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An analytic approach to probability tables for the unresolved resonance region

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Abstract. The Unresolved Resonance Region (URR) connects the fast neutron region with the Resolved Resonance Region (RRR). The URR is problematic since resonances are not resolvable experimentally yet the fluctuations in the neutron cross sections play a discernible and technologically important role: the URR in a typical nucleus is in the 100 keV – 2 MeV window where the typical fission spectrum peaks. The URR also represents the transition between R-matrix theory used to described isolated resonances and Hauser-Feshbach theory which accurately describes the average cross sections. In practice, only average or systematic features of the resonances in the URR are known and are tabulated in evaluations in a nuclear data library such as ENDF/B-VII.1. Codes such as AMPX and NJOY can compute the probability distribution of the cross section in the URR under some assumptions using Monte Carlo realizations of sets of resonances. These probability distributions are stored in the so-called PURR tables. In our work, we begin to develop a scheme for computing the covariance of the cross section probability distribution analytically. Our approach offers the possibility of defining the limits of applicability of Hauser-Feshbach theory and suggests a way to calculate PURR tables directly from systematics for nuclei whose RRR is unknown, provided one makes appropriate assumptions about the shape of the cross section probability distribution.

1. Introduction

For neutron induced reactions below 20 MeV incident energy, the Unresolved Resonance Region (URR) connects the fast neutron region with the Resolved Resonance Region (RRR). In the RRR, R-matrix theory is used to describe the shape and correlations between resolved resonances in the cross sections. In the fast region, Hauser-Feshbach theory with the Width Fluctuation Correction (WFC) accurately describes the cross sections. In between, the URR is problematic: here the resonances are not resolvable experimentally yet the fluctuations in the neutron cross sections play a discernible and technologically important role. Indeed, the URR in a typical nucleus is in the 100 keV – 2 MeV window, where the typical fission spectrum peaks.

In practice, only average or systematic features of the resonances in the URR are known and these are tabulated in evaluations in a nuclear data library such as ENDF/B-VII.1 [1]. With judicious application of nuclear reaction phenomenology, one can compute the average cross sections in the URR region (see pp. 343-350 of the ENDF Format manual [2]). In fact, one can go further than just the average cross section. Several processing codes, notably NJOY [3], AMPX [4], CALENDF [5] and GRUCON [6], offer one the ability to compute the probability distribution function (PDF) for the total cross section at a fixed incident energy $\wp(\sigma_{(n,\mathrm{tot})}|E)$ as well as the conditional probabilities for the neutron induced reactions (n,x), $\wp(\sigma_{(n,x)}|\sigma_{(n,\mathrm{tot})},E)$. From these $\wp$'s, one can compute self-shielding factors, Bondarenko factors, cross section bands, etc..

Processing codes adopt a Monte Carlo approach to computing probability distributions. They generate an ensemble of "resonance ladders", namely a simulated set of levels for the compound nucleus populated by the incident neutron accompanied by the resonance widths of these states. These simulated resonances are generated using the average parameters in the ENDF formatted files. These realizations of simulated resonances are used to reconstruct a sample cross sections and from the ensemble of reconstructed cross sections, the probability distribution of the cross section is determined. These Monte-Carlo approaches are cumbersome and time consuming, often dominating the time taken to process a single evaluation. In this contribution, we ask whether it is possible to compute the PDF x, $\wp(\sigma_x|E)$, analytically?

Our proposed scheme is straightforward, we assume that the cross section PDF can be approximated with some suitably shaped multivariate PDF, say a multi-variate log-normal, Poisson or χ^2 distribution, as these are consistent with the constraint that $\sigma_x>0$. We then compute $\langle\sigma_x\rangle$ and $\mathrm{cov}(\sigma_x,\sigma_y)=\langle\sigma_x\sigma_y\rangle-\langle\sigma_x\rangle\langle\sigma_y\rangle$ and convert these to a form appropriate for our assumed PDF.

For this scheme to work we must compute the average cross section and the cross section covariance. The average cross section is already known in both the URR [2] and from the Hauser-Feshbach formula with the Width Fluctuation Correction (WFC). Surprisingly, both URR and the Hauser-Feshbach theory with the WFC use same basic theory, but with practical differences. Both assume have narrow isolated resonances so that the weak

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coupling approximation is valid and we may treat the resonances with the Single Level Breit-Wigner (SLBW) approximation. Both approaches assume the average cross section may be computed with an ensemble average of resonances, assuming that the resonance widths follow a Porter-Thomas (χ^2) distribution. In the URR, the degree-of-freedom ν of the χ^2 distribution is specified by the evaluator. In the WFC of the Hauser-Feshbach theory, ν is determined from a phenomenological prescription such as that in Ref. [7]. The actual cross section average is then given essentially by the Hauser-Feshbach equation in both cases but the details of the averaging procedure differ in practice. In the URR, the MC2-II algorithm [8] is used while in the fast region the WFC is used as given e.g., by Gruppelaar [9]. Given that both use essentially the same approach, we should be able to make the fast and average URR cross sections agree. More importantly, we should be able to use this common approach as a guide for computing the covariance.

2. The average cross section

We begin by reviewing the origins of the Width Fluctuation Correction (WFC) for the compound nuclear cross section. This discussion motivates our approach to the cross section correlation $\langle\sigma_{ab}\sigma_{cd}\rangle$ in Sect. 3.

Here we follow the derivation in Ref. [9]. Assuming that we have narrow isolated resonances, $\Gamma \ll D \ll \Delta E$ where Γ is a typical resonance width, D is the mean resonance spacing and ΔE is the typical energy scale of measurements. In this case the Single Level Breit Wigner (SLBW) approximation is valid and we have the total channel cross section of

$$\sigma_c = \frac{4\pi g_c}{k_c^2}\sum_\mu \left\{\sin^2\phi_c + \frac{\Gamma_{c\mu}}{\Gamma_\mu}\left(\psi_\mu\cos 2\phi_c + \chi_\mu \sin 2\phi_c\right)\right\} \tag{1}$$

and the partial channel reaction cross section of

$$\sigma_{ab} = \frac{4\pi g_a}{k_a^2}\sum_\mu \frac{\Gamma_{a\mu}\Gamma_{b\mu}}{\Gamma_\mu^2}\psi_\mu. \tag{2}$$

Here the profile functions ψ and χ are

$$\psi_\mu + i\chi_\mu = \frac{\Gamma_\mu^2/4}{(E-E_0)^2+\Gamma_\mu^2/4} + i\frac{(E-E_0)\Gamma_\mu/2}{(E-E_0)^2+\Gamma_\mu^2/4}. \tag{3}$$

These channel cross sections must of course be added appropriately to compute the total, capture, elastic or any other reaction cross section.

Consider now the energy average of a reaction cross section in the SLBW approximation:

$$\langle\sigma_{ab}\rangle = \frac{1}{\Delta E}\int_{E-\Delta E/2}^{E+\Delta E/2} dE'\sigma_{ab}(E') \tag{4}$$

If we assume that we have narrow isolated resonances, then $\Delta E \gg \Gamma_\mu$ and

$$\langle\sigma_{ab}\rangle \approx \frac{4\pi g_a}{\Delta E k_a^2}\sum_\mu \frac{\Gamma_{a\mu}\Gamma_{b\mu}}{4} \times \int_{-\infty}^{\infty} dE' \frac{1}{(E-E_0)^2+\Gamma_\mu^2/4} \tag{5}$$

The SLBW reaction cross section has poles in both the upper and lower half-planes of the complex energy surface. Therefore we will consider a semi-circular contour integral with the contour closing in the upper half plane, enclosing all the poles in the cross section above the real axis. Performing this integral we easily arrive at

$$\langle\sigma_{ab}\rangle \approx \frac{2\pi g_a}{\Delta E k_a^2}\sum_\mu \frac{\Gamma_{a\mu}\Gamma_{b\mu}}{\Gamma_\mu} \tag{6}$$

We assume that the number of resonances is large and that we may replace the sum over resonances with an ensemble average. So, we replace

$$\sum_\mu \frac{\Gamma_{a\mu}\Gamma_{b\mu}}{\Gamma_\mu} \approx \frac{\Delta E}{D}\left\langle\left\langle \frac{\Gamma_a\Gamma_b}{\Gamma}\right\rangle\right\rangle. \tag{7}$$

The ensemble average $\langle\langle\cdot\rangle\rangle$ is an average over all possible values of the widths, which are assumed to have a Porter-Thomas or χ^2 distribution with ν degrees of freedom, $\wp^{PT}(x|\nu)$. For $a \neq b$:

$$\left\langle\left\langle \frac{\Gamma_a\Gamma_b}{\Gamma}\right\rangle\right\rangle = \int_0^\infty d\Gamma_a\, \wp^{PT}\left(\frac{\Gamma_a}{\overline{\Gamma}_a}\middle|\nu_a\right) \times \int_0^\infty d\Gamma_b\, \wp^{PT}\left(\frac{\Gamma_b}{\overline{\Gamma}_b}\middle|\nu_b\right) \times \prod_{c\neq a,b}\int_0^\infty d\Gamma_c\, \wp^{PT}\left(\frac{\Gamma_c}{\overline{\Gamma}_c}\middle|\nu_c\right)\frac{\Gamma_a\Gamma_b}{\Gamma} \tag{8}$$

and for $a = b$:

$$\left\langle\left\langle \frac{\Gamma_a^2}{\Gamma}\right\rangle\right\rangle = \int_0^\infty d\Gamma_a\, \wp^{PT}\left(\frac{\Gamma_a}{\overline{\Gamma}_a}\middle|\nu_a\right) \times \prod_{c\neq a}\int_0^\infty d\Gamma_c\, \wp^{PT}\left(\frac{\Gamma_c}{\overline{\Gamma}_c}\middle|\nu_c\right)\frac{\Gamma_c^2}{\Gamma} \tag{9}$$

with

$$\langle\langle\Gamma_c\rangle\rangle = \int_0^\infty d\Gamma_c\, \wp^{PT}\left(\frac{\Gamma_c}{\overline{\Gamma}_c}\middle|\nu_c\right)\Gamma_c = \overline{\Gamma}_c. \tag{10}$$

The integrals in Eqs. (8)–(9), can be done numerically, as is done in most processing codes (actually using the same MC^2-II algorithm) or performed analytically follow Gruppelaar [9]. Using the fact that

$$\frac{1}{\Gamma} = \int_0^\infty dt e^{-\Gamma t} = \int_0^\infty dt e^{-\sum_c \Gamma_c t} \tag{11}$$

and the result

$$\mathcal{J}_n(t,\overline{\Gamma}_c,\nu_c) = \int_0^\infty d\Gamma_c\, \wp^{PT}\left(\frac{\Gamma_c}{\overline{\Gamma}_c}\middle|\nu_c\right)(\Gamma_c)^n e^{-\Gamma_c t} = \left(\frac{2\overline{\Gamma}_c}{\nu_c}\right)^n \frac{\Gamma(\frac{\nu_c}{2}+n)}{\Gamma(\frac{\nu_c}{2})}\left(1+\frac{2t\overline{\Gamma}_c}{\nu_c}\right)^{-(n+\nu_c/2)}, \tag{12}$$

we obtain the usual

$$\left\langle\left\langle \frac{\Gamma_a\Gamma_b}{\Gamma}\right\rangle\right\rangle = \frac{\overline{\Gamma}_a\overline{\Gamma}_b}{\overline{\Gamma}}\mathcal{W}_{ab}. \tag{13}$$

Here $\mathcal{W}_{ab}$ is the WFC factor:

$$\mathcal{W}_{ab} = \left(1 + \delta_{ab}\frac{2}{\nu_a}\right) \times \int_0^\infty dx \prod_c \left(1 + \frac{2\overline{\Gamma}_c}{\nu_c\overline{\Gamma}}x\right)^{-(\delta_{ac}+\delta_{bc}+\nu_c/2)}. \quad (14)$$

With these, we obtain the energy average reaction cross section

$$\langle\sigma_{ab}\rangle = \frac{2\pi g_a}{k_a^2 D}\frac{\overline{\Gamma}_a\overline{\Gamma}_b}{\overline{\Gamma}}\mathcal{W}_{ab}. \quad (15)$$

Since we are in the weak coupling limit, we have $T_c \approx 2\pi\overline{\Gamma}_c/D$ and we recover the usual Hauser-Feshbach equation:

$$\langle\sigma_{ab}\rangle = \frac{g_a}{k_a^2}\frac{T_a T_b}{\sum_c T_c}\mathcal{W}_{ab}. \quad (16)$$

3. Cross section correlations

Now consider the cross section correlation $\langle\sigma_{ab}\sigma_{cd}\rangle$. Again we assume that we have narrow isolated resonances and as before, the energy average in the cross section correlation can be approximated

$$\langle\sigma_{ab}\sigma_{cd}\rangle \approx \frac{1}{\Delta E}\left(\frac{4\pi g_a}{k_a^2}\right)\left(\frac{4\pi g_c}{k_c^2}\right) \times \sum_{\mu\nu}\int_{-\infty}^{\infty}\left[\frac{\Gamma_{a\mu}\Gamma_{b\mu}/4}{(E'-E_\mu)^2+\Gamma_\mu^2/4}\right] \times \left[\frac{\Gamma_{c\nu}\Gamma_{d\nu}/4}{(E'-E_\nu)^2+\Gamma_\nu^2/4}\right] dE' \quad (17)$$

Again, this has poles in both the upper and lower half planes so we perform. the contour integration as before. Since we have assumed narrow isolated resonances, we find

$$\langle\sigma_{ab}\sigma_{cd}\rangle \approx \frac{\pi/4}{\Delta E}\left(\frac{4\pi g_a}{k_a^2}\right)\left(\frac{4\pi g_c}{k_c^2}\right)\sum_\mu \frac{\Gamma_{a\mu}\Gamma_{b\mu}\Gamma_{c\mu}\Gamma_{d\mu}}{\Gamma_\mu^3} \quad (18)$$

As before, we replace the sum over resonances with an ensemble average

$$\sum_\mu \frac{\Gamma_{a\mu}\Gamma_{b\mu}\Gamma_{c\mu}\Gamma_{d\mu}}{\Gamma_\mu^3} \approx \frac{\Delta E}{D}\left\langle\left\langle\frac{\Gamma_a\Gamma_b\Gamma_c\Gamma_d}{\Gamma^3}\right\rangle\right\rangle \quad (19)$$

Similar to before, we use

$$\frac{1}{\Gamma^3} = \int_0^\infty dt_1\int_0^\infty dt_2\int_0^\infty dt_3 e^{-\Gamma(t_1+t_2+t_3)} \quad (20)$$

and assume Porter-Thomas distributions with degree of freedom ν. We arrive at

$$\left\langle\!\!\left\langle\frac{\Gamma_a\Gamma_b\Gamma_c\Gamma_d}{\Gamma^3}\right\rangle\!\!\right\rangle = \overline{\Gamma}_a\overline{\Gamma}_b\overline{\Gamma}_c\overline{\Gamma}_d\left(1+\frac{2\delta_{ab}}{\nu_a}\right)\left(1+\frac{2\delta_{cd}}{\nu_c}\right) \times \int_0^\infty dt_1\int_0^\infty dt_2\int_0^\infty dt_3\prod_f \times \left(1+\frac{2t\overline{\Gamma}_f}{\nu_f}\right)^{-\Delta} \quad (21)$$

with $t = t_1 + t_2 + t_3$ and $\Delta = \delta_{af} + \delta_{bf} + \delta_{cf} + \delta_{df} + \nu_f/2$. We can simplify this result further first rewriting the t's in cylindrical coordinates and integrating out the angular dependence. In analogy with the WFC factor above, we define $\mathcal{W}_{abcd}$ in terms of the integration result:

$$\mathcal{W}_{abcd} = \frac{\overline{\Gamma}^3}{\overline{\Gamma}_a\overline{\Gamma}_b\overline{\Gamma}_c\overline{\Gamma}_d}\left\langle\left\langle\frac{\Gamma_a\Gamma_b\Gamma_c\Gamma_d}{\Gamma^3}\right\rangle\right\rangle = \left(1+\frac{2\delta_{ab}}{\nu_a}\right)\left(1+\frac{2\delta_{cd}}{\nu_c}\right)\int_0^\infty dx\frac{x^2}{2}\prod_f \times \left(1+\frac{2\overline{\Gamma}_f}{\nu_f\overline{\Gamma}}x\right)^{-\Delta} \quad (22)$$

This is an intriguing result as this $\mathcal{W}_{abcd}$ factor looks very much like the WFC factor used in the average cross section.

We can now write down the covariance between the cross sections very compactly. First

$$\langle\sigma_{ab}\sigma_{cd}\rangle = \frac{\pi D}{\Gamma}\frac{\mathcal{W}_{abcd}}{\mathcal{W}_{ab}\mathcal{W}_{cd}}\langle\sigma_{ab}\rangle\langle\sigma_{cd}\rangle = \frac{2\pi^2}{T}\frac{\mathcal{W}_{abcd}}{\mathcal{W}_{ab}\mathcal{W}_{cd}}\langle\sigma_{ab}\rangle\langle\sigma_{cd}\rangle \quad (23)$$

using $T_c = 2\pi\overline{\Gamma_c}/D$. Therefore, in this model the cross section covariance is given by

$$\mathrm{cov}(\sigma_{ab},\sigma_{cd}) = \langle\sigma_{ab}\rangle\langle\sigma_{cd}\rangle\left(\frac{2\pi^2}{T}\frac{\mathcal{W}_{abcd}}{\mathcal{W}_{ab}\mathcal{W}_{cd}} - 1\right). \quad (24)$$

We note that there is nothing in this expression or the expressions for $\mathcal{W}_{ab}$ or $\mathcal{W}_{abcd}$ that keep the covariance positive. This indicates that this model has a limited range of applicability that we will investigate in the next section.

4. The behavior of fluctuation factors

To understand the behavior of both the WFC factor $\mathcal{W}_{ab}$ and the WFC-like factor $\mathcal{W}_{abcd}$, we consider a system with a four neutron channels with identical widths, a typical number active in the URR of a typical nucleus, and one gamma channel with $T_\gamma = 10^{-4}$. We use the Kawano-Talou systematics for ν [7]. Figure 1 shows the factors as a function of neutron transmission coefficient.

Raw plots of the factors are not very instructive. Therefore, consider the standard deviation of the cross section: $\Delta\sigma_{ab} = \sqrt{\mathrm{cov}(\sigma_{ab},\sigma_{ab})}$. In Fig. 2 we plot $\Delta\sigma_{ab}/\langle\sigma_{ab}\rangle$ as a function of T_n in this example. Clearly the fluctuations in the cross sections are very large for small T_c and diminish rapidly as T_c increases. We also note that the gamma channel, with its small T_γ exhibits relative fluctuations an order of magnitude larger than the neutron channels.

We now investigate how the model behaves as the number of channels increases at fixed $T_n = 0.2$. We know from Eq. (24) that the covariance has the possibility of going negative. In Fig. 3 we plot the relative variance of the elastic cross section $(\Delta\sigma_{aa}/\langle\sigma_{aa}\rangle)^2 = \mathrm{cov}(\sigma_{aa},\sigma_{aa})/\langle\sigma_{aa}\rangle^2$ for elastic scattering as a function of the number of open neutron channels. We see as the number of channels reaches becomes large the variance drops below zero, indicating a breakdown of the model. This in a way is no surprise as we are deeply in the strong coupling limit.

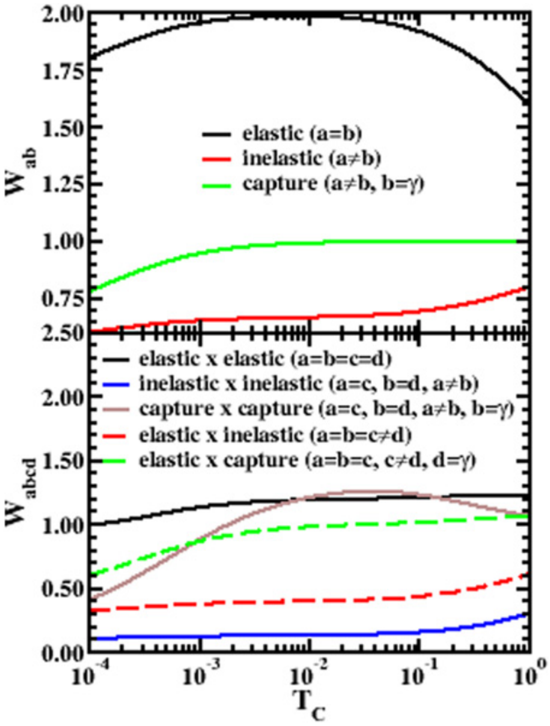

Figure 1. A comparison of the WFC and WFC-like factors $\mathcal{W}_{ab}$ and $\mathcal{W}_{abcd}$ as a function of neutron transmission coefficient. As described in the text, this calculation has four neutron channels and one gamma channel and $T_\gamma = 10^{-4}$. Here all channels are assumed to be neutron channels unless otherwise stated (e.g., channel "b" for capture).

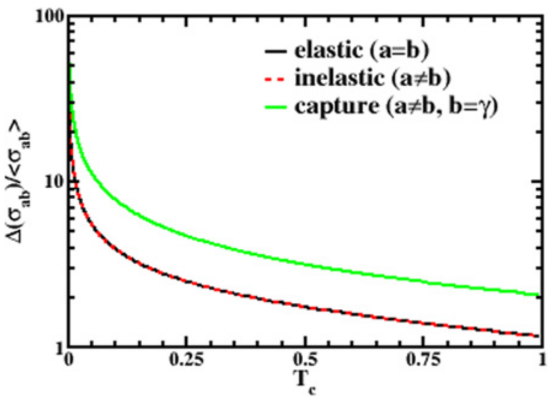

Figure 2. The relative variance of the reaction cross sections as a function of neutron transmission coefficient. Here all channels are assumed to be neutron channels unless otherwise stated (e.g. channel "b" for capture).

5. Outlook

We have outlined the beginnings of a scheme to compute the compound nuclear cross section probability distribution function in the URR region. Our approach offers the possibility of defining the limits of applicability

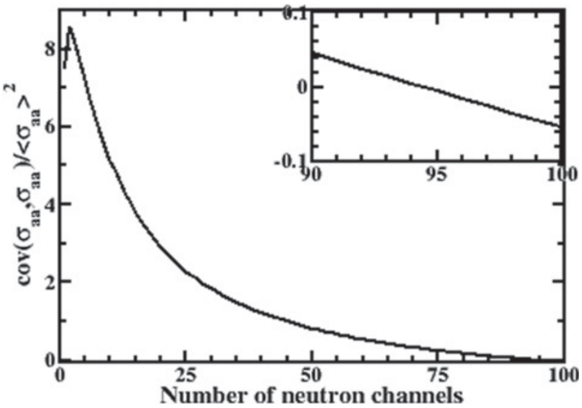

Figure 3. Plot of the relative variance of the elastic scattering cross section as a function of the number of neutron channels. In the inset, we show the region at high channel number, showing the breakdown of the approach in the strong coupling limit.

of Hauser-Feshbach theory and suggests a way to calculate PURR tables directly from systematics for nuclei whose RRR is unknown, provided one makes appropriate assumptions about the shape of the cross section probability distribution. This scheme should also be applicable to unstable nuclei where no resonances can be measured in practical experiments. To complete this program, we must fully characterize the region of applicability and test it against other probability table generations tools.

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