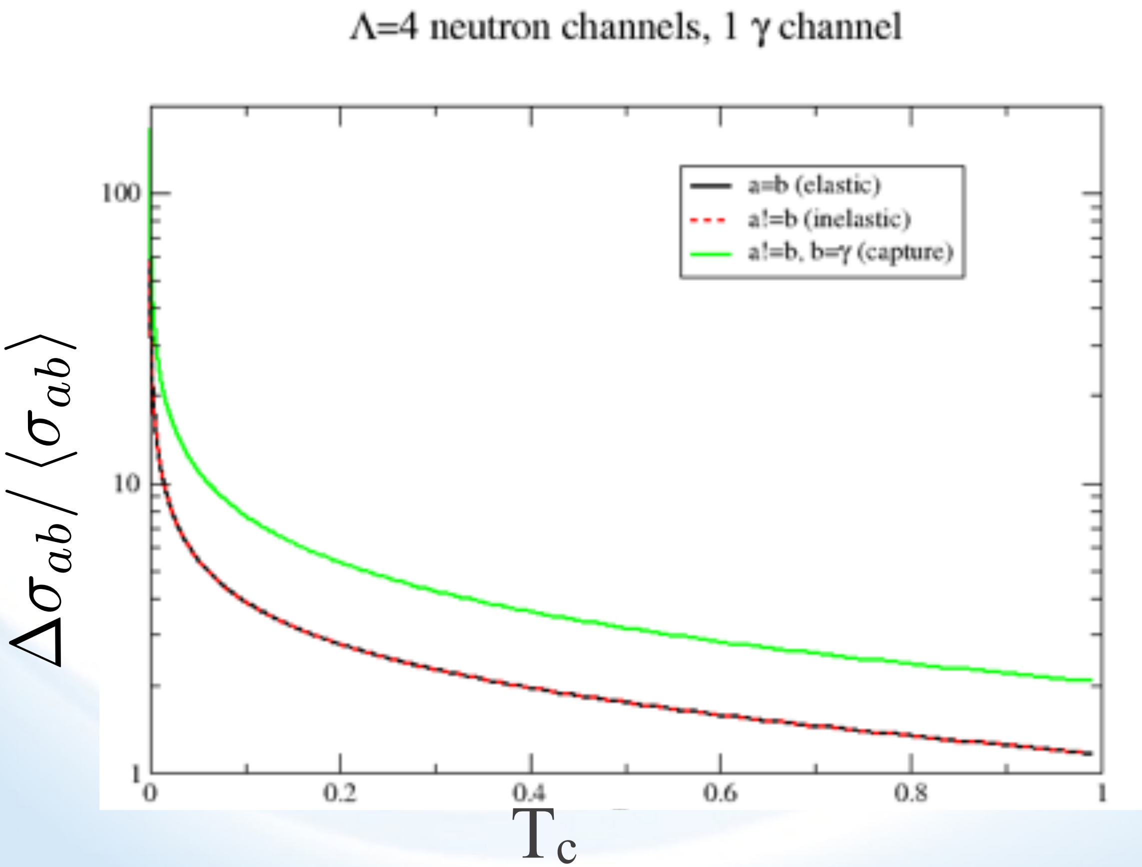


Gg=1e-4 eV

Compound nuclear cross section variance

$$\mathrm{cov}(\sigma_{ab},\sigma_{cd}) = \langle\sigma_{ab}\rangle\langle\sigma_{cd}\rangle\left(\frac{\pi\Delta E}{\Gamma}\frac{\mathcal{W}_{abcd}}{\mathcal{W}_{ab}\mathcal{W}_{cd}} - 1\right)$$

$$= \langle\sigma_{ab}\rangle\langle\sigma_{cd}\rangle\left(\frac{2\pi^2}{T}\frac{\mathcal{W}_{abcd}}{\mathcal{W}_{ab}\mathcal{W}_{cd}} - 1\right)$$

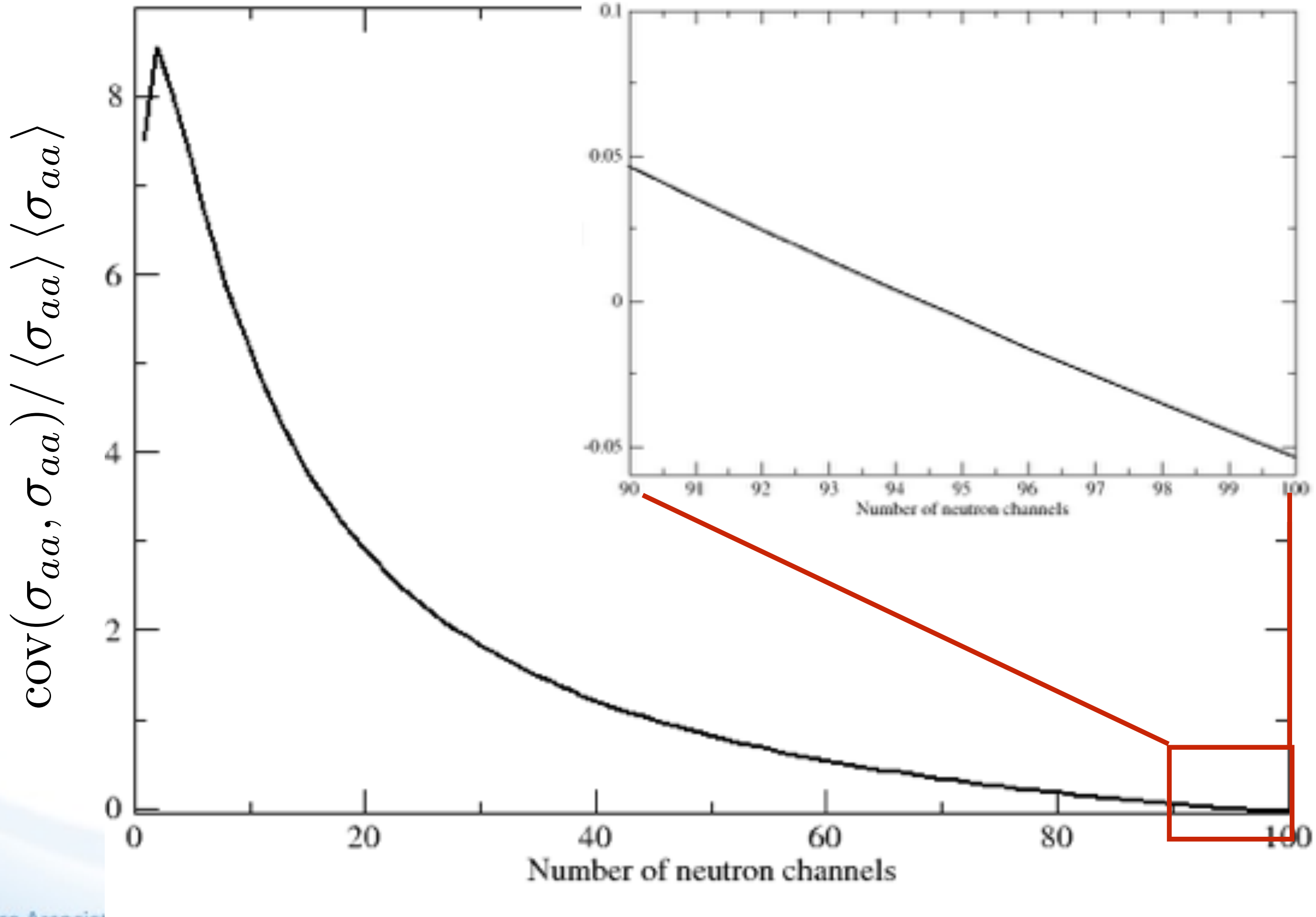


Gg=1e-4 eV

- Since all n widths same, elastic & inelastic variance same
- Capture cross section small, relative variances huge

The model breaks down in strong coupling limit :(

Gn=0.2 eV, Gg=1e-4 eV



We have made a big step toward analytic cross section PDFs

- We have a scheme, based on Moldauer's approach to compute the compound nuclear cross section covariance
- Still we must:
  - Fully characterize region of applicability
  - Finish testing vs. GOE realizations of cross section
- Note: scheme should be applicable to URR and RRR of unstable nuclei where no resonances can be measured in practical experiment