Validation of R-Matrix Limited Based Reconstruction Capability for RXSP Code

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1. Introduction

RXSP (Reactor Cross Sections Processing code) is a code being developed by REAL(Reactor Engineering Analysis Laboratory) group in Tsinghua University starting from the year 2008, which is intended to convert the evaluated nuclear data into continuous energy nuclear data libraries in ACE format [1].

Reconstructing point-wise cross sections from resonance parameters in ENDF-6 files is the most essential function in RXSP code. At the very beginning of this development, it is capable of resonance reconstruction based on all R-Matrix approximated formalism, i.e. Single-Level Breit-Wigner (SLBW), Multi-Level Breit-Wigner (MLBW), Adler-Adler, as well as the most popular Reich-Moore formula, which consist of all available resolved resonance formalisms in the first version of ENDF/B-VII [2]. However, a more accurate R-Matrix Limited (also named Reich-Moore Limited) formalism is firstly applied to represent resonance characteristics for neutron-induced cross section in RRR (Resolved Resonance Range) of ^{35}Cl isotope in the latest ENDF/B-VII.1 data base. The reason for Cross Section Evaluation Working Group in Oak Ridge National Laboratory to highly recommend this lies in these aspects in accordance with ENDF-6 user manual [3] in the following.

The R-Matrix Limited representation is a more general multilevel and multichannel formulation; In addition to the normal elastic scattering and Coulomb reactions; Furthermore, it allows resonance angular distribution to be calculated; finally, it is also capable of computing derivatives of cross sections with respect to resonance parameters, which can be easily utilized in resonance parameter evaluation work.

2. Methods and Results

In order to extend the capability for RXSP code to deal with R-Matrix Limited based point-wise resonance cross sections reconstruction, the original format of parameters in RRR need to be known as well as the detailed computation procedure to get cross sections based on these parameters. Though the user manual of ENDF-6 format makes a list to illustrate the format of R-Matrix Limited based parameters, which will be overlooked in this section. However, the cross section generating from these parameters are described in detailed four steps in the following.

2.1 Cross Section Calculation

1) Energy-independent constants

In this step, the atomic mass of incoming neutron and target nuclide need to be defined, as well as a very important constant, i.e. statistical factor g_J being determined as follows:

$$g_{Ja} = \frac{2J+1}{(2i_a+1)(2i_b+1)} \quad (1)$$

J is the total spin of the compound nucleus system composed of incoming neutron and target nuclide, i_a and i_b standing for the spin of them respectively. The subscribe α is representative of reaction channel made up by neutron and the target nuclide.

2) Energy-dependent variables

ρ is the first energy-dependent factor need to be defined as neutron wave number k and scattering radius AP, which can be directly retrieved from File 2 in ENDF file.

$$\rho = k \times AP \quad (2)$$

$$k = \sqrt{\frac{2m_a m_b^2}{(m_a+m_b)^2}E} \quad (3)$$

Based on them, the hard-sphere penetration factor P, level shift factor S, and potential scattering phase shift factor ϕ can be given like this:

$$P_l = \begin{cases} \rho & l=0 \\ \dfrac{\rho^2 P_{l-1}}{(l-S_{l-1})^2 + P_{l-1}^2} & l \neq 0 \end{cases} \quad (4)$$

$$S_l = \begin{cases} 0 & l=0 \\ \dfrac{\rho^2 (l-S_{l-1}) P_{l-1}}{(l-S_{l-1})^2 + P_{l-1}^2} & l \neq 0 \end{cases} \quad (5)$$

$$\phi_l = \begin{cases} \rho & l=0 \\ \phi_{l-1} - \tan^{-1}\left(\dfrac{P_{l-1}}{l-S_{l-1}}\right) & l \neq 0 \end{cases} \quad (6)$$

These above formalisms are only for non-Coulomb reaction, the Coulomb reaction related expression can be referred in SAMMY manual [4].

3) Construct R-Matrix and other Matrixes

In order to generate point-wise cross section in RRR, R-Matrixes need to be constructed in terms of resonance parameters extracted from File 2 of ENDF file as follows:

$$R_{cc'} = \left[\sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\gamma - E - \frac{i}{2}\Gamma_{\lambda\gamma}} + R_c^{bkg}\delta_{cc'} \right] \delta_{JJ'} \quad (7)$$

$$\gamma_{\lambda c} = \sqrt{\frac{\Gamma_{\lambda c}}{2P_c(E)}} \quad (8)$$

For the reason for computational stability in calculating cross sections, X matrix is given in the following:

$$X = P^{\frac{1}{2}} L^{-1}\left(L^{-1} - R\right)^{-1} R P^{\frac{1}{2}} \quad (9)$$

$$L = (S - B) + iP \quad (10)$$

Where P and S are penetration factor and shift factor respectively, where B is the arbitrary boundary constant at the channel radius AP. Thus, the various cross sections are written in terms of X .

4) Generate point-wise cross sections

The calculated cross sections (elastic scattering, inelastic scattering, absorption, capture) are expressed in terms of X through equation (11) to (14) in the following, by summing over spin groups (over total spin J), and then summing over all channels in accordance with those particles pairs and spin groups.

$$\sigma_{n,elastic} = \frac{4\pi}{k_n^2} \sum_J g_{Jn} \sum_c \left\{ \begin{array}{l} \sin^2\phi_c \left(1 - 2X_{cc}^{i}\right) \\ - X_{cc}^{r} \sin(2\phi_c) \\ + \sum_{c'} {X_{cc'}^{i}}^2 + {X_{cc'}^{r}}^2 \end{array} \right\} \quad (11)$$

$$\sigma_{n,inelastic} = \frac{4\pi}{k_n^2} \sum_J g_{Jn} \sum_c \sum_{c'} {X_{cc'}^{i}}^2 + {X_{cc'}^{r}}^2 \quad (12)$$

$$\sigma_{n,absorption} = \frac{4\pi}{k_n^2} \sum_J g_{Jn} \sum_c \left\{ X_{cc}^{i} - \sum_{c'} {X_{cc'}^{i}}^2 + {X_{cc'}^{r}}^2 \right\} \quad (13)$$

$$\sigma_{n,capture} = \frac{4\pi}{k_n^2} \sum_J g_{Jn} \sum_{inc\ c} \left\{ X_{cc}^{i} - \sum_{all\ c'} {X_{cc'}^{i}}^2 + {X_{cc'}^{r}}^2 \right\} \quad (14)$$

Fission cross section can be obtained by subtracting capture cross section from total absorption cross section. And total cross section can be computed by summation of elastic scattering, inelastic scattering, and absorption cross section.

2.2 Code Development

The resonance reconstruction capability in RXSP code applies inverted stack method [5] to obtain energy grid of point-wise cross sections. Only these three types of cross sections (elastic scattering, capture and fission) can be directly computed by resonance formula from the resonance parameters. Consequently, certain values for the relative error of these three types of cross section are treated as convergence criteria. However, the new R-Matrix Limited formula expands the capacity of computing other types of cross sections including some charged particle emission reaction. Thus, RXSP code adds relative errors of other competitive cross sections into the convergence criteria, but the detailed reaction types depends on the specific resonance parameters in the practical nuclear data processing applications.

2.3 Numerical Results

^{35}Cl is the only one isotope which is represented by R-Matrix Limited format in ENDF/B-VII.1 data library. However, this isotope has been used in the validation of R-Matrix Limited based reconstruction capability in RXSP code [6]. Here the paper validates it by using ^{56}Fe and ^{16}O, which are very important in reactor physical simulations, the resonance parameters in ENDF-formatted file being retrieved from CIELO project [7]. To validate the accuracy of processing R-Matrix Limited formulae, the SAMMY code is used as the reference in this paper. Therefore, elastic scattering, absorption, along with inelastic scattering cross sections are illustrated through Fig. 1 to Fig.3 for ^{56}Fe and Fig. 4 to Fig. 6 for ^{16}O.

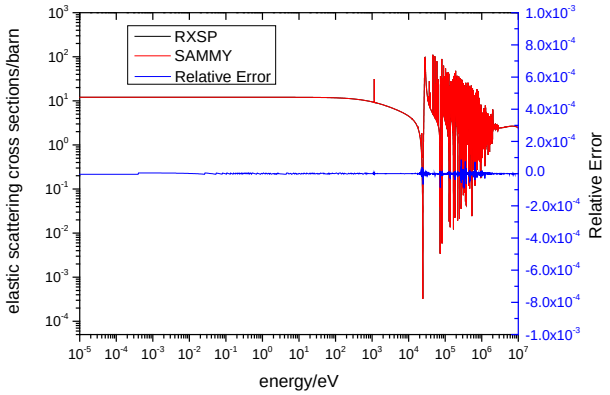

Fig. 1. Elastic scattering cross sections for ^{56}Fe

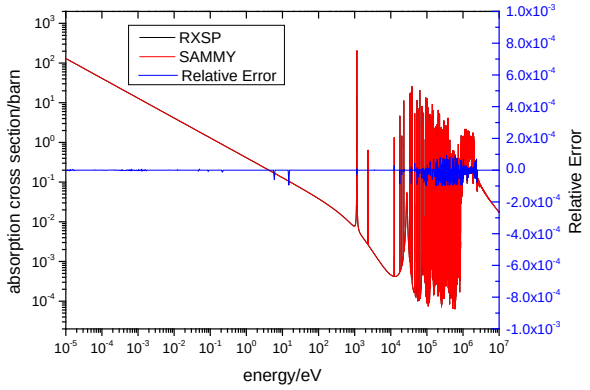

Fig. 2. Absorption cross sections for ^{56}Fe

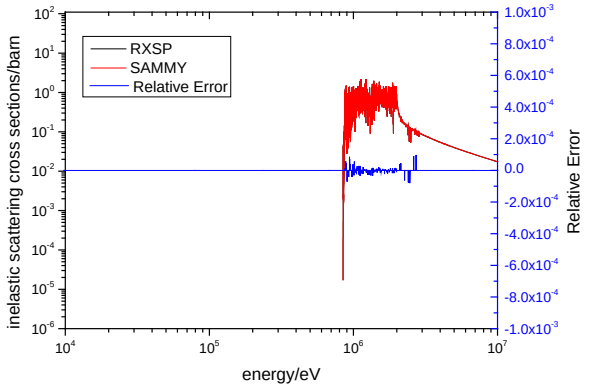

Fig. 3. Inelastic scattering cross sections for ^{56}Fe

As seen for Fig.1 to Fig.3, elastic scattering, absorption and inelastic scattering cross sections are calculated by RXSP and SAMMY code in the resolved resonance energy range of 10^{-5}eV-2MeV for the isotope of ^{56}Fe. They agree with each other very well for the results of both codes, their maximal relative error being less than 10^{-4}.

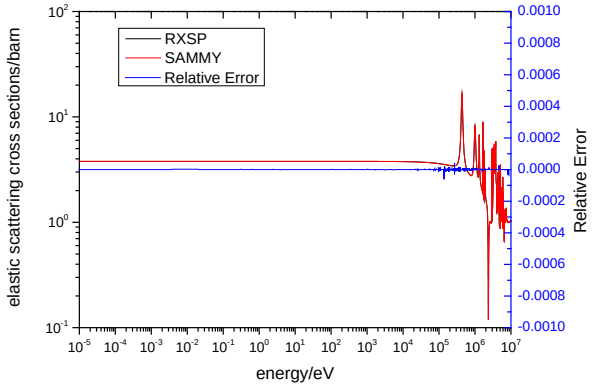

Fig. 4. Elastic scattering cross sections for ^{16}O

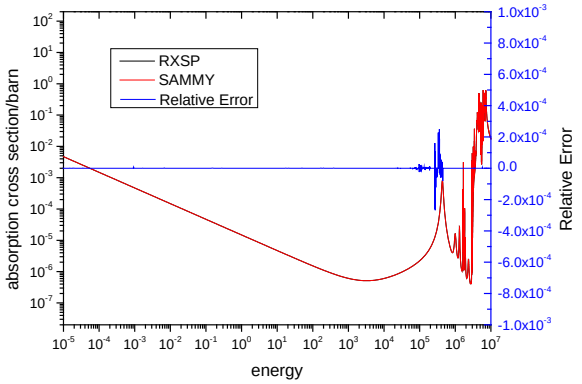

Fig. 5. Absorption cross sections for ^{16}O

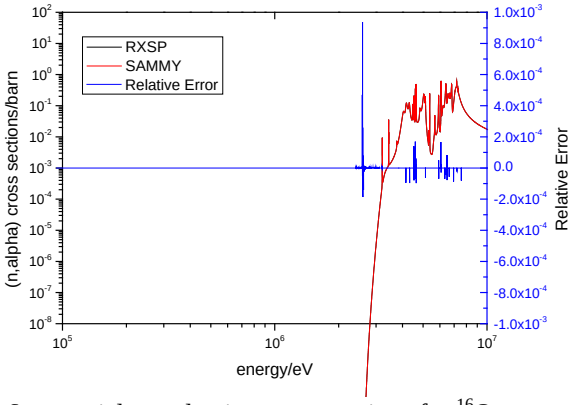

Fig. 6. α-particle production cross sections for ^{16}O

It is shown that from Fig. 4 to Fig.6 that the point-wise cross sections including elastic scattering, absorption and inelastic scattering cross sections are computed for the resolved resonance energy range of 10^{-5}eV-6.12MeV for ^{16}O isotope, by using RXSP code as well as SAMMY. They show the same trend with that of ^{56}Fe, where their difference is so small that absolute value of relative error being within the range of 10^{-4}, except that in certain location, the relative error is still less than 10^{-3}. It is noted that α-particle production cross sections of ^{16}O can be directly generated based on R-Matrix Limited resonance parameters, while it is impossible for any other resonance parameters, i.e. SLBW,MLBW, Adler-Adler and even Reich-Moore.

3. Conclusions

R-Matrix Limited formalism and associated resonance parameters are analyzed and implemented in RXSP code to extend its resonance reconstruction capability, which is validated by comparing reconstructed point-wise cross sections generated from RXSP and SAMMY code for ^{56}Fe and ^{16}O.

4. Acknowledgements

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