Random-matrix approach for generating cross sections and probability table in the unresolved resonance region

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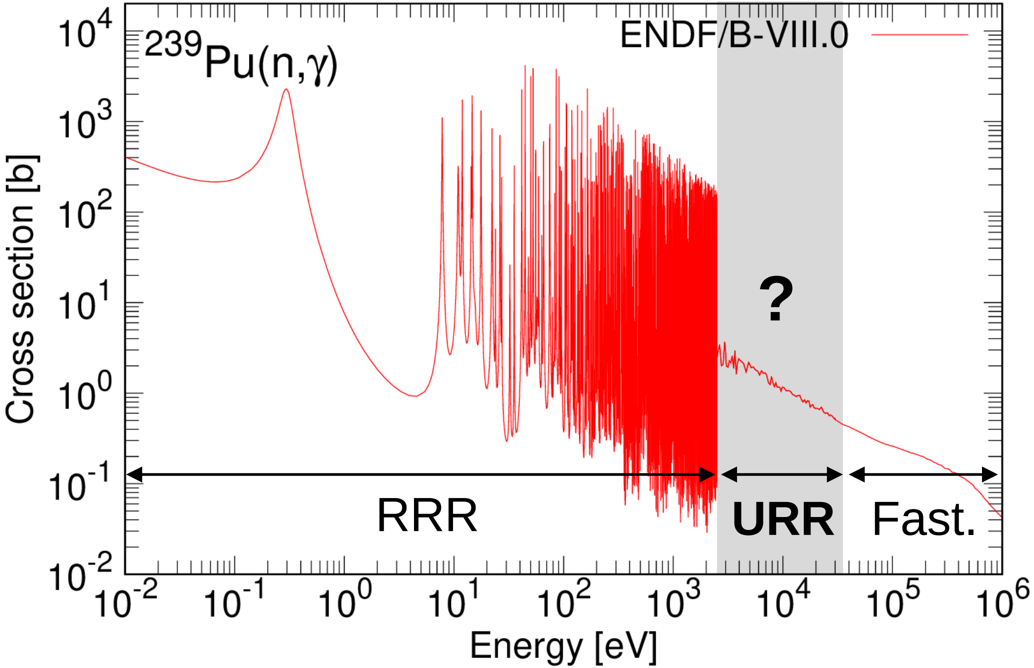
Cross section in theoretical approaches



Resolved resonance region (RRR)

- Individual resonances can be seen
- Expressed in R-matrix formalism by using resonance parameters

Fast energy region

- Smooth cross section because resonance width is bigger than the spacing
- Calculated by Hauser-Feshbach theory

Unresolved resonance region (URR)

- Resonances overlap and cannot be separated from one another
- **No commonly used theoretical model**

Importance of URR and probability table

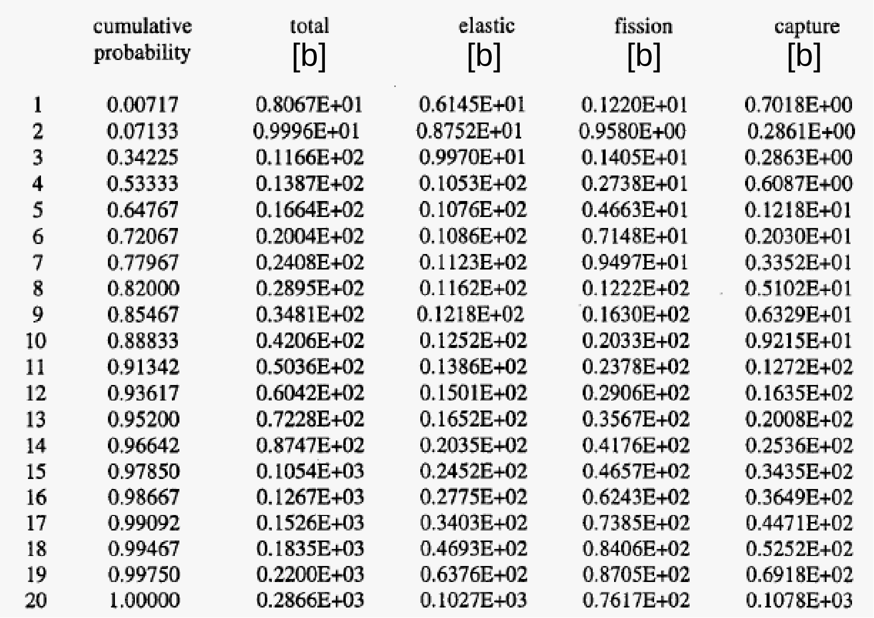
Self-shielding: Neutrons are easily captured at resonance peaks, and the neutron flux decreases at resonance energies. → Impacts on reaction rate

We need to take into account resonances in URR as well !

- A probability table which represents the probabilistic distribution of cross sections is employed in Monte-Carlo approaches

- Assume Wigner and chi-square distributions for the resonance spacing and width, respectively

A theoretical approach is required to calculate the cross sections in URR without these kinds of assumptions



	cumulative probability	total [b]	elastic [b]	fission [b]	capture [b]
1	0.00717	0.8067E+01	0.6145E+01	0.1220E+01	0.7018E+00
2	0.07133	0.9996E+01	0.8752E+01	0.9580E+00	0.2861E+00
3	0.34225	0.1166E+02	0.9970E+01	0.1405E+01	0.2863E+00
4	0.53333	0.1387E+02	0.1053E+02	0.2738E+01	0.6087E+00
5	0.64767	0.1664E+02	0.1076E+02	0.4663E+01	0.1218E+01
6	0.72067	0.2004E+02	0.1086E+02	0.7148E+01	0.2030E+01
7	0.77967	0.2408E+02	0.1123E+02	0.9497E+01	0.3352E+01
8	0.82000	0.2895E+02	0.1162E+02	0.1222E+02	0.5102E+01
9	0.85467	0.3481E+02	0.1218E+02	0.1630E+02	0.6329E+01
10	0.88833	0.4206E+02	0.1252E+02	0.2033E+02	0.9215E+01
11	0.91342	0.5036E+02	0.1386E+02	0.2378E+02	0.1272E+02
12	0.93617	0.6042E+02	0.1501E+02	0.2906E+02	0.1635E+02
13	0.95200	0.7228E+02	0.1652E+02	0.3567E+02	0.2008E+02
14	0.96642	0.8747E+02	0.2035E+02	0.4176E+02	0.2536E+02
15	0.97850	0.1054E+03	0.2452E+02	0.4657E+02	0.3435E+02
16	0.98667	0.1267E+03	0.2775E+02	0.6243E+02	0.3649E+02
17	0.99092	0.1526E+03	0.3403E+02	0.7385E+02	0.4471E+02
18	0.99467	0.1835E+03	0.4693E+02	0.8406E+02	0.5252E+02
19	0.99750	0.2200E+03	0.6376E+02	0.8705E+02	0.6918E+02
20	1.00000	0.2866E+03	0.1027E+03	0.7617E+02	0.1078E+03

Table 1. Probability table for ^{239}Pu at an incident neutron energy of 430 eV and a temperature of 300 degrees Kelvin [based on ENDF/B-V, Rev. 2]

L. L. Carter et al., LA-UR-98-0026 (1998).

Research objective and approach

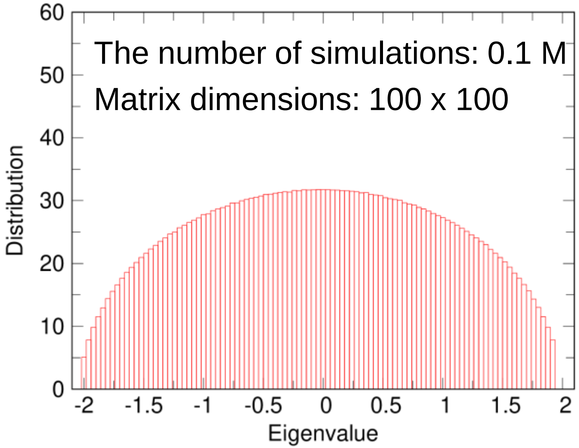
Develop a theoretical model to obtain cross sections in URR and employ them to create the probability table

Random-matrix approach

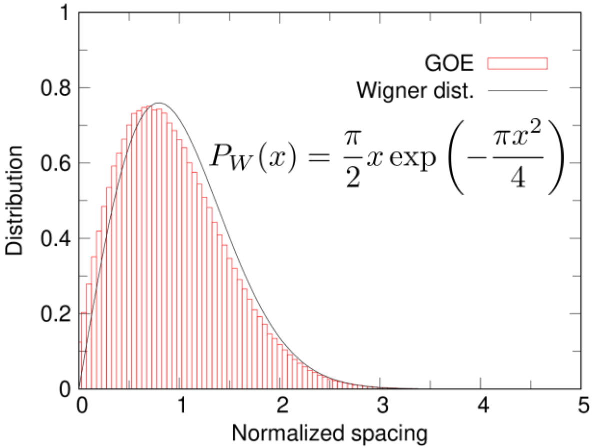
Gaussian Orthogonal Ensemble (GOE)

- Real symmetric matrix
- Matrix elements are Gaussian distributed random numbers

Eigenvalue distribution



Distribution of spacing of each eigenvalue



S matrix calculated using GOE

$$S_{ab}^{(\mathrm{GOE})} = \delta_{ab} - 2i\pi \sum_{\mu\nu} W_{a\mu}(D^{-1})_{\mu\nu} W_{\nu b}$$

E : energy in units of λ

(Does not represent incident neutron energy!)

$$D_{\mu\nu} = E\delta_{\mu\nu} - H_{\mu\nu}^{(\mathrm{GOE})} + i\pi \sum_{c} W_{\mu c} W_{c\nu}$$

$H_{\mu\nu}^{(\mathrm{GOE})}$: Random matrix

J. J. M. Verbaarschot et al., Phys. Rep. 129, 367 (1985).

T. Kawano et al., Phys. Rev. C92, 044617 (2015).

Input parameters

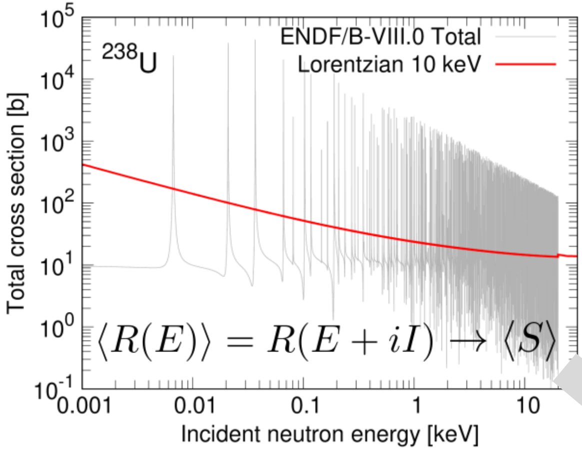
- The number of levels N
- The number of channels Λ
  - The number of inelastic scattering channels is determined by possible number of neutron partial waves and the corresponding excited levels
- Neutron, photon, and fission transmission coefficients T_n, T_γ, T_f

How to smoothly connect 2 regions

The S matrix smoothly connects between RRR and fast energy regions

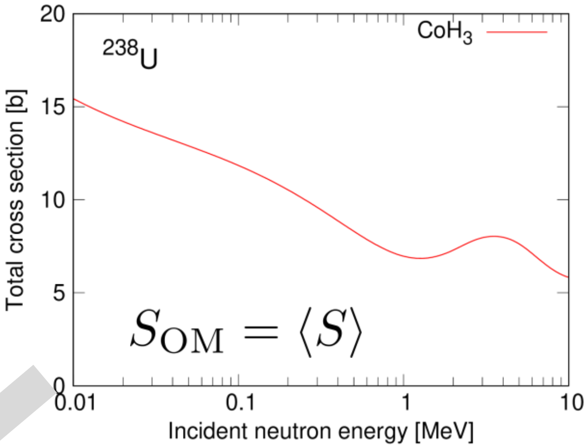
Between RRR and URR

1. Obtain the energy-averaged R matrix in RRR (ENDF/B-VIII.0)
2. Determine the optical model parameters to reproduce $\langle R(E) \rangle$



Between URR and fast energy regions

☑ We can consistently use the same treatments as those used in the Hauser-Feshbach model and (coupled-channel) optical model in CoH_3



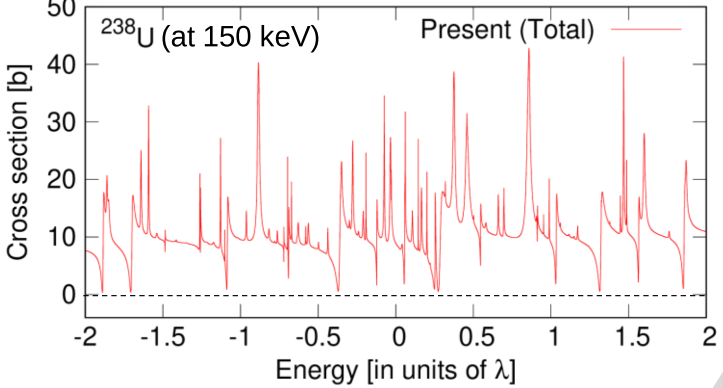
Key input parameters:

Transmission coefficients $T = 1 - |\langle S \rangle|^2$

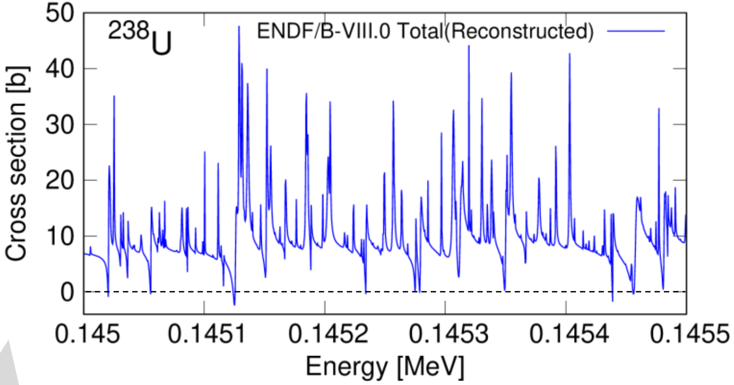
Calculated cross sections

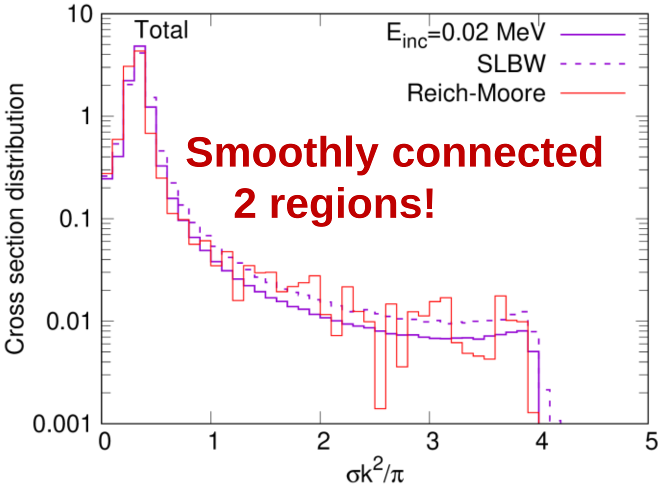
Phys. Rev. C112, 064608 (2025).

GOE-S-matrix model (**unitarity is guaranteed!**)

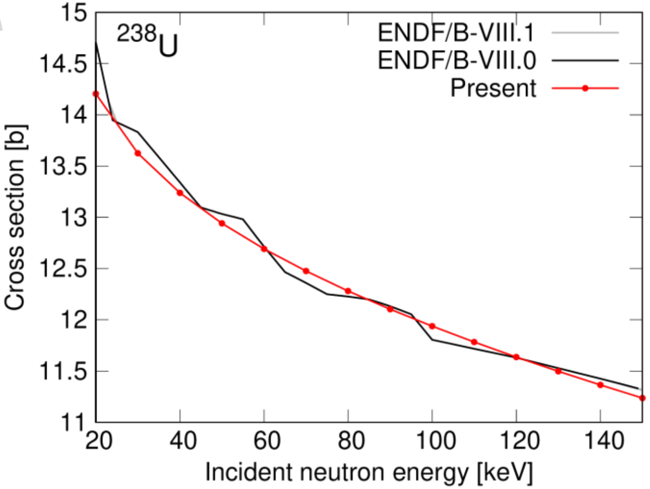


Single-level Breit-Wigner formula (unitarity is not guaranteed)



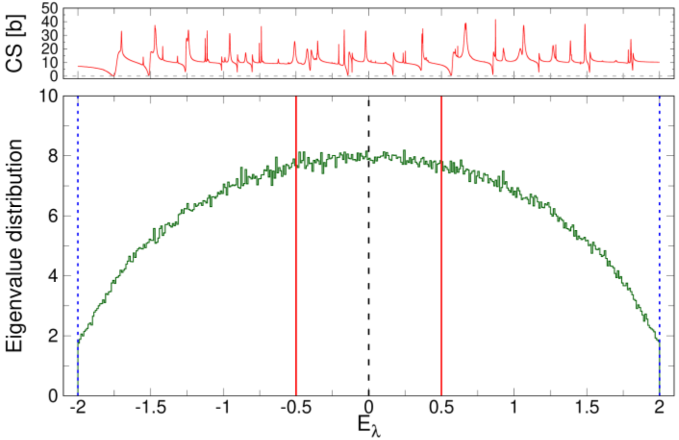


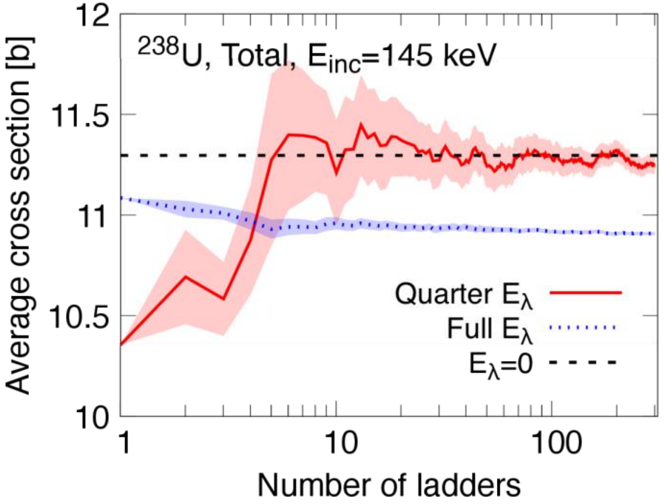
Smoothly connected 2 regions!

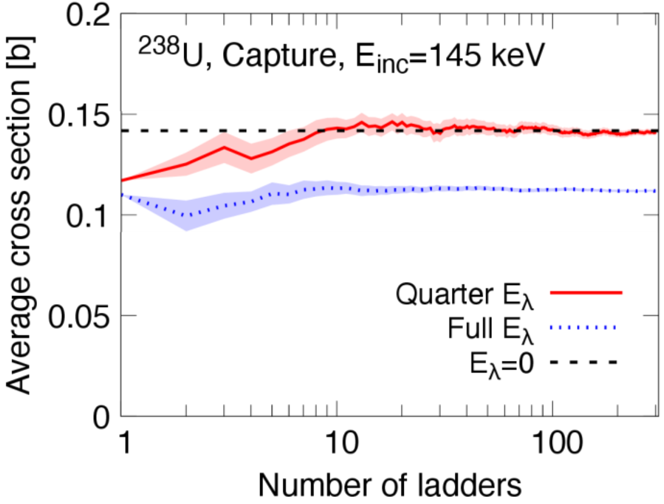


Selected energy range

- The eigenvalue distribution corresponds to the level density.
- The convergence behavior depends on the level density.
- Compared the convergence of the cross sections using the full E_λ range and the quarter E_λ range.





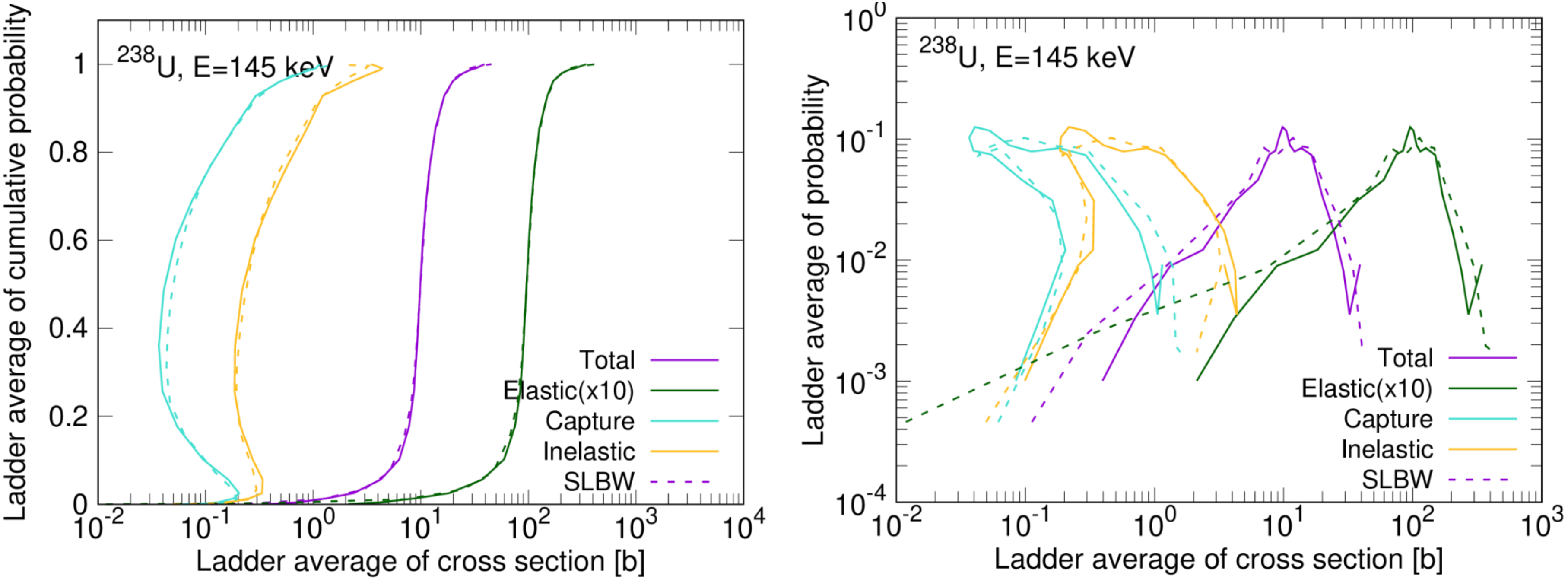


We restrict the energy range to E_λ = — λ/2 to λ/2.

Calculated probability tables

J. Nucl. Sci. Technol. (published)

The number of ladders: 10000



- No significant differences are observed between the GOE calculation and the single-level Breit-Wigner result.
- Small ladder average of cross sections are seen in the SLBW results due to the negative cross sections.

Conclusions

- **We developed a new theoretical model to obtain cross sections in URR and employ them to create the probability table.**

- The input transmission coefficients are determined that the S matrix smoothly connects between RRR and higher energy regions.

- The average cross sections converge to evaluate data by restricting the range to $E_\lambda = -\lambda/2$ to $\lambda/2$.

- The main difference in probability table between our new approach and the SLBW comes from the unitarity condition.

Future work

- Introduce the temperature effect (Doppler broadening)

Acknowledgements

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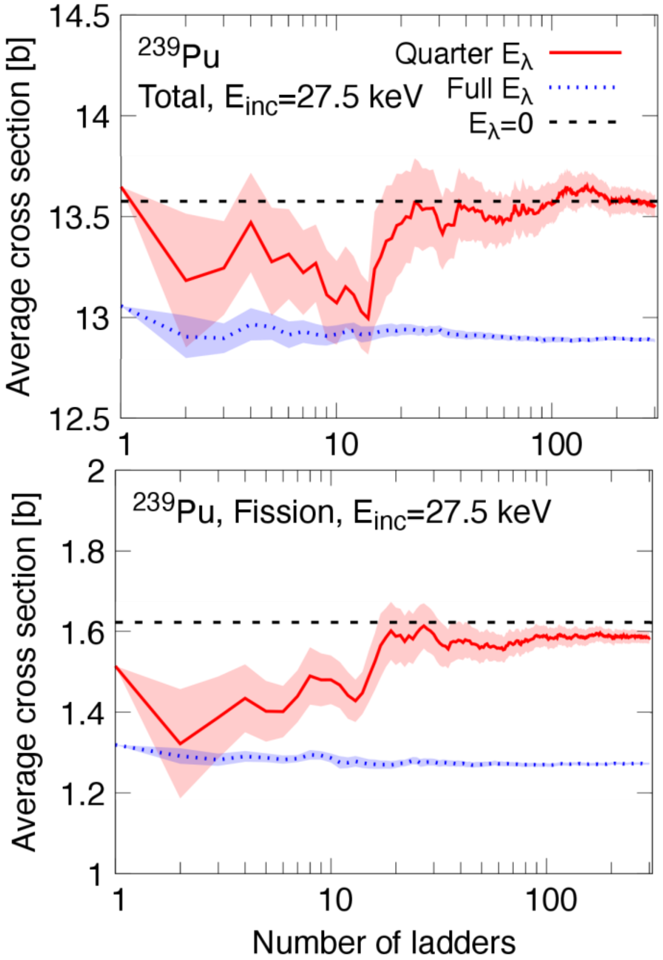
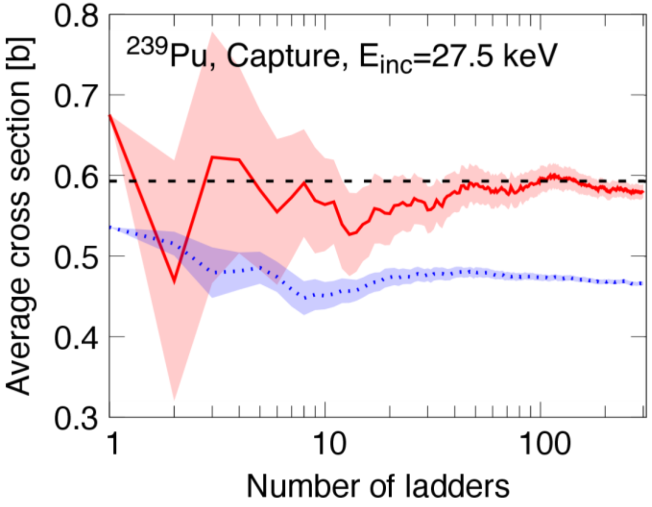
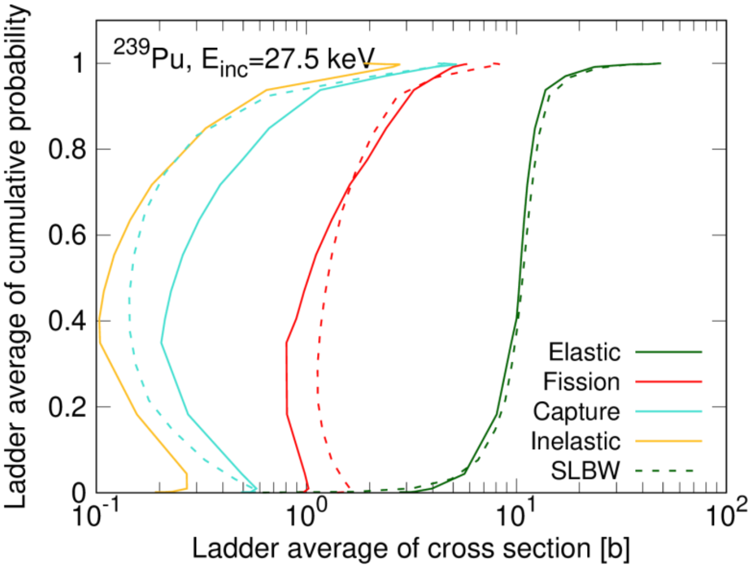
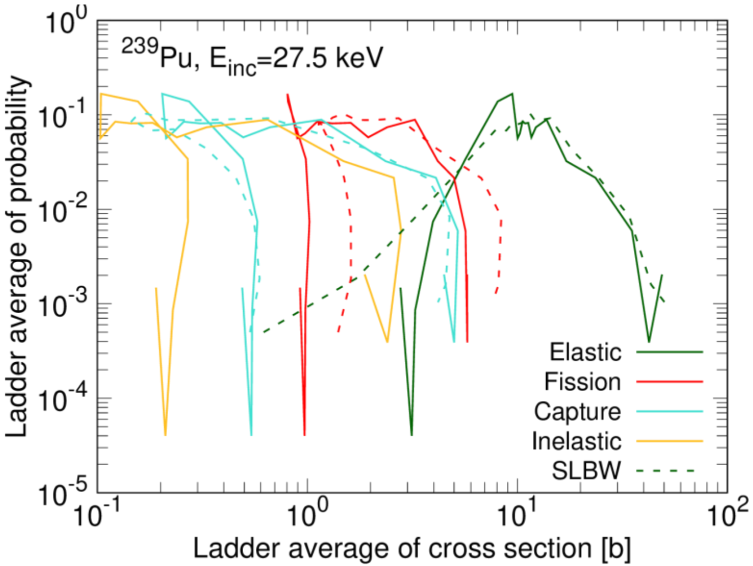
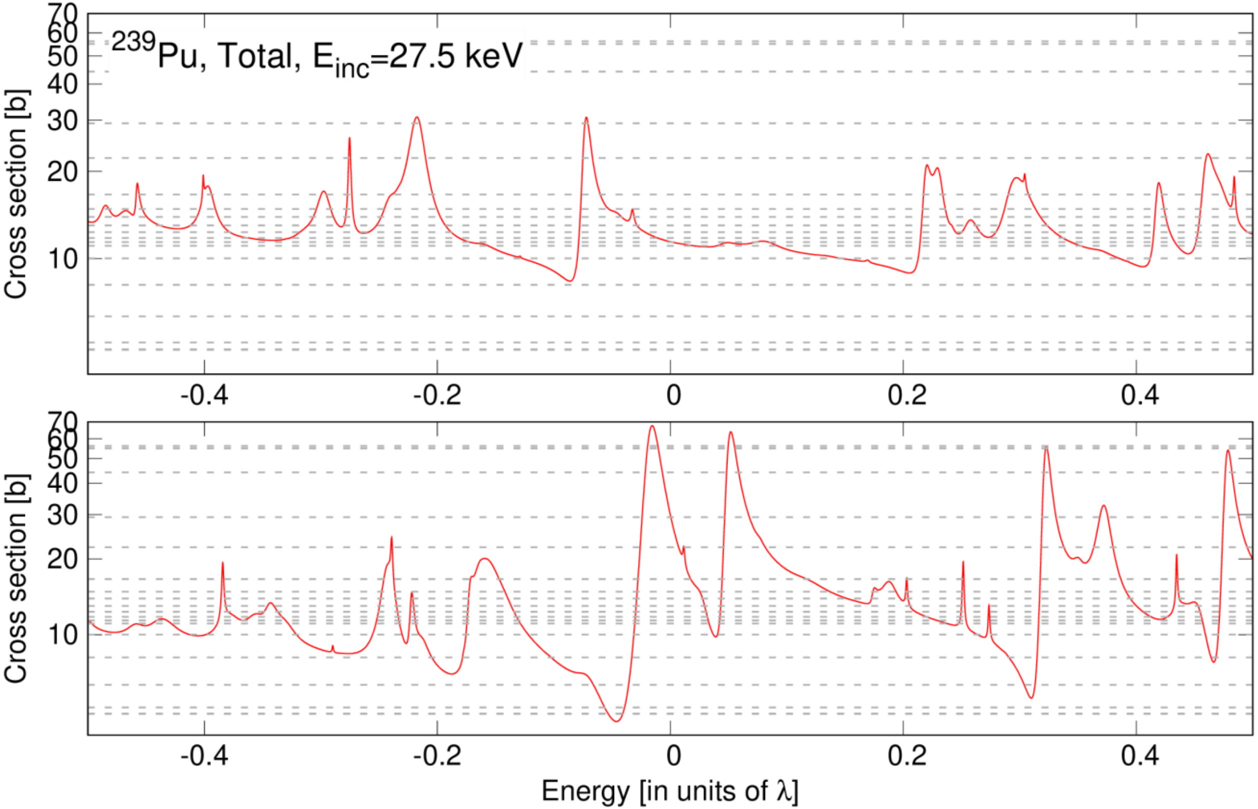

^{239}Pu
Total, E_{inc}=27.5 keV
Quarter E_λ
Full E_λ
E_λ=0
Average cross section [b]
14.5
14
13.5
13
12.5
1
10
100
^{239}Pu, Fission, E_{inc}=27.5 keV
Average cross section [b]
2
1.8
1.6
1.4
1.2
1
1
10
100
Number of ladders


^{239}Pu, Capture, E_{inc}=27.5 keV
Average cross section [b]
0.8
0.7
0.6
0.5
0.4
0.3
1
10
100
Number of ladders


^{239}Pu, E_{inc}=27.5 keV
Ladder average of cumulative probability
Ladder average of cross section [b]
0
0.2
0.4
0.6
0.8
1
10^{-1}
10^{0}
10^{1}
10^{2}
Elastic
Fission
Capture
Inelastic
SLBW


^{239}Pu, E_{inc}=27.5 keV
Ladder average of probability
Ladder average of cross section [b]
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{-1}
10^{0}
10^{1}
10^{2}
Elastic
Fission
Capture
Inelastic
SLBW



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