Updates to R-matrix Evaluations of Fissile Actinides: $^{233,235}U$, ^{239}Pu

Marco T. Pigni
Nuclear Data and Criticality Safety
Oak Ridge National Laboratory, Oak Ridge, TN

Nuclear Data Week – Cross Section Evaluation Working Group (CSEWG) meeting
Brookhaven National Laboratory, November 4–8 2019, Upton, NY

Introduction

Importance and Significance of Cross Section Fluctuations

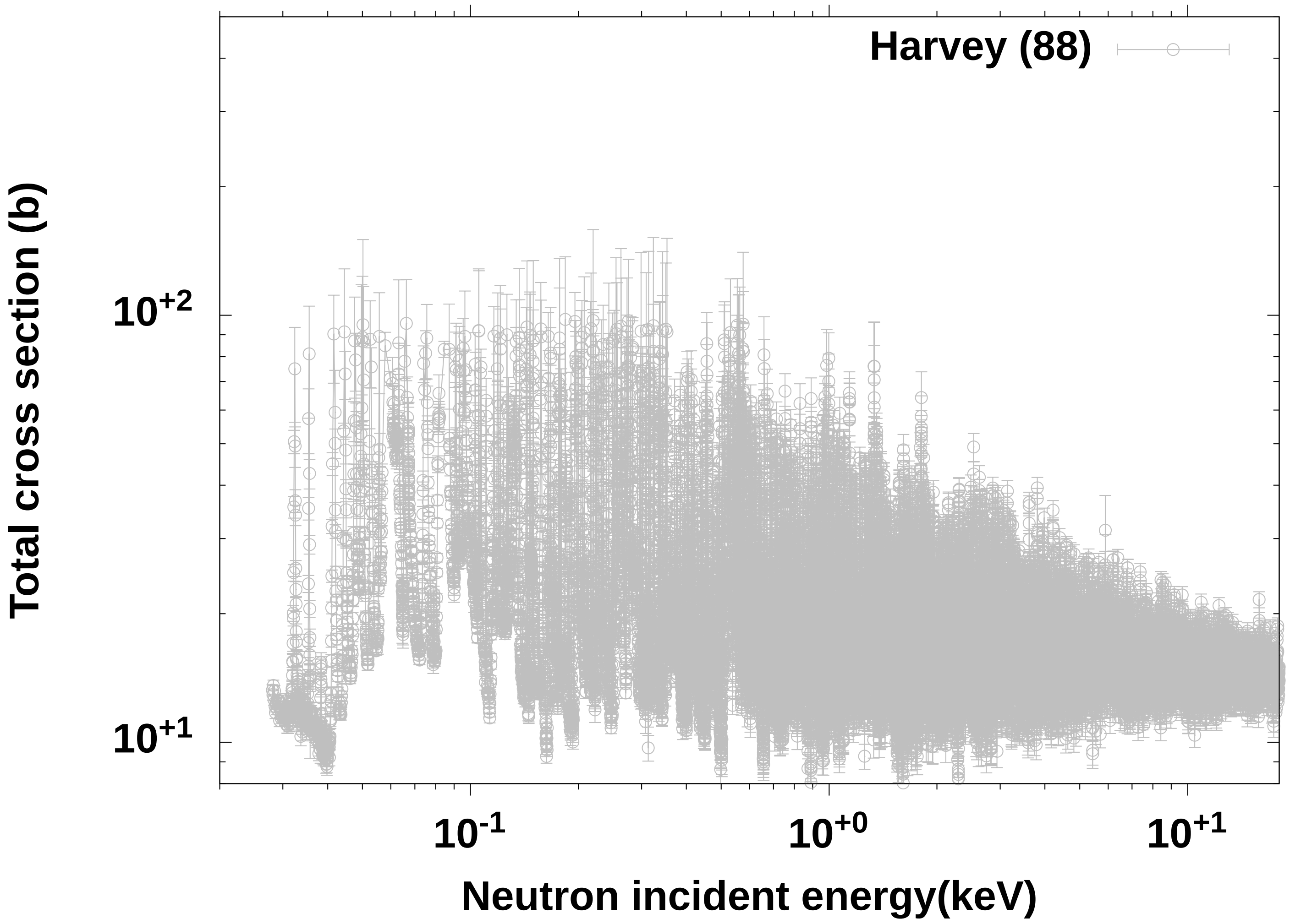
- Criticality benchmark calculations are highly sensitive to cross section fluctuations (usually in the keV neutron energy region for fissile actinides)
  - Average resonance parameters and related probability tables are commonly used to generate cross section fluctuations
- Measured cross sections possess a rapidly varying resonant behavior depending on the incident neutron energy
  - At low energies, the resonance-like structure from the quasi-bound state of the compound nucleus can be measured fairly easy since the experimental resolution is higher than the spacing of the level states
  - However, as the energy increases, the number of levels is so large that only fluctuations related to very closely-spaced levels can be measured
- These data are generally evaluated with a relatively simple method (R-matrix theory)
- For resonance that cannot be resolved experimentally, the cross section fluctuations are usually described in terms of S-matrix elements calculated from average quantities obtained from R-matrix analyses

Motivation and Overarching Goals

To Establish the Highest Fidelity Nuclear Evaluated Data

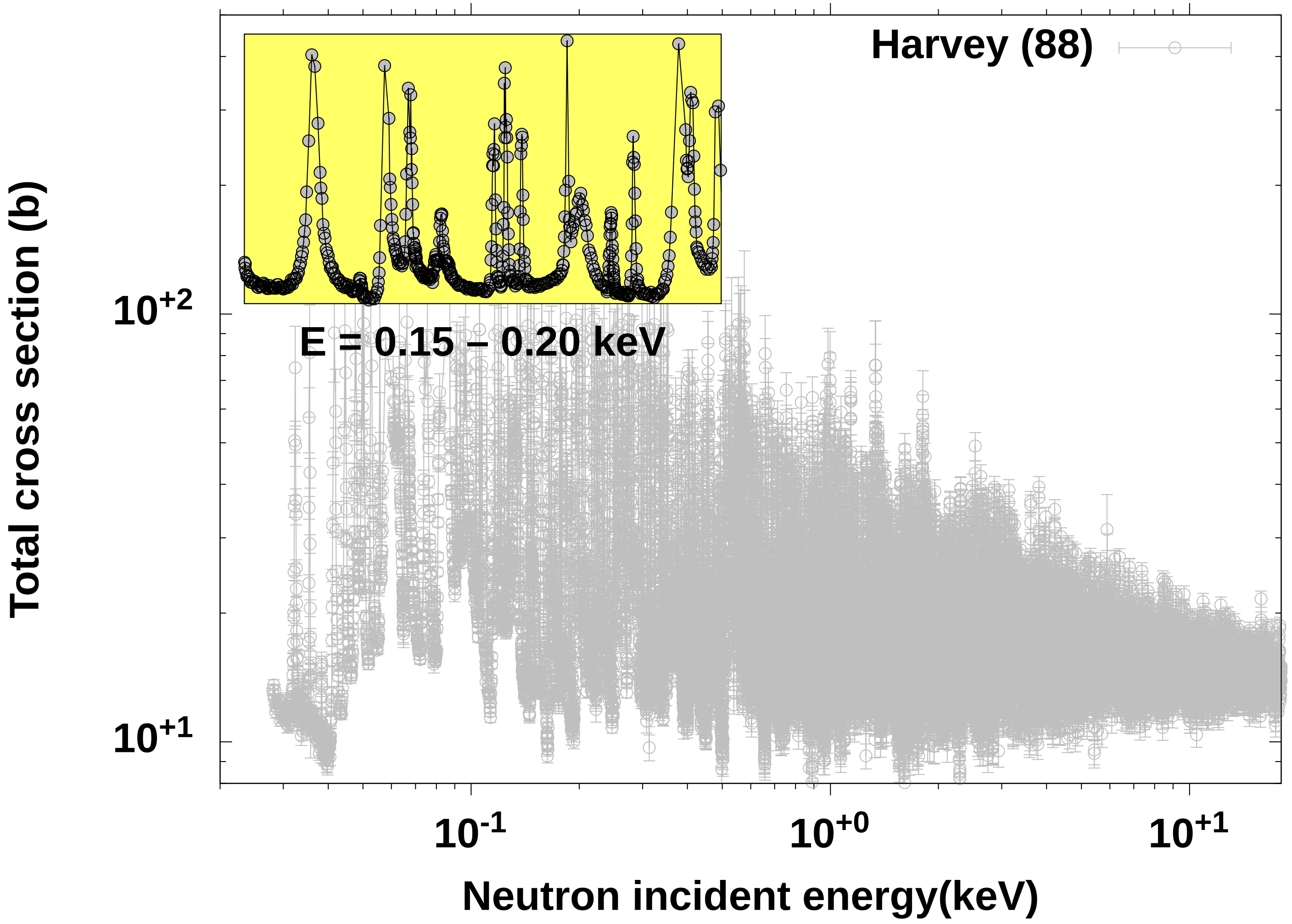
- Evaluated data files do not entirely describe the cross section fluctuations available in measured data
  - This information could improve the performance in benchmark calculations
- High-fidelity description of measured data in neutron energy regions where fluctuations are important and relevant for applications
- Fluctuating cross sections evaluated within a consistent theoretical formalism
  - The energy averaged cross sections are defined in terms of the average resonance parameters simply because the Single Level Breit Wigner approximation is used
- Inclusion of fluctuating cross section aiming to limit the size of the evaluated data files as well as maintaining performance in benchmark calculations

Experimental Data
Fluctuations in Measured Cross Section (n+^{239}Pu)



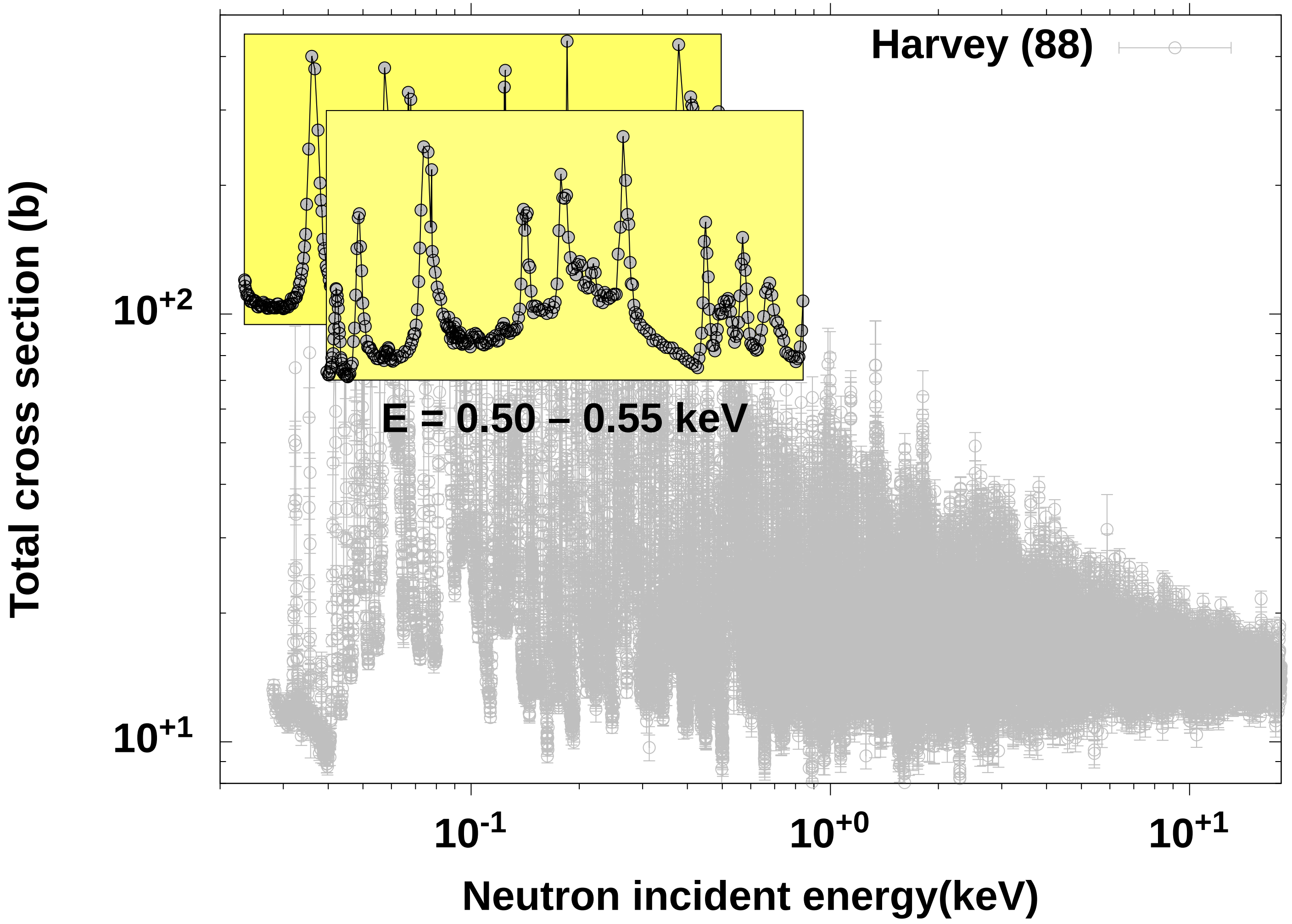
Experimental Data

Fluctuations in Measured Cross Section (n+^{239}Pu)



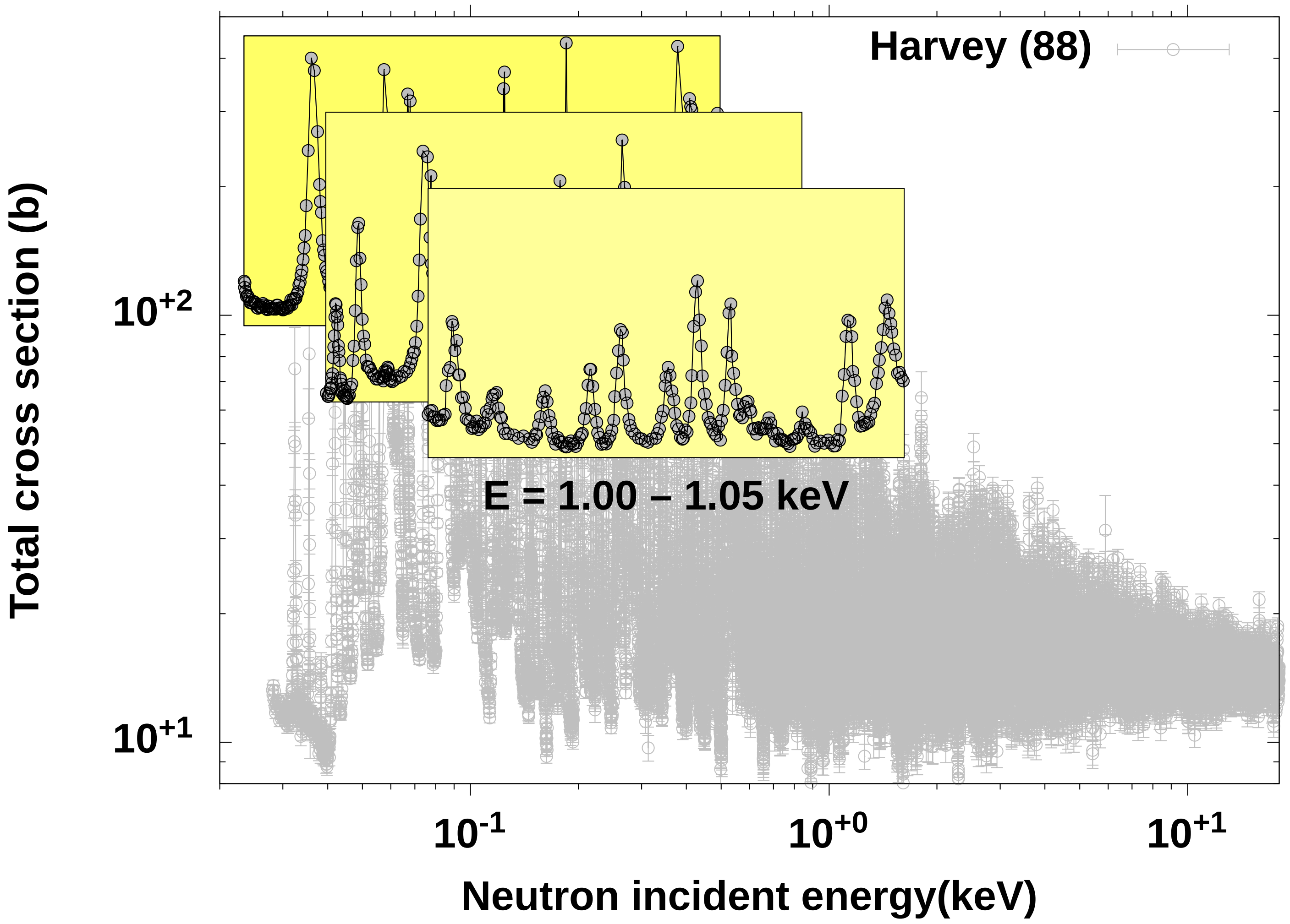
Experimental Data

Fluctuations in Measured Cross Section ($n+^{239}Pu$)



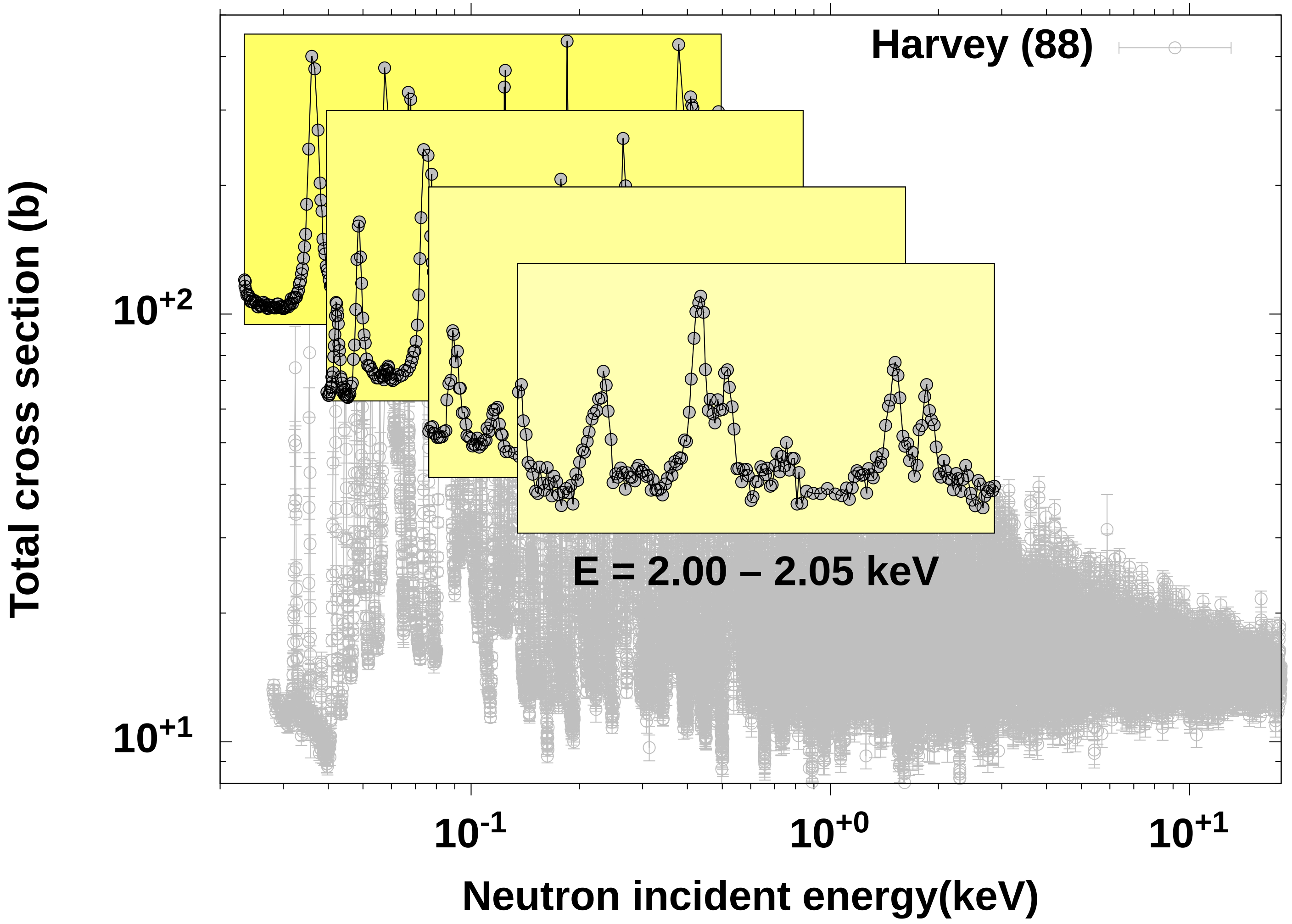
Experimental Data

Fluctuations in Measured Cross Section (n+^{239}Pu)



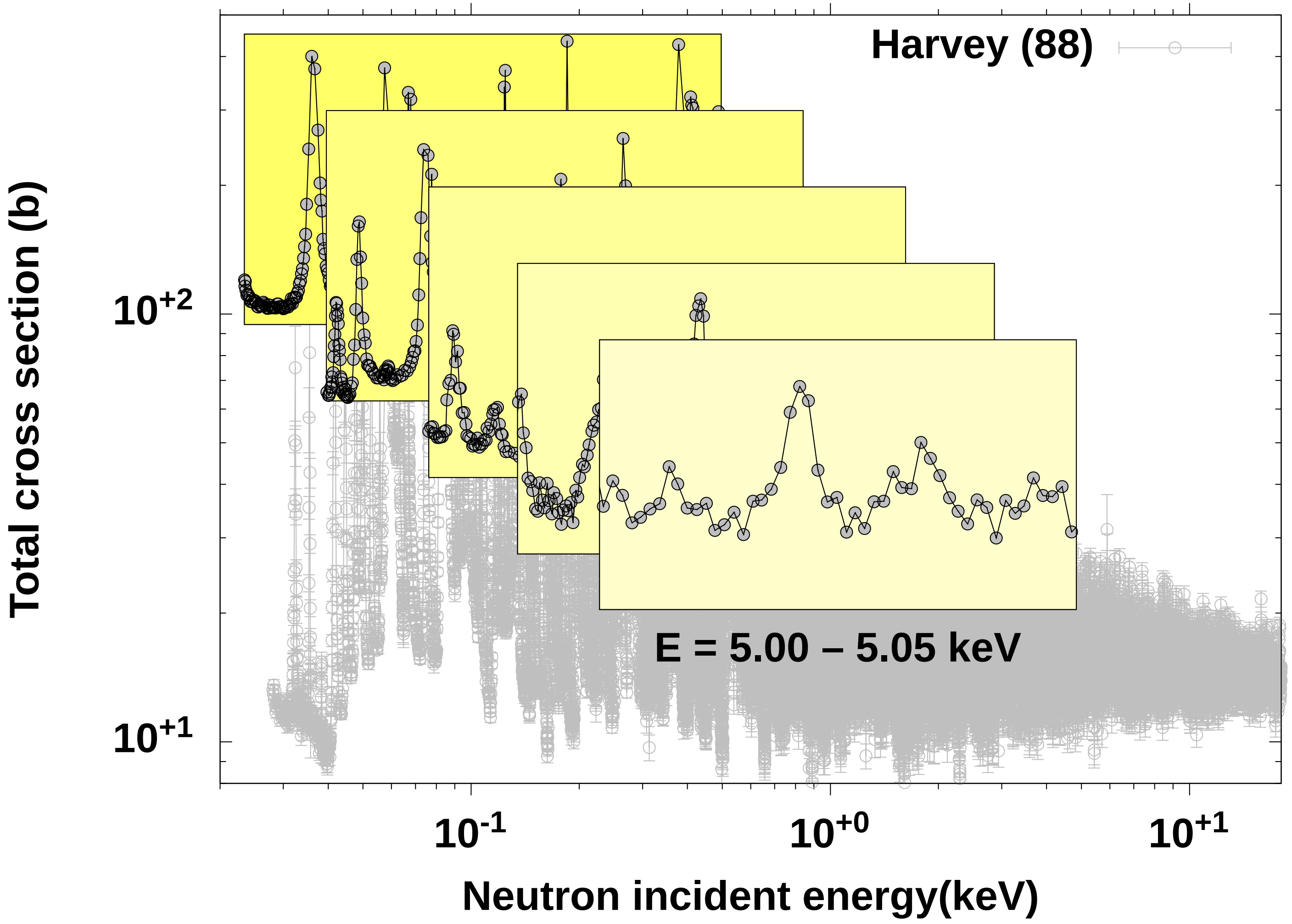
Experimental Data

Fluctuations in Measured Cross Section (n+^{239}Pu)



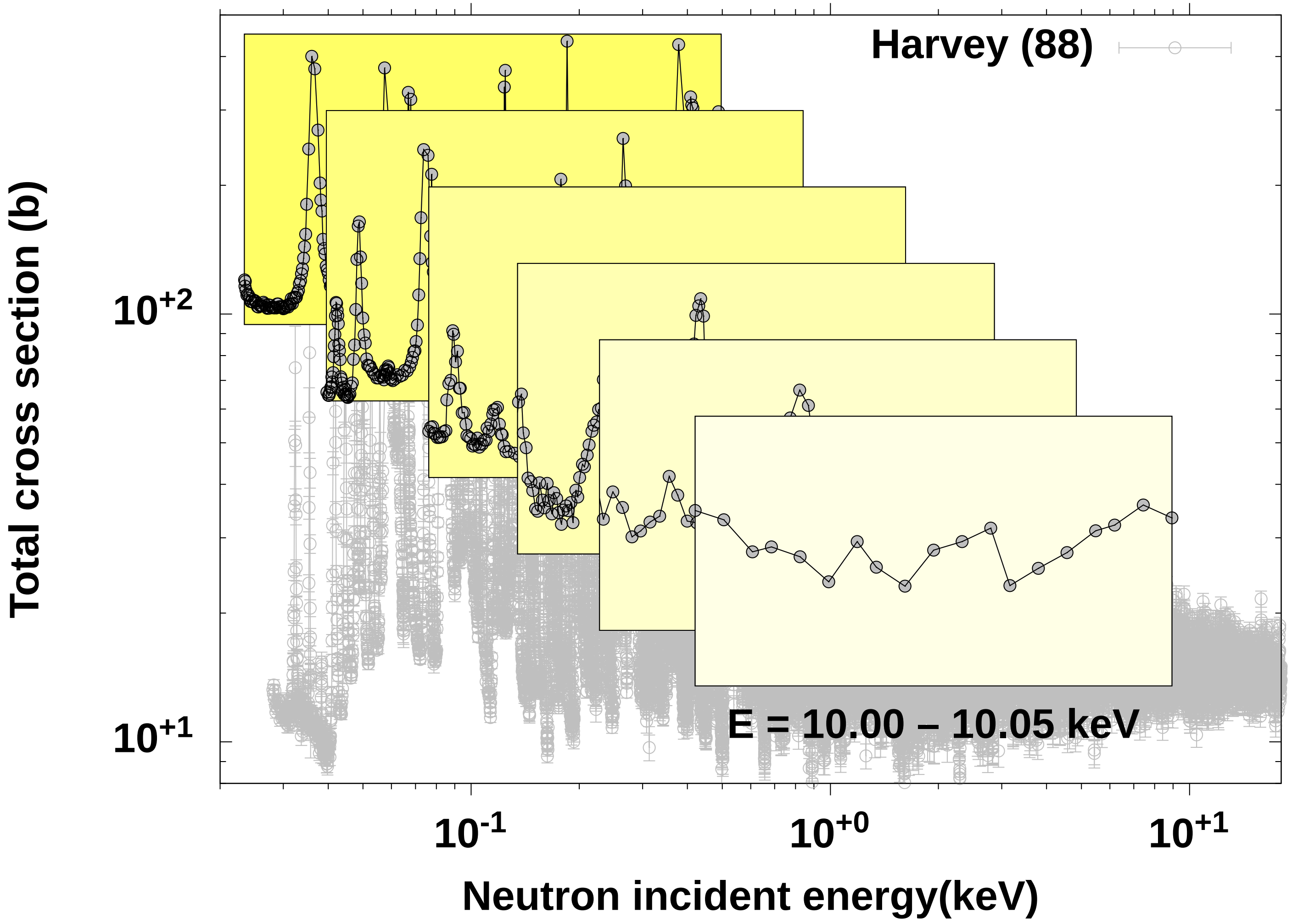
Experimental Data

Fluctuations in Measured Cross Section (n+^{239}Pu)



Experimental Data

Fluctuations in Measured Cross Section (n+^{239}Pu)



Theory: S-matrix Elements

Reich-Moore Representation of the Reduced R-matrix Function

All physical quantities defined by γ_λ (reduced-width amplitudes) and E_λ (resonance energies)

$$\mathrm{R}_{cc'}(E) = \sum_\lambda \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E - \imath\gamma_{\lambda\gamma}} \tag{1}$$

and the S-matrix elements are given by

$$\mathrm{S}_{cc'}(E) = e^{-\imath(\phi_c+\phi_{c'})}\sqrt{P_c}\{[\mathbf{1}-\mathbf{R}(\mathbf{L}-\mathbf{B})]^{-1}[\mathbf{1}-\mathbf{R}(\mathbf{L}^*-\mathbf{B})]\}_{cc'}\sqrt{P_{c'}}\,, \tag{2}$$

where ϕ_c is the hard-sphere phase-shift and $L_{cc'} = (S_c + \imath P_c)\delta_{cc'}$ is related to S_c (hard-sphere shift factor) and P_c (hard-sphere penetrability) for chosen B_c (boundary parameters)

The cross section for the entrance channel c (neutron) and exit channel c' (neutron, γ, …) is

$$\sigma_{cc'}(E) = \frac{\pi}{k_c^2} g_c \,|\, \delta_{cc'} - \mathrm{S}_{cc'} \,|^2 \tag{3}$$

where g_c is the statistical spin factor

Link S-matrix Function to Average Total Cross Sections

Lorentzian Energy Averaging

The total cross section averaged over the energy interval I can be calculated from the average S-matrix elements S_{cc} with a Lorentzian weight function

$$\langle \mathsf{S}_{cc}(E)\rangle = \int_{-\infty}^{+\infty} dE' \frac{I/\pi}{(E'-E)^2+\imath I^2} \mathsf{S}_{cc}(E') \tag{4}$$

Since there are no poles above the real axis due to the causality of the S matrix

$$\langle \mathsf{S}_{cc}(E)\rangle = \mathsf{S}_{cc}(E+\imath I) \tag{5}$$

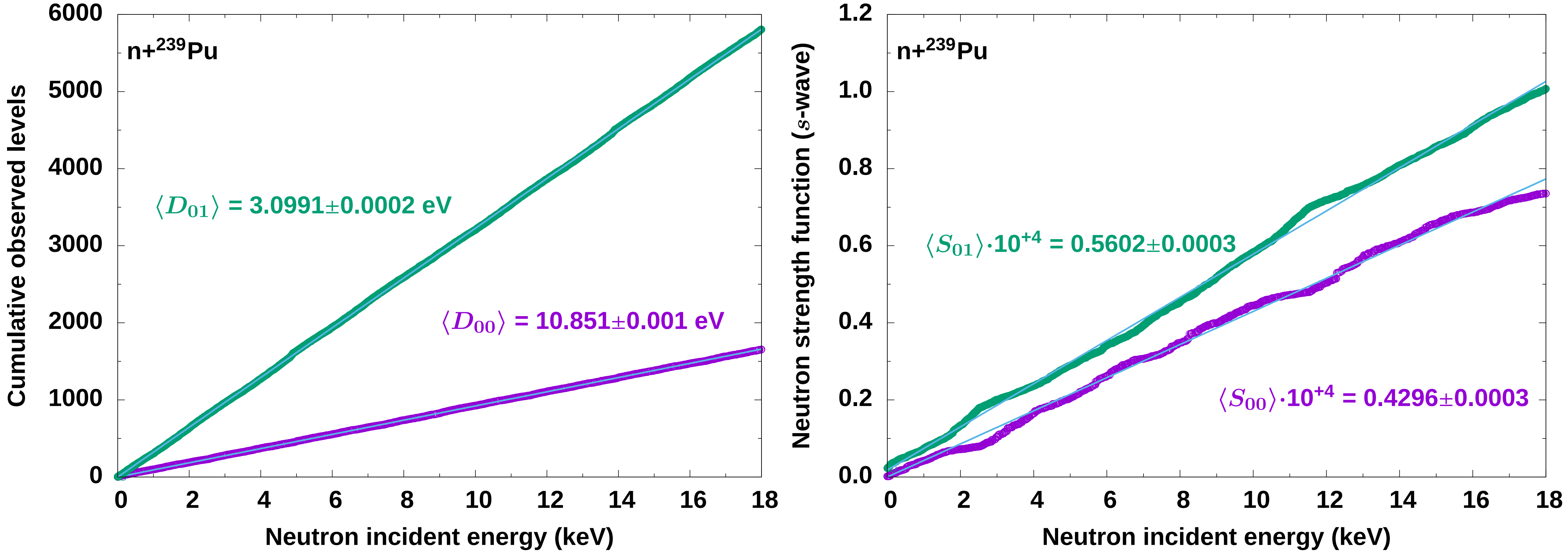
A common approximation is to average only the R-matrix function

$$\langle \mathsf{S}_{cc}(E)\rangle \approx e^{-2\imath\phi_c}\sqrt{P_c}[1-\langle \mathsf{R}_{cc}\rangle(L_c-B_c)]^{-1}[1-\langle \mathsf{R}_{cc}\rangle(L_c^*-B_c)]\sqrt{P_c}\,, \tag{6}$$

where $\langle \mathsf{R}_{cc}(E)\rangle \equiv \mathsf{R}_{cc}(E+\imath I)$ and the energy dependence of ϕ_c, P_c and L_c is neglected

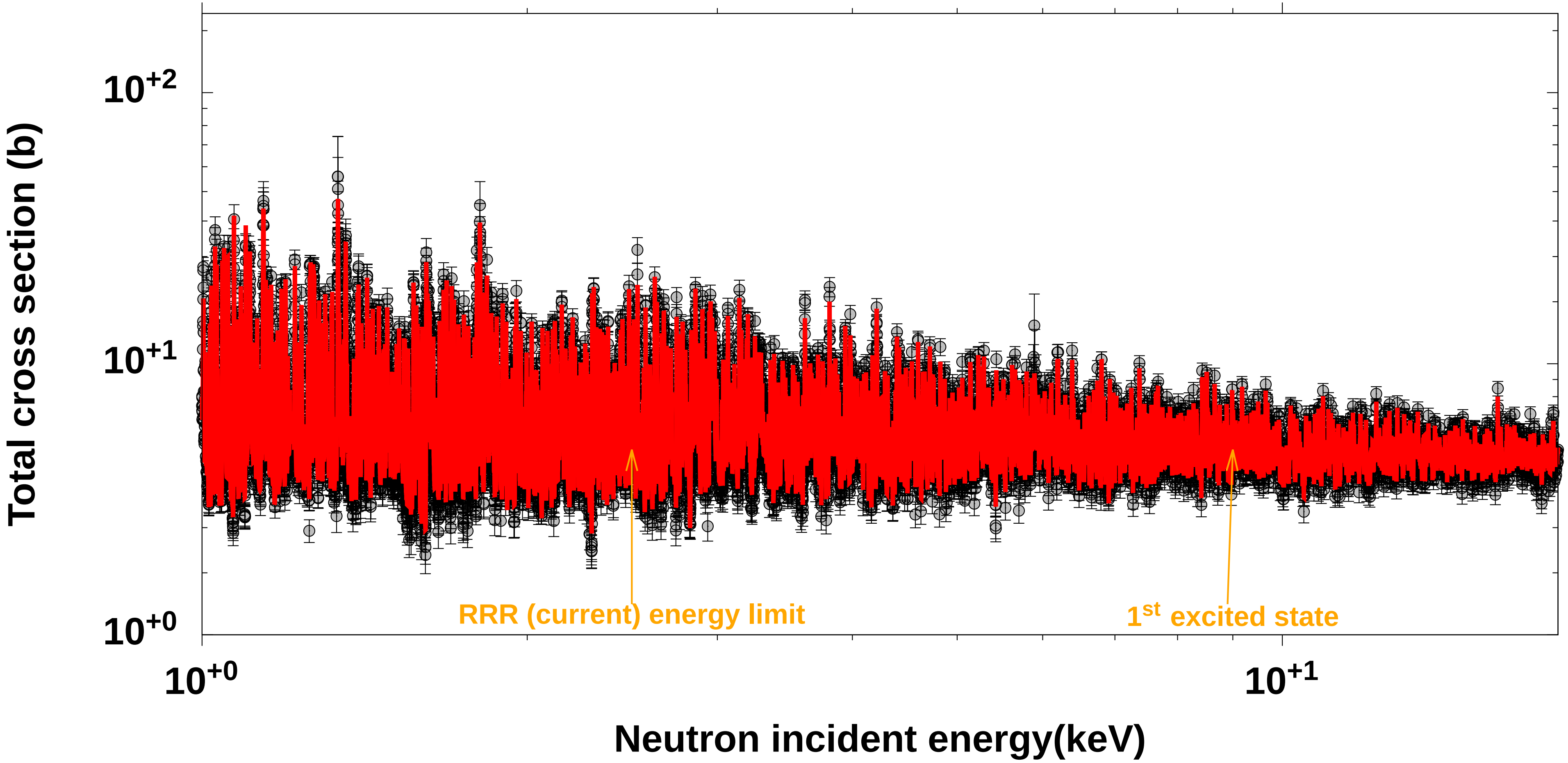
Extrapolating Energy Levels and Resonance Amplitudes

Statistics from Resonance Parameters below 2.5 keV



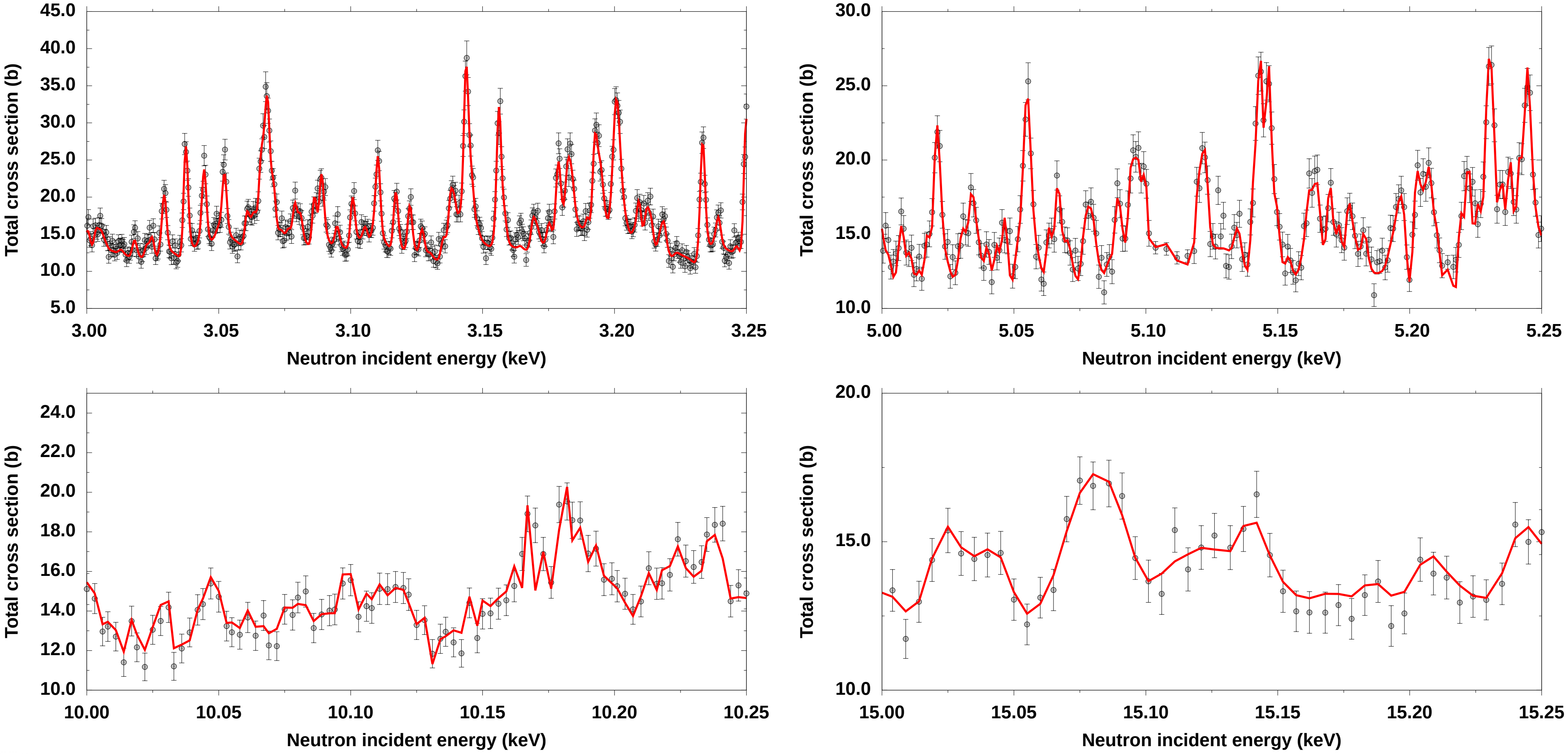
^{239}Pu Total Cross Section in the Resonance Region

Fit to Measured Data

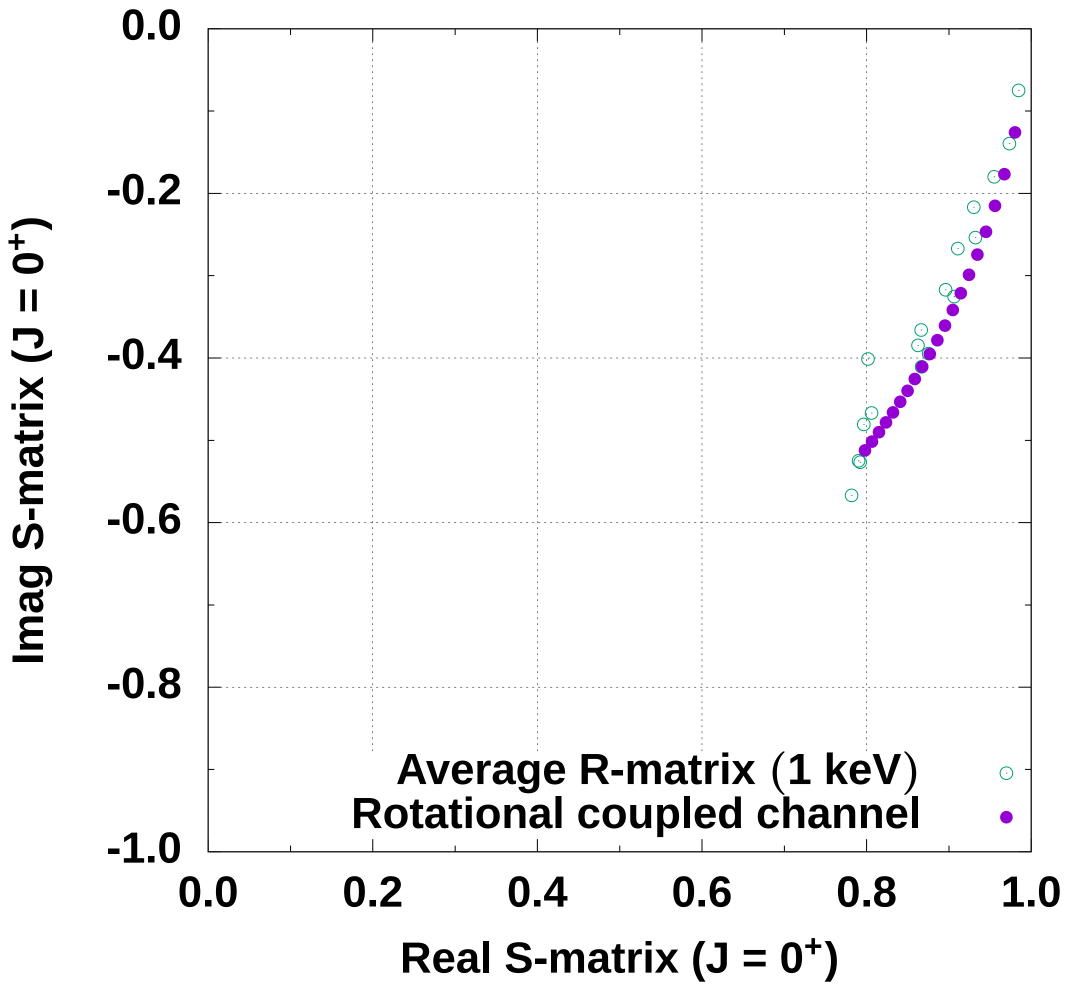


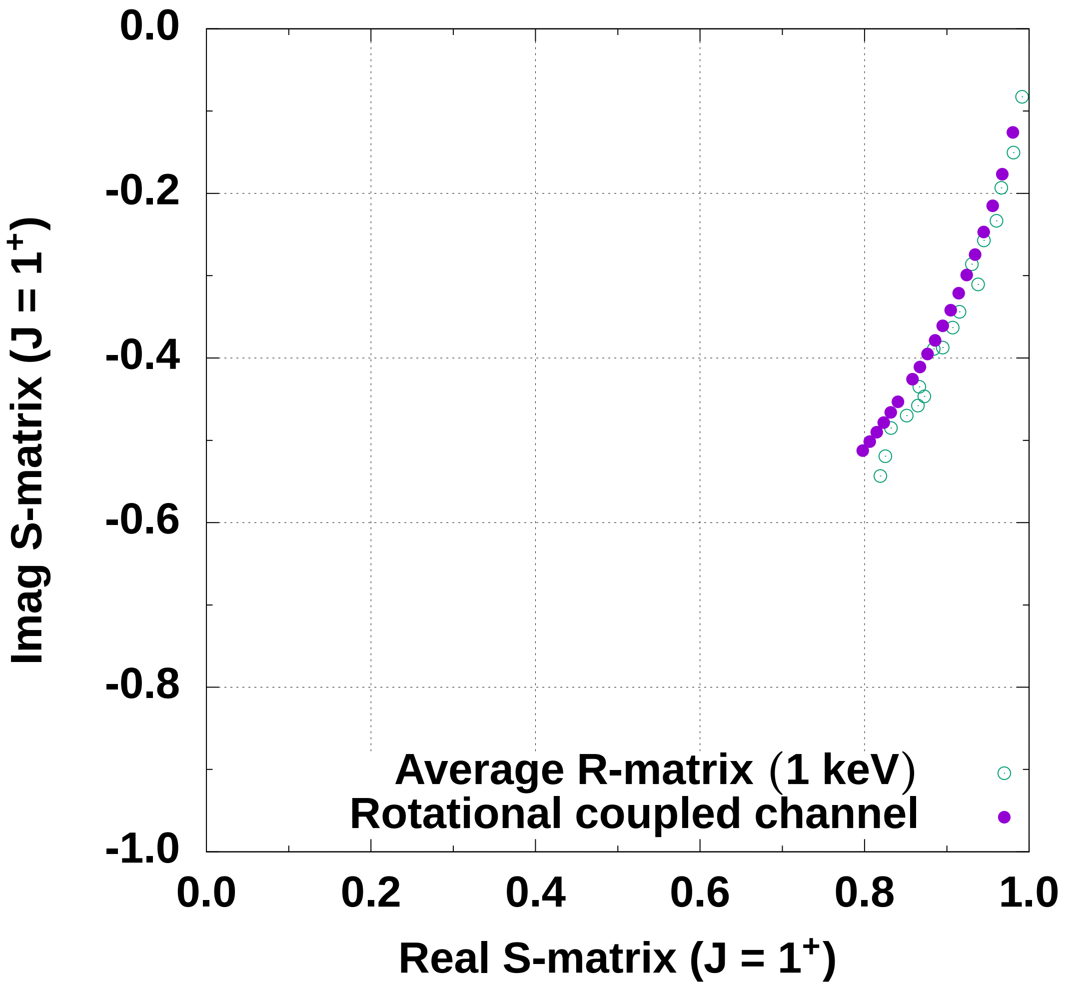
^{239}Pu Total Cross Section in the Resonance Region

Fit to Measured Data



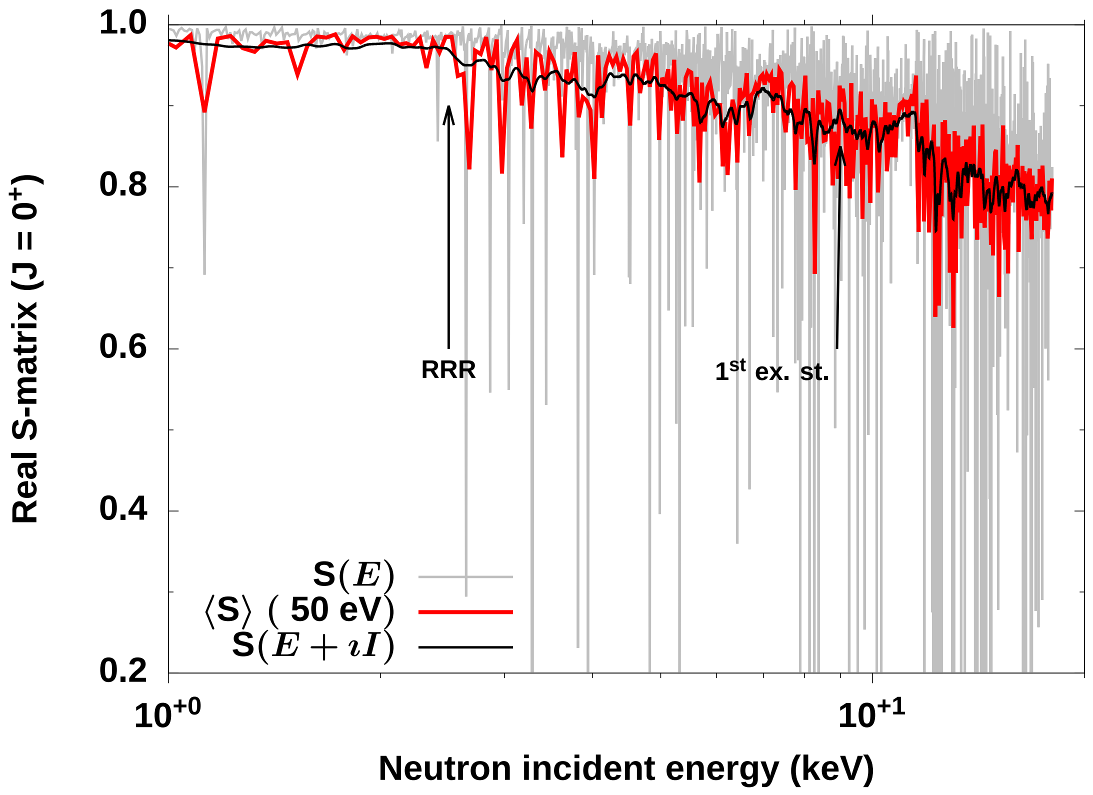
Link R-matrix to Optical Model Calculations

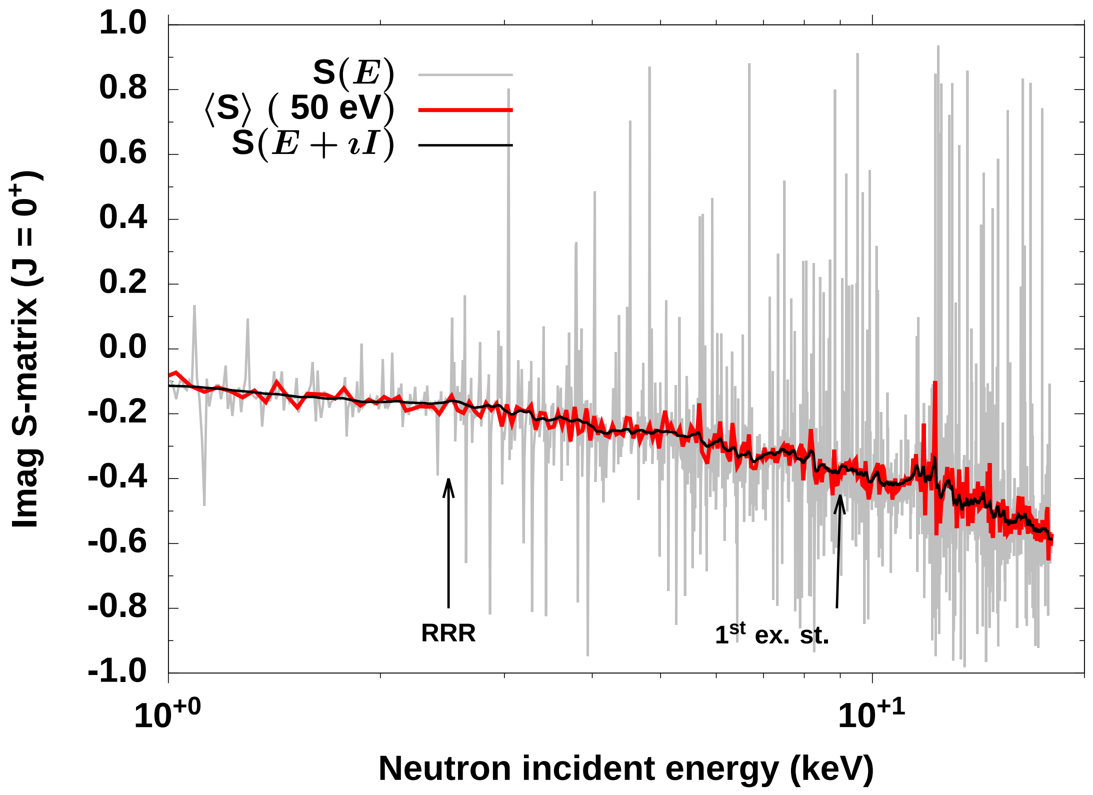




S-matrix Elements from Extrapolated Populations

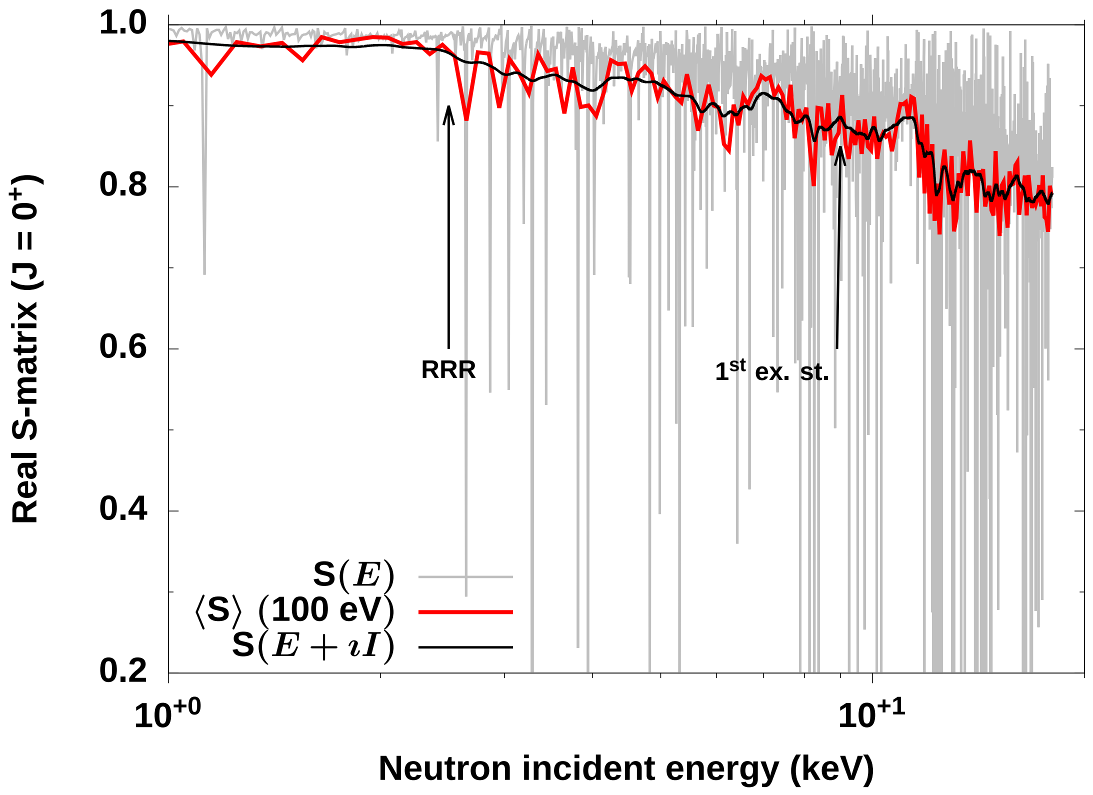
Real and Imaginary Components (J=0$^+$ Population)

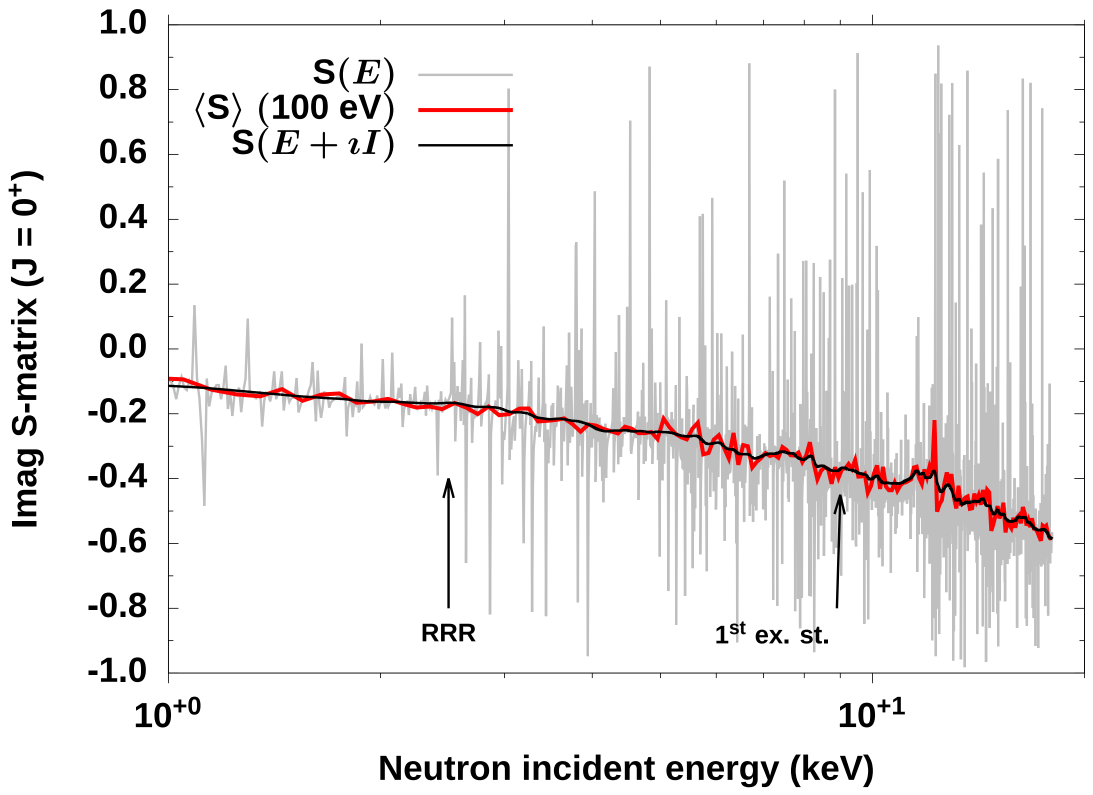




S-matrix Elements from Extrapolated Populations

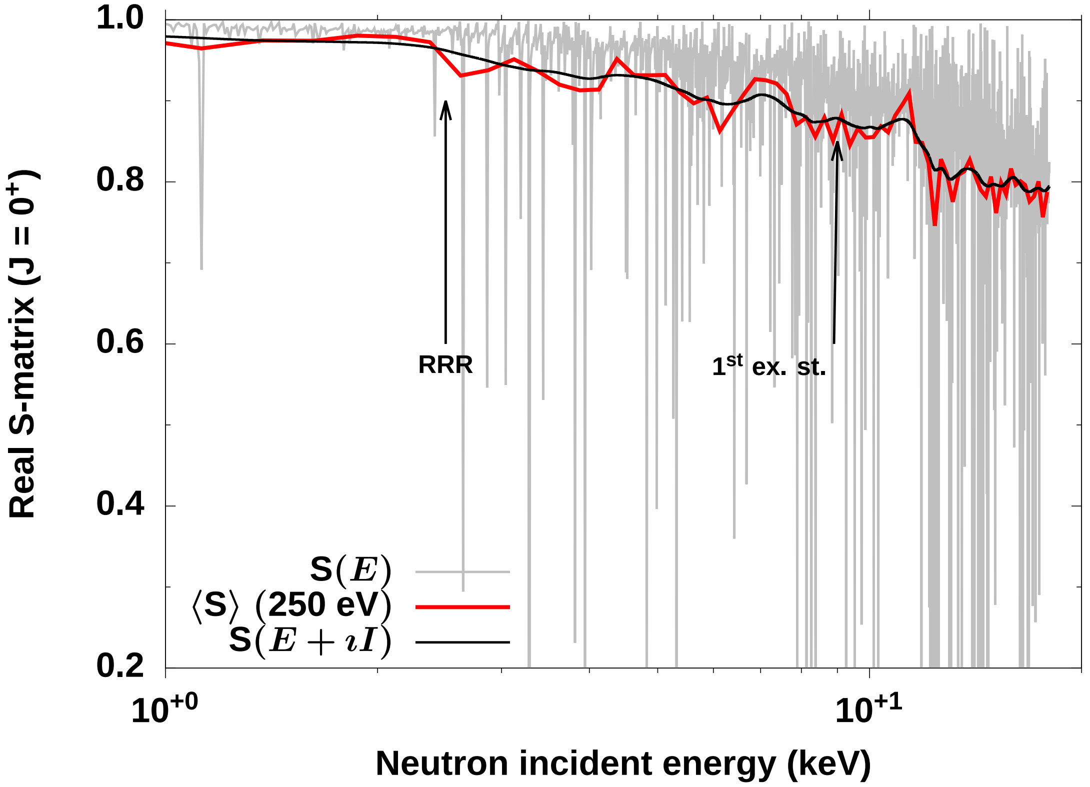
Real and Imaginary Components (J=0+ Population)

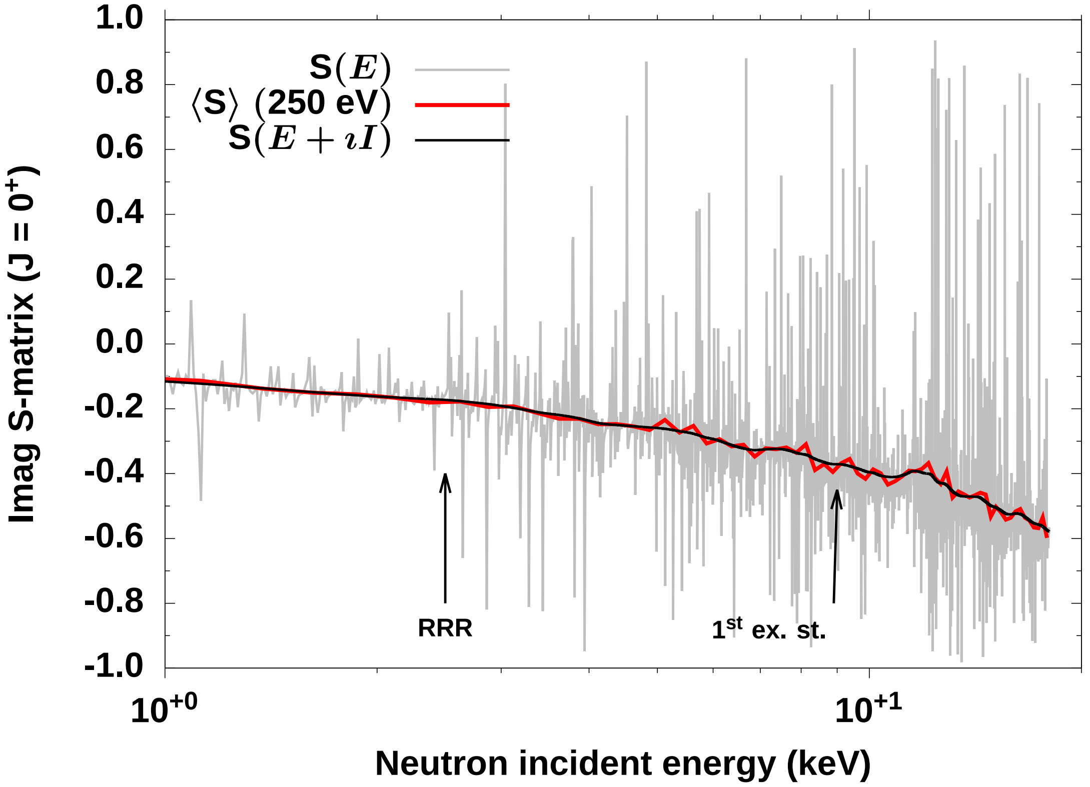




S-matrix Elements from Extrapolated Populations

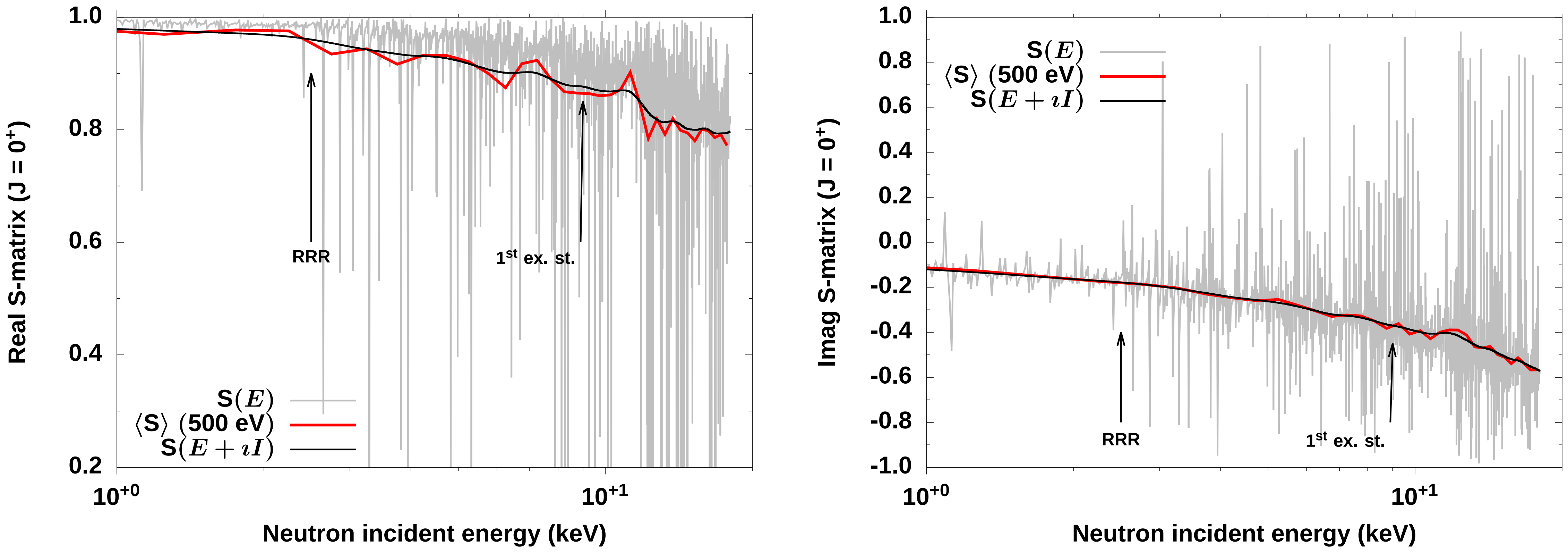
Real and Imaginary Components (J=0$^+$ Population)





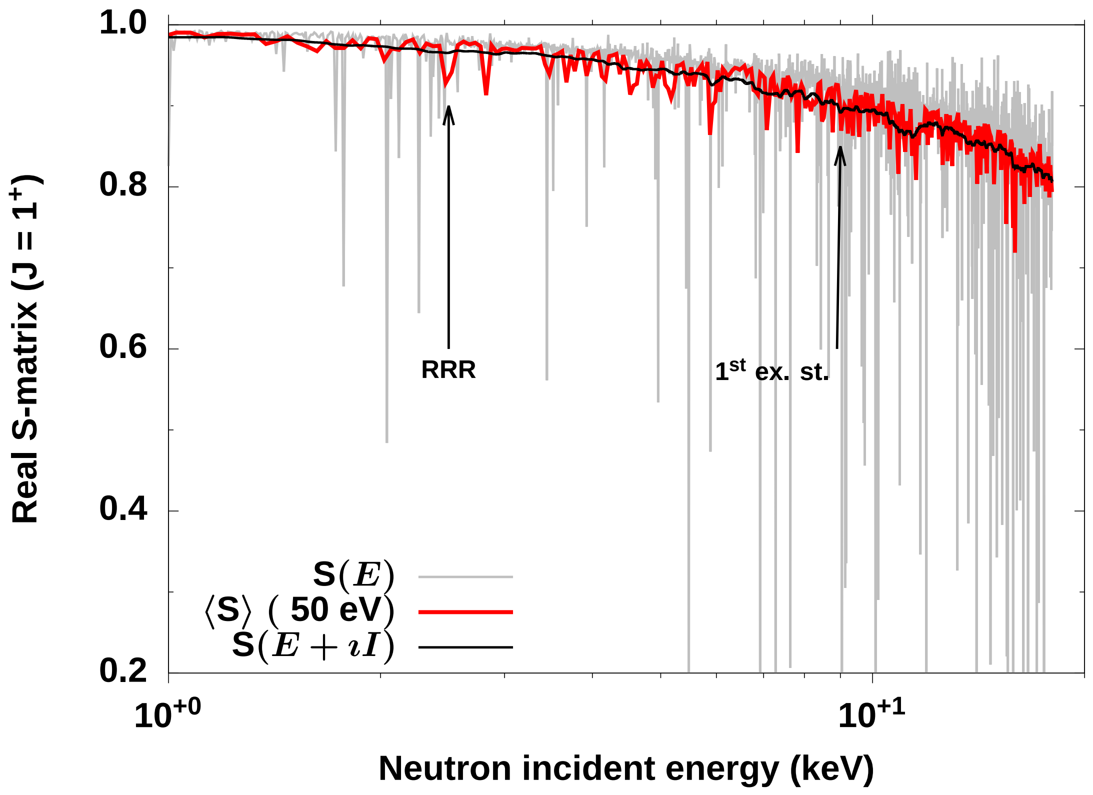
S-matrix Elements from Extrapolated Populations

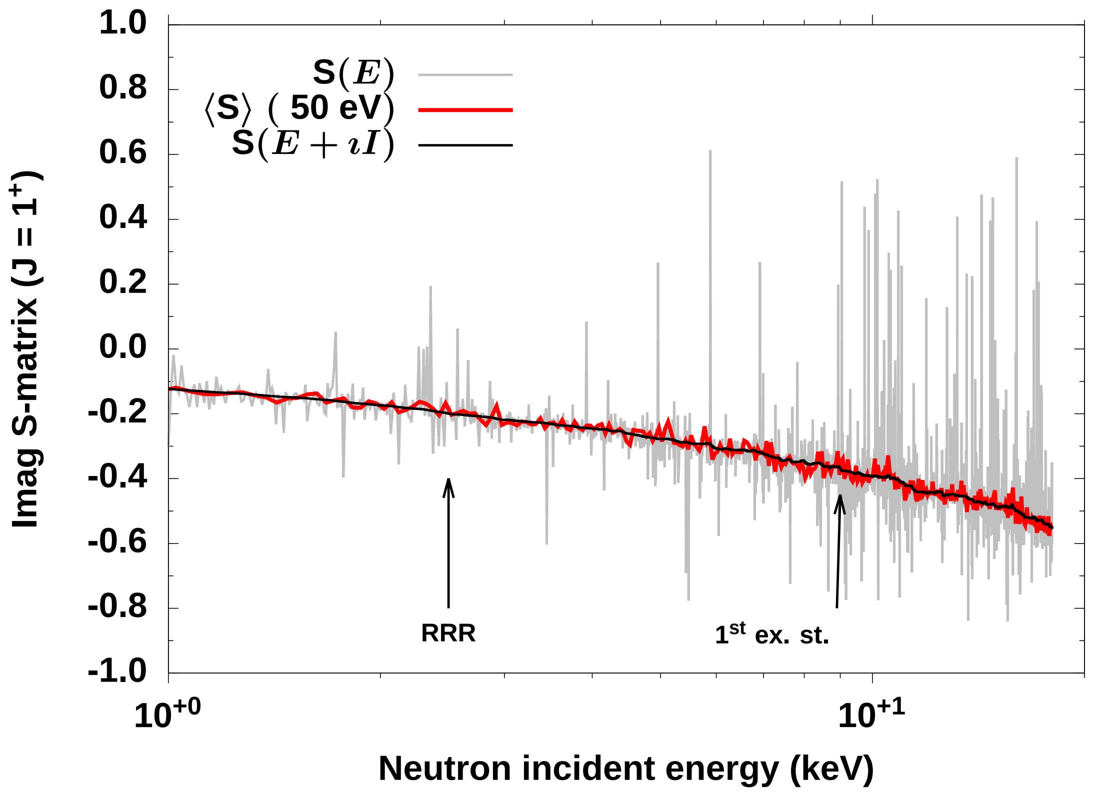
Real and Imaginary Components (J=0$^+$ Population)



S-matrix Elements from Extrapolated Populations

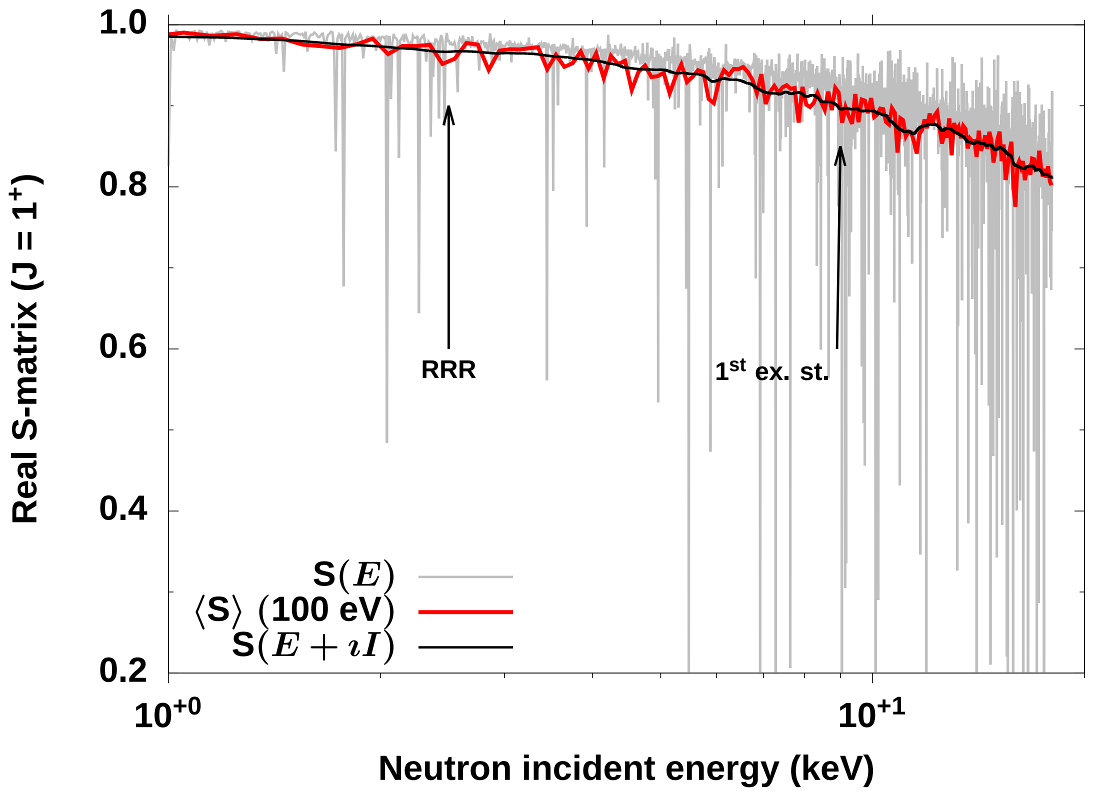
Real and Imaginary Components (J=1$^+$ Population)

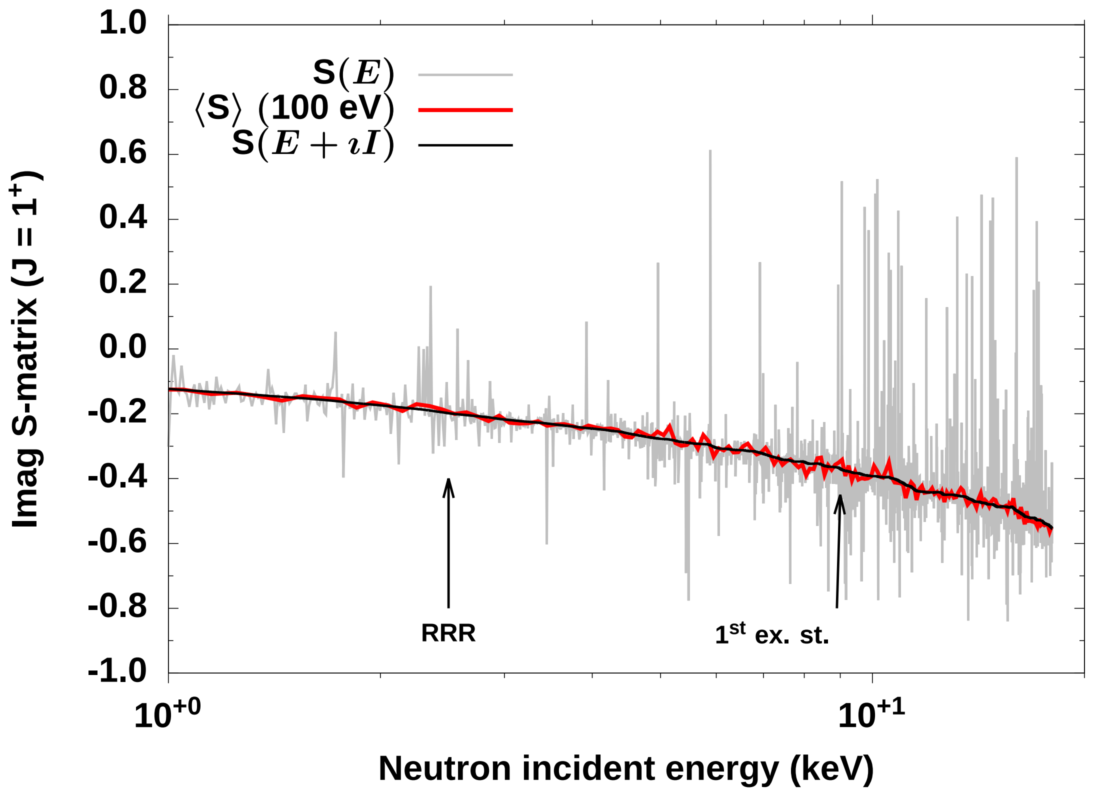




S-matrix Elements from Extrapolated Populations

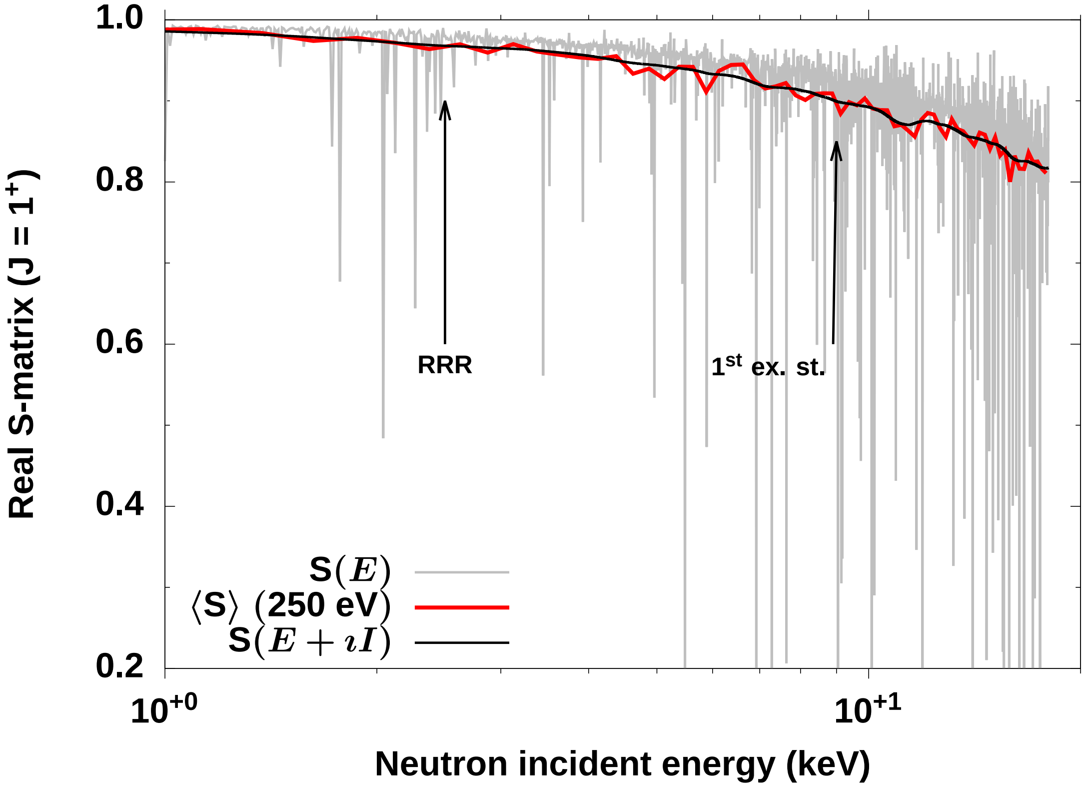
Real and Imaginary Components (J=1+ Population)

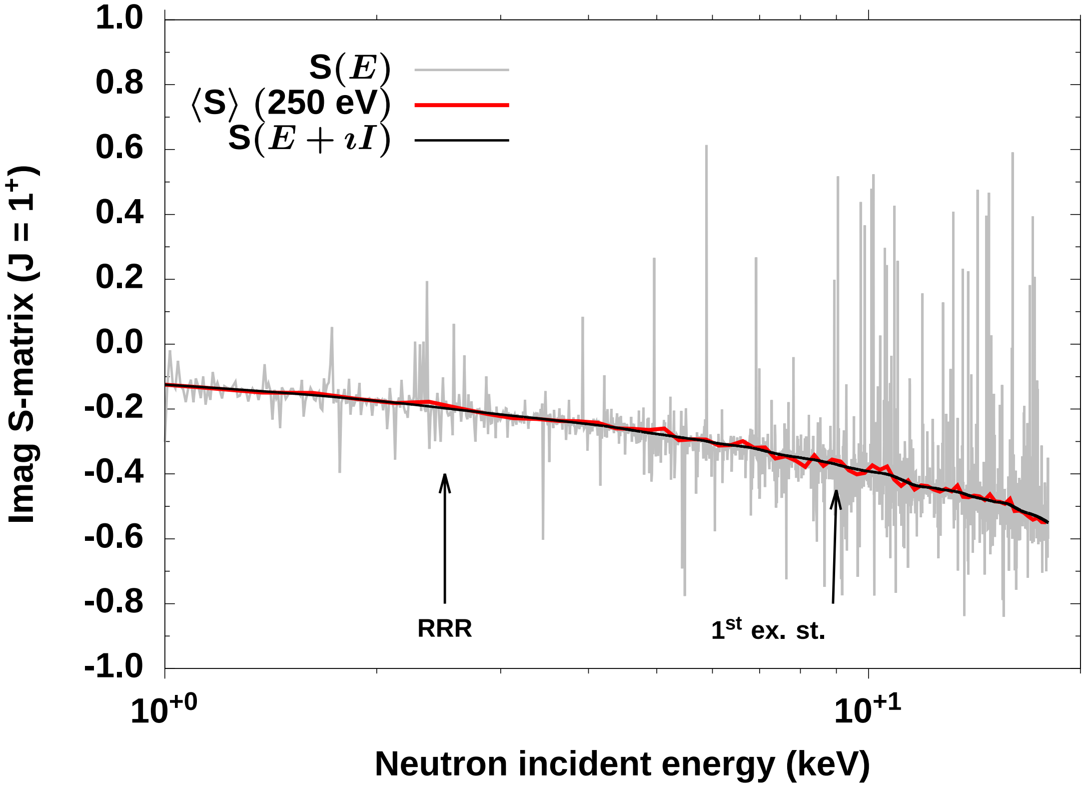




S-matrix Elements from Extrapolated Populations

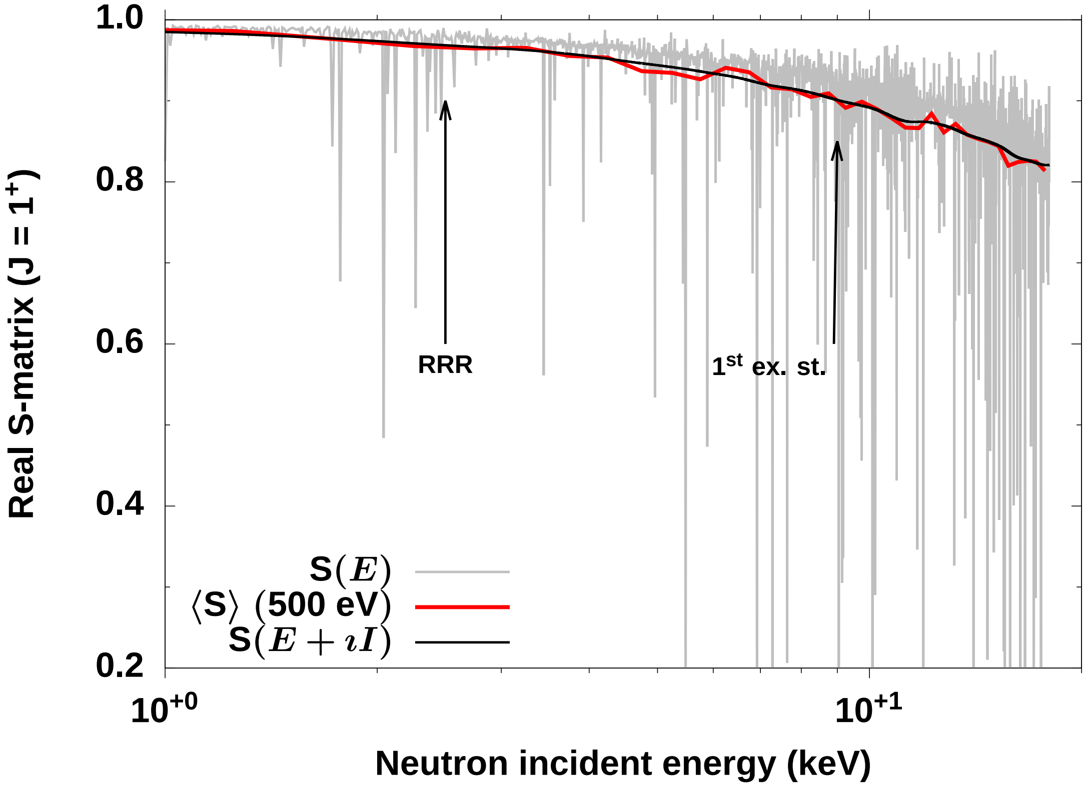
Real and Imaginary Components (J=1$^+$ Population)

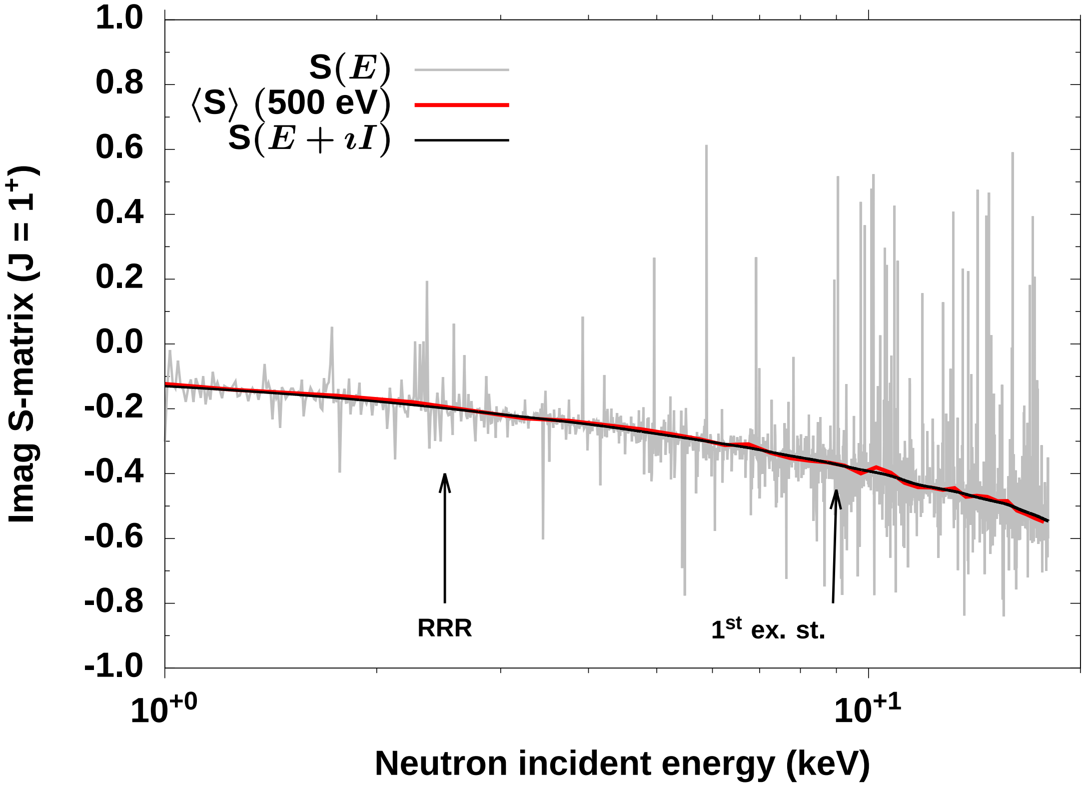




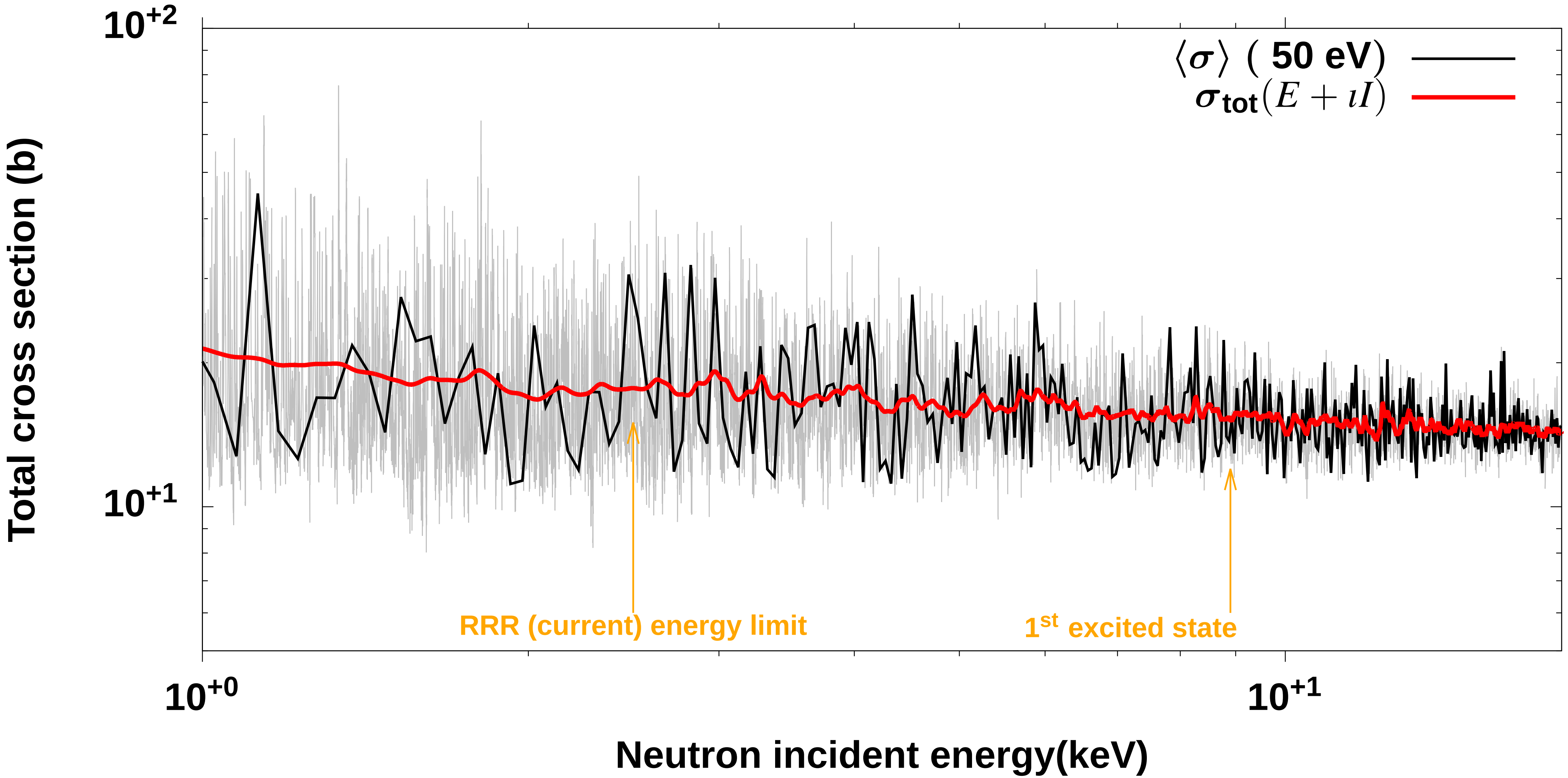
S-matrix Elements from Extrapolated Populations

Real and Imaginary Components (J=1$^+$ Population)

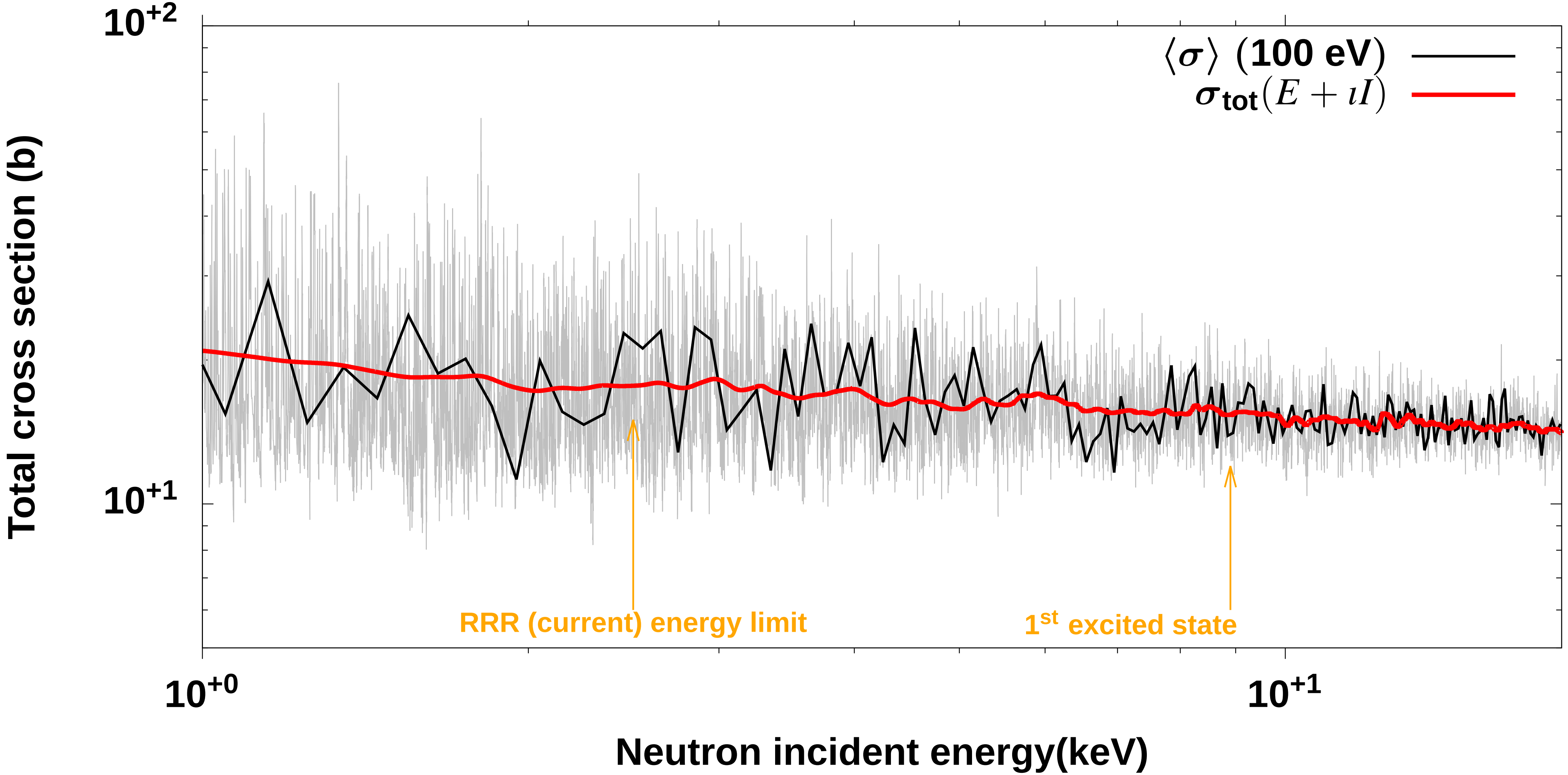




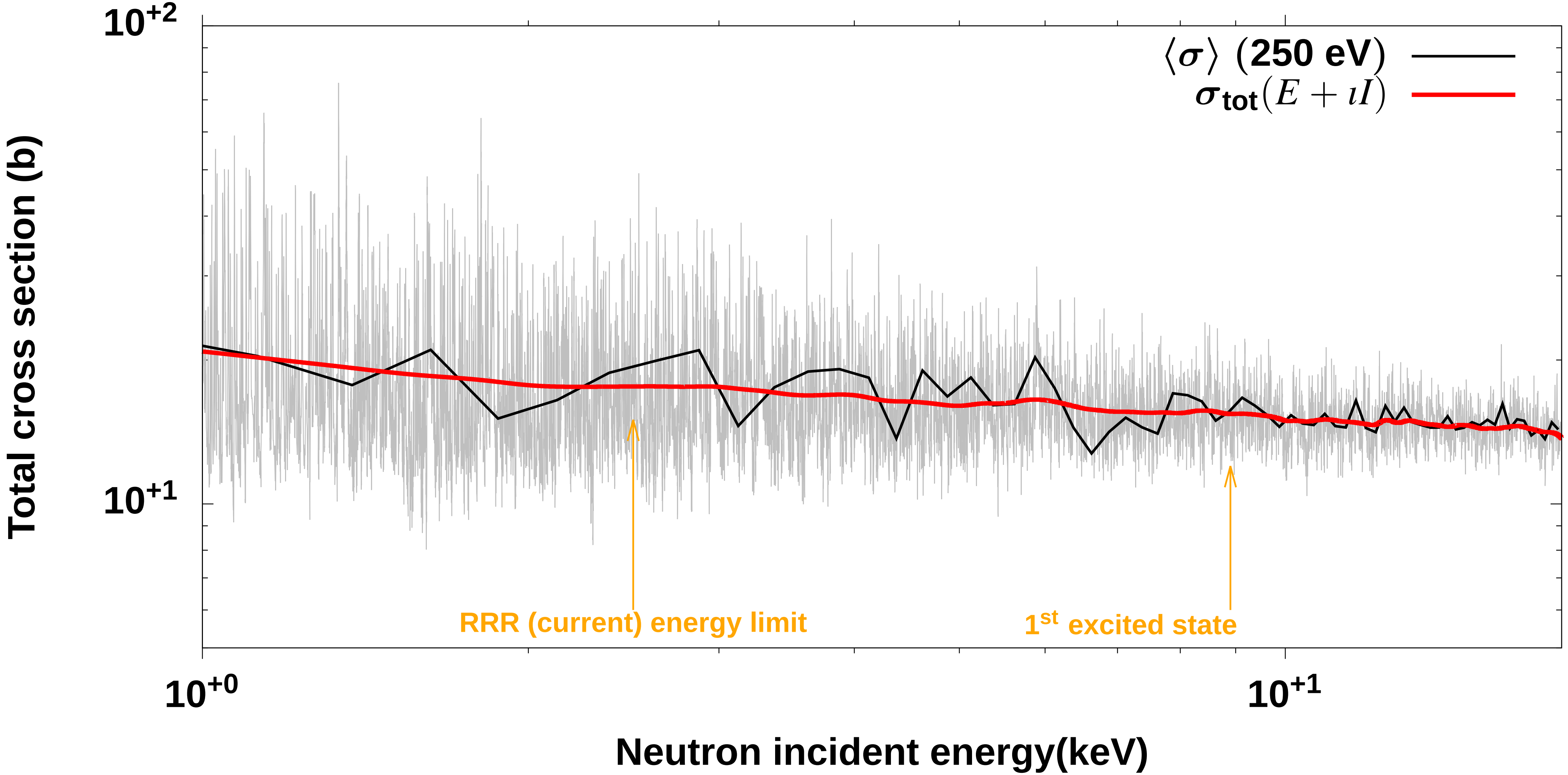
^{239}Pu Energy-average Total Cross Section



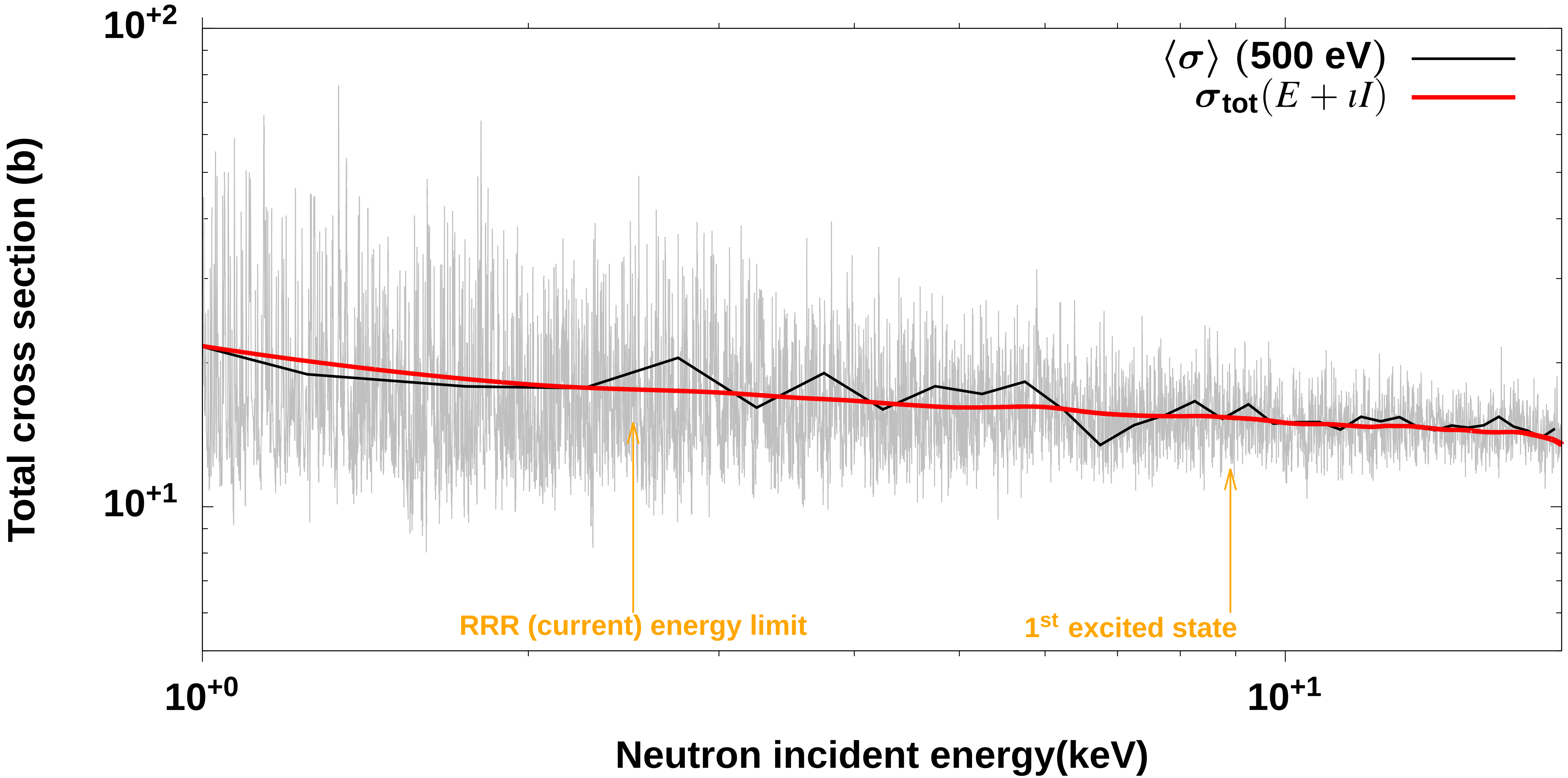
^{239}Pu Energy-average Total Cross Section



^{239}Pu Energy-average Total Cross Section



^{239}Pu Energy-average Total Cross Section



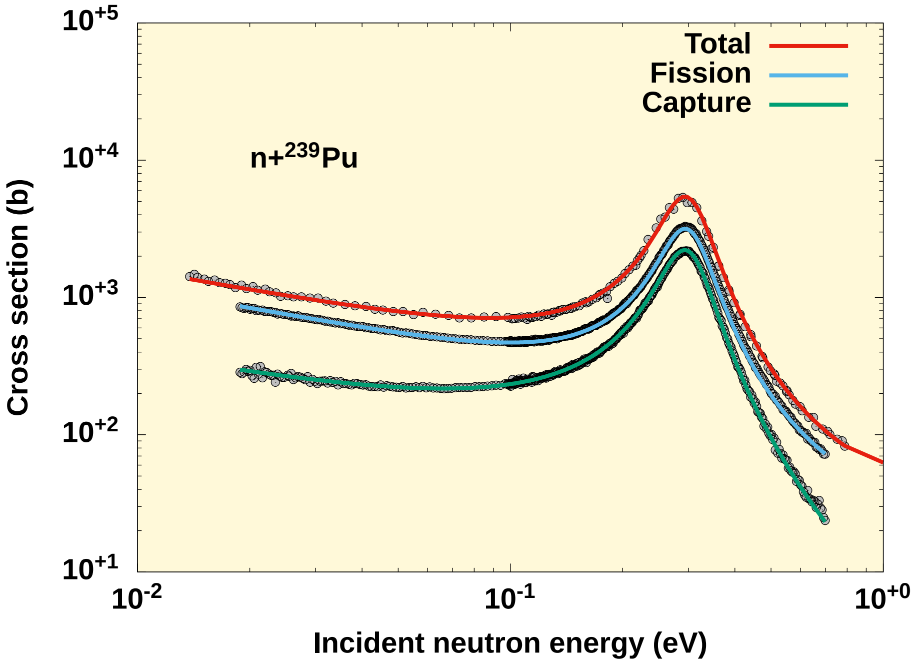
Resolving Key Issues in the Intermediate Structure Region

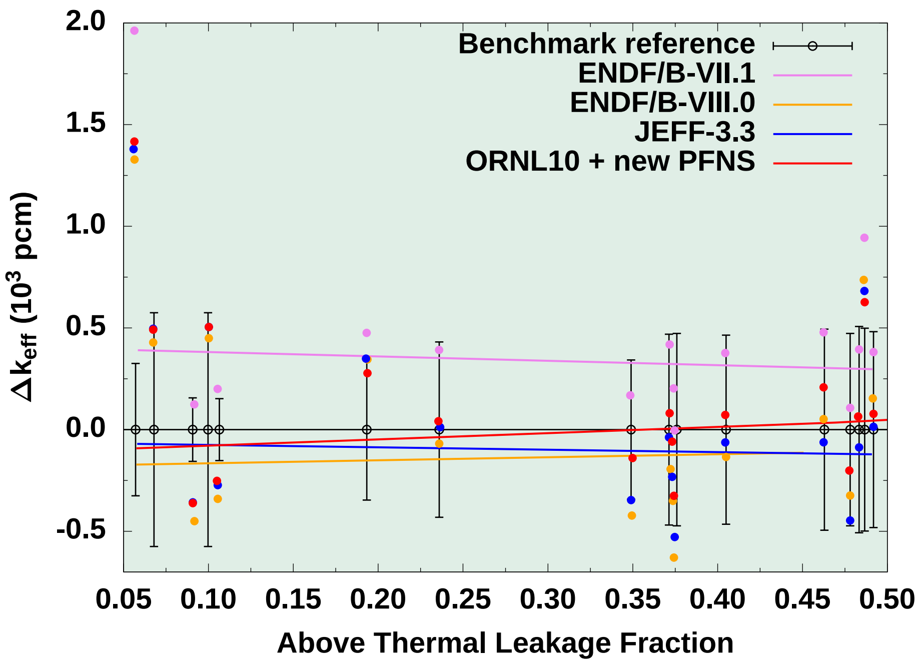
- The intermediate structure observed in the measured data can be described by including in the evaluated data files average cross sections calculated from the average S-matrix function
- With a proper energy grid the average cross sections can be broadened and calculated at the desired temperature
- In the case of selected applications for which the temperature dependence is particularly important and sensitive to the fluctuations, the resonance parameters could be used instead of the average cross sections
- Theoretical development to rigorously quantify the shape and compound component of the cross sections might be still needed

Coupling the Thermal and RRR Region to New PFNS

- **Background:** The recently released ENDF/B-VIII.0 was based on evaluations performed within the international collaboration CIELO aiming to improve nuclei of fundamental importance such as ^{235}U and ^{239}Pu. The ^{235}U R-matrix evaluation (ORNL) was updated with the latest thermal constants and prompt fission neutron spectra (PNFS) improving the benchmark performance of the thermal solutions. However, for ^{239}Pu evaluation the focus was in the high energy range and the prediction on the thermal solution benchmarks was underpredicted

- **Results:** Within IAEA coordinated research activities, newly evaluated PFNS showed a reduction of 1.8% on the average energy : PFNS(⟨Eav⟩=2.08 MeV). This changes were combined to recent work on ^{239}Pu R-matrix evaluation (ORNL) aimed to update the thermal constants. This led to improved benchmark performance in the thermal solutions





Conclusion and Remarks

- A procedure to accurately model the measured cross section fluctuations for inclusion into evaluated nuclear data files was developed and tested on ^{239}Pu total cross sections
- The procedure consisted on defining population of levels as well as related amplitudes extrapolated from the systematics of the resonance parameters in the resolved resonance region
- By using realistic population of extrapolated levels, the fit of measured total cross section produced a continuous S-matrix function S(E) in Reich-Moore approximation
- The S-matrix function averaged over a suitable energy interval was used to obtain averaged cross sections consistent with the measured data
- Transmittable formatted files (ENDF, GNDS) with LSSF=1 will consist on
  - File 3 : smoothed cross sections
  - File 2 : average resonance parameters fitted to the energy bins defined in File 3
- Capability to store probability tables is a way to show the fluctuating cross sections

Acknowledgments

This work was supported by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy

Thank you!