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Practical Method for Estimating Neutron Cross Section Covariances in the Resonance Region

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Recent evaluations of neutron cross section covariances in the resolved resonance region reveal the need for further research in this area. Major issues include declining uncertainties in multigroup representations and proper treatment of scattering radius uncertainty. To address these issues, the present work introduces a practical method based on kernel approximation using resonance parameter uncertainties from the Atlas of Neutron Resonances. Analytical expressions derived for average cross sections in broader energy bins along with their sensitivities provide transparent tool for determining cross section uncertainties. The role of resonance-resonance and bin-bin correlations is specifically studied. As an example we apply this approach to estimate (n,γ) and (n,el) covariances for the structural material ^{55}Mn.

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I. INTRODUCTION

There are several issues with neutron cross section covariances in the resolved resonance region. Probably the most important is decline of uncertainties of covariances in broad multigroup representations. The other issues include proper inclusion of scattering radius uncertainty and discrepancies in processed covariances in the ENDF file 32 produced by NJOY [1] and PUFF [2].

This work addresses these issues by developing a transparent formalism for cross section covariances based on resonance parameter uncertainties of Atlas of Neutron Resonances [3]. The full covariance matrix is constructed with a thermal region based directly on experimental data, scattering radius uncertainty is handled explicitly, and by using ENDF file 33 we would bypass file 32 processing issue. The full account of this work can be found in Ref. 4.

II. METHODOLOGY

We proceed in three steps. First, kernel approximation is invoked for single resonance or a group of resonances which are described by average cross section in suitable energy bin. Then, the uncertainty of this average cross section is computed from resonance parameter sensitivities folded with resonance parameter uncertainties, allowing explicit inclusion of resonance-resonance correlations. Finally covariance matrix is constructed by combining these bins together.

1. Average Cross Sections

For a single resonance at energy E_0, capture cross section as a function of the incident neutron energy E in the single-level Breit-Wigner (SLBW) can be expressed as

$$\sigma_\gamma(E) = \pi \lambda\!\!\!^{-2} \frac{g\Gamma_n\Gamma_\gamma}{(E-E_0)^2 + \frac{1}{4}\Gamma^2}. \tag{1}$$

Here, $\lambda\!\!\!^{-}$ is the de Broglie wavelength of the incoming neutron, g is the spin statistical factor, and Γ_n, Γ_γ, and Γ are the neutron, radiative and total widths, respectively. The capture kernel is defined as the integral

$$A_\gamma = \int_{-\infty}^{+\infty} \sigma_\gamma(E)dE = 2\pi^2 \lambda\!\!\!^{-2} g\frac{\Gamma_n\Gamma_\gamma}{\Gamma}. \tag{2}$$

The average cross section due to several resonances located in one energy bin with the energy width of $\Delta E = E_1 - E_2$ can be approximated as

$$\begin{aligned}\bar{\sigma}_\gamma &= \tfrac{1}{\Delta E}\textstyle\int_{E_1}^{E_2} \sigma_\gamma(E)dE \approx \tfrac{1}{\Delta E}\int_{-\infty}^{+\infty} \sigma_\gamma(E)dE \\ &\approx \sum_r a_r \tfrac{g_r\Gamma_{nr}\Gamma_{\gamma r}}{\Gamma_r}\ .\end{aligned} \tag{3}$$

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Here the summation goes over all resonances r in the energy interval ΔE where a_r is defined as $a_r = 2\pi^2\lambda\!\!\!^{-2}/\Delta E$.

Within the SLBW formalism the elastic scattering cross section for a single resonance can be expressed as

$$\sigma_n(E) = \sum_l 4\pi\lambda\!\!\!^{-2}(2l+1)\sin^2\phi_l + \pi\lambda\!\!\!^{-2} g \frac{\Gamma_n^2 - 2\Gamma_n\Gamma\sin^2\phi_l + 2(E-E_0)\Gamma_n\sin(2\phi_l)}{(E-E_0)^2+\frac{1}{4}\Gamma^2}, \quad (4)$$

where ϕ_l is the phase shift, l being the orbital momentum. The term containing $2(E-E_0)\Gamma_n\sin(2\phi_l)$ describes interference between potential and resonance scattering which is negative at $E < E_0$ and positive at $E > E_0$. These negative and positive contributions are approximately equal and they cancel out if one computes the average elastic scattering cross section by integrating the cross section over a broad energy interval around the resonance energy E_0.

Considering that potential scattering is slowly varying function of energy and the dominant contribution to integral of the resonance term comes from relatively narrow energy range (compared to E) around E_0 one gets

$$\bar{\sigma}_n \approx \sigma_n^{pot}(\bar{E}) + \sum_r a_r \frac{g_r\Gamma_{nr}(\Gamma_{nr} - 2\Gamma_r\sin^2\phi_{lr})}{\Gamma_r}, \quad (5)$$

where $\bar{E} \approx E_0$ and σ_n^{pot} is the potential scattering cross section.

2. Covariances

Sensitivity to the resonance parameter can be computed as

$$\frac{\partial\bar{\sigma}}{\partial p_{i,r}} = \sum_{r'} \frac{\partial\bar{\sigma}_{r'}}{\partial p_{i,r}} = \frac{\partial\bar{\sigma}_r}{\partial p_{i,r}}, \quad (6)$$

where $i = \gamma, n$. We note that the sensitivity for only one resonance remains on the right hand side and we neglect contributions from the imperfect knowledge of the resonance energy E_0 and spin J. Using these sensitivities the uncertainty of the average cross section can be obtained as

$$< \delta\bar{\sigma}\delta\bar{\sigma} > = \sum_{i,r,i',r'} \frac{\partial\bar{\sigma}}{\partial p_{i,r}} < \delta p_{i,r}\delta p_{i',r'} > \frac{\partial\bar{\sigma}}{\partial p_{i',r'}}, \quad (7)$$

where $< \delta p_{i,r}\delta p_{i',r'} >$ is the covariance of resonance parameters.

Using Eq. (3) sensitivities of the average capture cross section can be expressed as

$$\frac{\partial\bar{\sigma}_\gamma}{\partial\Gamma_n} = ag\frac{\partial}{\partial\Gamma_n}\frac{\Gamma_n\Gamma_\gamma}{\Gamma} = ag\frac{\Gamma_\gamma^2}{\Gamma^2} = \bar{\sigma}_\gamma\frac{\Gamma_\gamma}{\Gamma}\frac{1}{\Gamma_n}, \quad (8)$$

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At low energies, the 3rd term in Eq. (5) can be neglected and thus sensitivities of the average elastic resonance scattering cross section $\bar{\sigma}_n^{res}$ with respect to the resonance parameters can be obtained as

$$\frac{\partial\bar{\sigma}_n^{res}}{\partial\Gamma_n} = ag\frac{\partial}{\partial\Gamma_n}\frac{\Gamma_n^2}{\Gamma} = ag\frac{\Gamma_n}{\Gamma}\frac{\Gamma+\Gamma_n}{\Gamma} = \bar{\sigma}_n^{res}\frac{\Gamma+\Gamma_\gamma}{\Gamma}\frac{1}{\Gamma_n}, \quad (10)$$

$$\frac{\partial\bar{\sigma}_n^{res}}{\partial\Gamma_\gamma} = ag\frac{\partial}{\partial\Gamma_\gamma}\frac{\Gamma_n^2}{\Gamma} = -ag\frac{\Gamma_n^2}{\Gamma^2} = -\bar{\sigma}_n^{res}\frac{\Gamma_\gamma}{\Gamma}\frac{1}{\Gamma_\gamma}. \quad (11)$$

Using Eq. (4) and neglecting d-wave, sensitivity of potential scattering cross section σ_n^{pot} to scattering radius can be obtained as

$$\frac{\partial\sigma_n^{pot}}{\partial R'} = \frac{8\pi}{k}\left\{\sin\phi_0\cos\phi_0 + 3\left(1 - \frac{1}{1+(kR')^2}\right)\sin\phi_1\cos\phi_1\right\}. \quad (12)$$

The elastic scattering cross section uncertainty is obtained by quadratic summation of contributions from both the resonance scattering and the potential scattering.

Table 1. ^{55}Mn cross sections uncertainties and scattering radius.

thermal capture cross section, σ_γ	13.36 b ± 0.8%
thermal elastic cross section, σ_n	2.06 b ± 3%
scattering radius, R'	4.5 fm ± 17.8%

III. APPLICATION TO ^{55}MN

Evaluation of covariances is carried out in three steps. First, we establish energy bins by suitably subdividing the entire resonance region, then determine correlations within these bins and compute uncertainties of average cross sections, and finally determine bin-bin correlations and construct a complete covariance matrix.

Thermal region is treated independently assuming full correlation with adopted uncertainties given in Table 1. This table also shows the value of $\Delta R'$ in the resonance region, which was considered to be twice the value in the thermal region of Ref. 3.

1. ^{55}Mn(n, γ) Covariances

When doing energy binning an evaluator proceeds iteratively, starts with estimates, computes averages from kernels and compares them with correct values obtained by processing ENDF file 2 in MLBW representation with NJOY. Once good agreement is reached the binning is considered to be completed. The outcome of our procedure is shown in Fig. 1.

Relative uncertainties shown in Fig. 2 depend on values of resonance-resonance correlations which were adopted uniformly in each energy bin. Several options

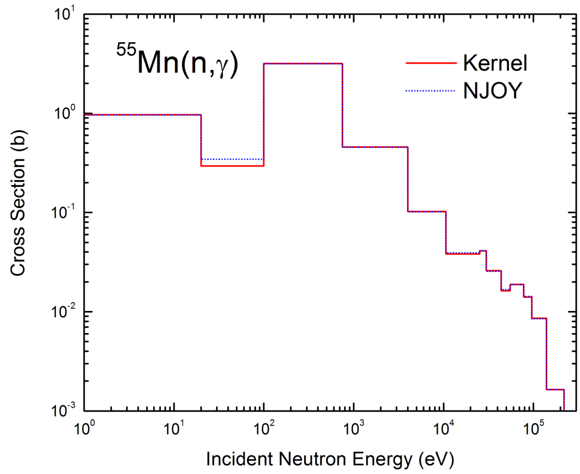

Fig. 1. (Color online) Comparison of average cross sections for ^{55}Mn capture obtained from kernels (above 100 eV) and from NJOY.

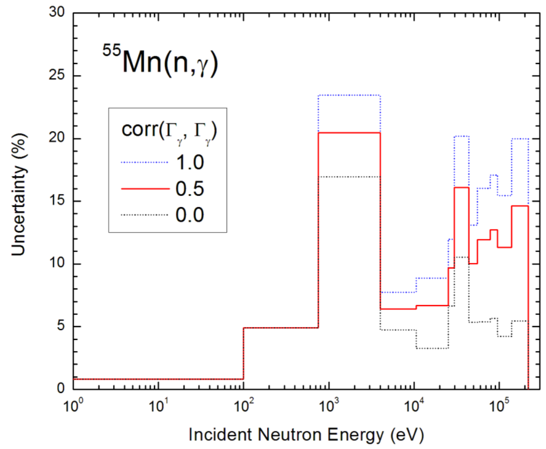

Fig. 2. (Color online) Relative uncertainties of average cross sections for ^{55}Mn capture for different values of corr$(\Gamma_\gamma, \Gamma_\gamma)$.

were tested: corr$(\Gamma_\gamma, \Gamma_\gamma)$ = 0, 0.5, 1.0, that is, uncorrelated, 50% and fully correlated, respectively. One can see that impact at high energies is very strong and uncorrelated option should be excluded to prevent uncertainty decline. In the absence of detailed knowledge we estimated these correlation coefficients to be 0.5.

A full covariance matrix was produced by using the above uncertainties, adding bin-bin correlation coefficients and converting this information into ENDF file 33. Then, NJOY was used to process the covariances into 33-group representation. The result is shown in Fig. 3 where resonance-resonance and bin-bin correlations are set to 0.5.

2. ^{55}Mn(n, el) Covariances

Figure 4 shows average elastic scattering cross sections from kernels compared with correct values produced by NJOY using MLBW representation. It is seen that our

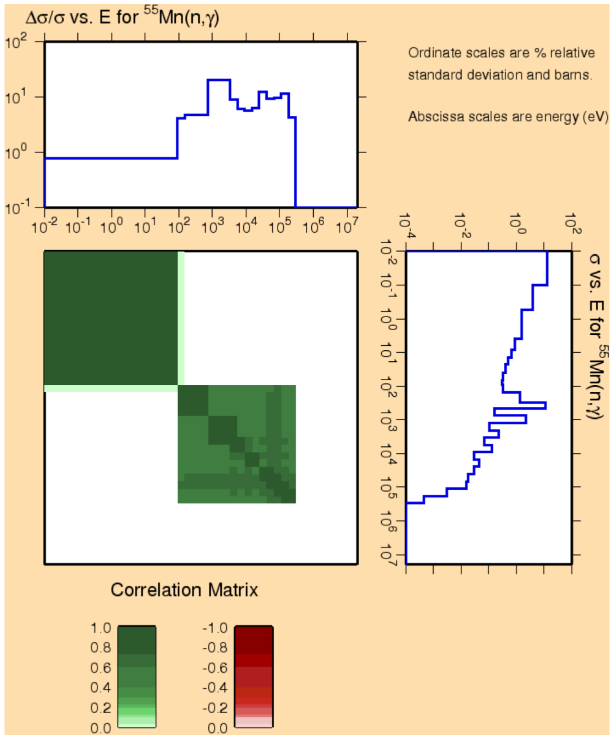

Fig. 3. (Color online) Covariances for ^{55}Mn capture in 33-energy groups where resonance-resonance and bin-bin correlation coefficients are 0.5.

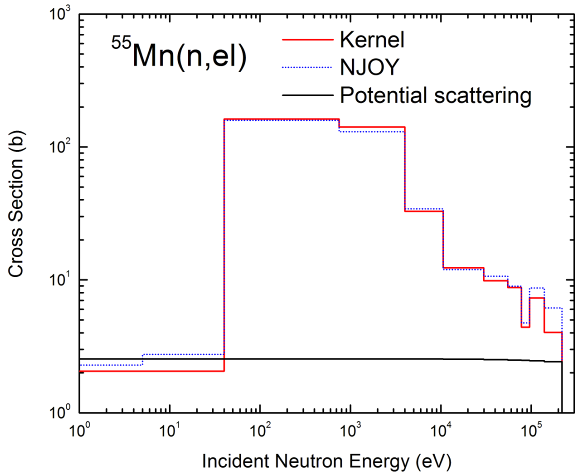

Fig. 4. (Color online) Comparison of average cross sections for ^{55}Mn elastic scattering obtained from kernels (above 40 eV) and from NJOY.

results agrees well with NJOY calculations and reasonable agreement was reached, suggesting that our approximation is sound.

Figure 5 shows relative uncertainties of average scattering cross sections. One can see that impact of resonance-resonance correlations is relatively small. This can be understood by the fact that, as a rule, there is only one strong elastic resonance in each energy bin. Contribution of scattering radius uncertainty, $\Delta R'$ to the uncertainty of the average elastic cross

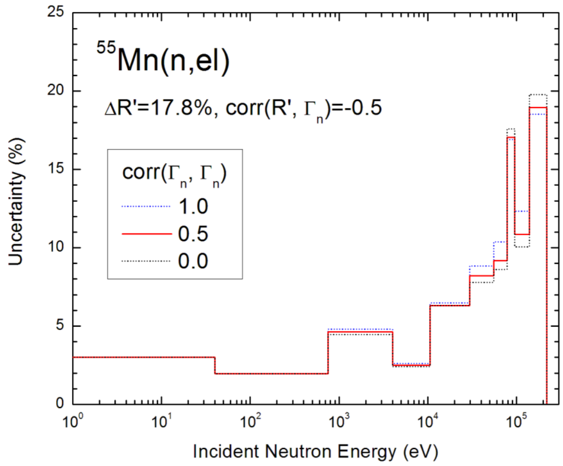

Fig. 5. (Color online) Uncertainties of average cross sections for ^{55}Mn elastic scattering for three different values of corr(Γ_n, Γ_n).

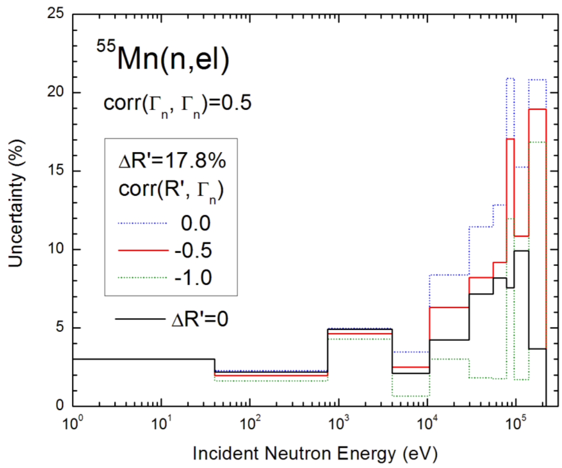

Fig. 6. (Color online) Uncertainties of average cross sections for ^{55}Mn elastic scattering for different values of corr(R', Γ_n).

section is examined in Fig. 6. At high energies, where σ_n^{res} becomes comparable to σ_n^{pot}, the scattering radius uncertainty contributes to the overall uncertainty quite considerably, depending on adopted correlation. Figure 7 shows final covariances for resonance-resonance and bin-bin correlation coefficients set to 0.5.

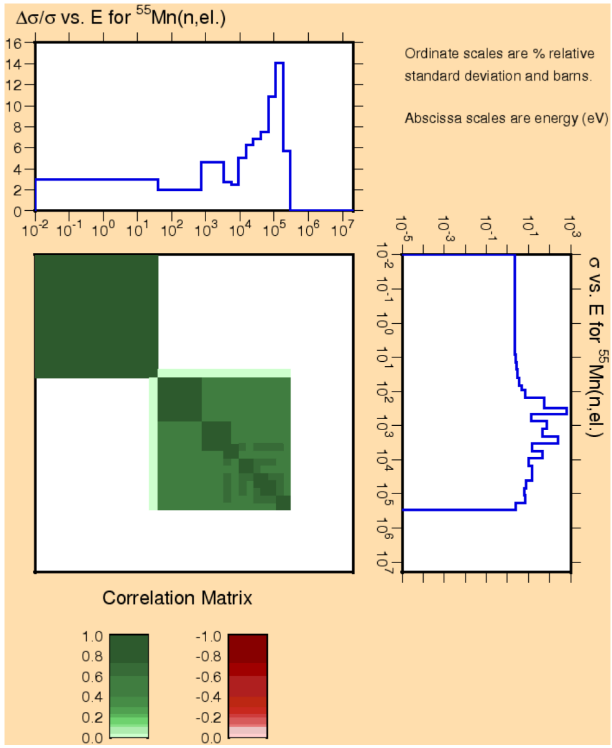

Fig. 7. (Color online) Covariances for ^{55}Mn(n, el) in 33-energy groups; resonance-resonance and bin-bin correlation coefficients are 0.5.

Practical application of this formalism was illustrated on covariances for ^{55}Mn. The formalism works well in particular for capture and the results look plausible. Contribution from potential scattering to uncertainty of elastic scattering cross sections is significant especially at high resonance energies.

IV. CONCLUSIONS

We developed formalism for producing ENDF file 33 covariances in the resonance region based on the kernel approximation for capture and elastic scattering and using data from the Atlas of Neutron Resonances. The formalism is transparent and based on analytical expressions.

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