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EXTENSION OF THE APPLICATION OF THE GENERALIZED POLE REPRESENTATION TO THE TREATMENT OF RESONANCE CROSS SECTIONS*

by

C. Jammes and R. N. Hwang
Argonne National Laboratory
Reactor Analysis Division
9700 S. Cass Avenue
Argonne, IL 60439

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DISCLAIMER

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Christian JAMMES* and Richard N. HWANG
Reactor Analysis Division
Argonne National Laboratory
Argonne (United States)
jammes@ra.anl.gov; b10561@ra.anl.gov

(*) Permanent address: CEA , Cadarache (France)
cjammes@cea.fr

Abstract

One reliable and convenient way of processing the cross sections in the resolved energy region is by use of the generalized pole representation, whereby the Doppler-broadening calculation can be carried out rigorously using the analytical approach. So far, its applications have been limited to cases with resonance parameters specified by the Reich-Moore formalism. Although such an approach, in principle, can be extended to all three remaining representations of resolved resonance parameters specified by the ENDF data format, there is no computational tool for handling such a task at present. Given that Breit-Wigner formalisms are probably the most widely used by any evaluated nuclear data library to represent cross sections, a special effort has to be made to convert the single level and multilevel Breit-Wigner resonance parameters to pole parameters. A FORTRAN computer code BW2PR has been developed for this purpose. Extensive calculations have been performed to demonstrate that the proposed method ensures the conservation of the information contained originally in Breit-Wigner resonance parameters. This will make it possible to apply the exact Doppler–broadening method to a larger collection of nuclides.

1 Introduction

This paper describes a part of our recent efforts to up-grade our cross section processing capabilities in the VIM Monte Carlo code (Prael, 1975) for reactor physics and criticality safety-related applications. It is quite apparent that the accuracy requirement for the computed point-wise cross sections in the base libraries must also be enhanced accordingly if the Monte Carlo approach is to be used as the ultimate computational standard. Our knowledge of nuclear data has been significantly improved in recent years, particularly in the resolved energy range where a dramatic extension of resonance data has been made for many nuclides of practical interest. Treatment of the resolved resonances in order to accurately account for the self-shielding effect and the related Doppler effect always constitutes one of the major tasks in processing of cross sections. The key issue is to compute the cross sections at any given energy and temperature that will accurately reflect the rigor of the state-of-the-art nuclear data. In our view, the surest way to achieve this objective is via the analytical approach.

As described in earlier work (Hwang, 1987), the Doppler-broadening of cross sections in the resolved resonance region can be rigorously treated using the generalized pole representation in the momentum domain. It has been shown that conversion of Reich-Moore resonance parameters (Reich, 1958) to pole parameters allows an exact Doppler-broadening without losing the rigor of the Reich-Moore formalism in representing the energy behavior of cross sections. As with the single Breit-Wigner, the multilevel Breit-Wigner and the Adler-Adler formalisms (Rose, 1997), the

generalized pole representation allows expression of cross sections as a linear combination of the traditional Voigt profiles (Solbrig, 1961). Consequently, not only is the incompatibility between the Reich-Moore representation and the existing codes based on the resonance integrals concepts circumvented, but also the high degree of accuracy, unlikely attainable via the commonly used numerical methods, can be achieved analytically. The generalized pole representation also makes it possible to take into account the second order Doppler effect (Hwang, 1998a) due to the weakly energy-dependent hard sphere shift factor. The use of that recently developed formalism is specially recommended if it is applied to systems like thermal reactors in which the treatment of the low energy limit requires as much accuracy as possible.

The case in point here is whether the same approach is also extendable to alternative cross section formalisms other than that of the Reich-Moore also widely used in the existing data files. Three other formalisms also in use are the single level Breit-Wigner (SLBW), multilevel Breit-Wigner (MLBW), and Adler-Adler formalisms. Of the three, the Adler-Adler formalism is seldom used because its applicability is limited to the s-wave resonances of few fissile isotopes in the low energy region. In contrast, approximately 90% of all resonant isotopes in most nuclear data files are specified by the SLBW or MLBW parameters. However, for the most important nuclides, the MLBW formalism is apparently preferred to the SLBW formalism that represents the limiting case when the resonances are well isolated. In the JEF 2.2 library, SLBW resonance parameters are almost systematically replaced by MLBW ones. The MLBW formalism is an enhancement in the sense that it accounts for the interference effect between each resonance for the scattering and total cross sections. That effect can be fully described by an additional interference cross section. The fission and radiative capture cross sections are identically represented in the two Breit-Wigner formalisms. Consequently, it will be seen that the conversion into pole parameters is formally similar for those two formalisms except for the treatment of the so-mentioned interference cross section.

The purpose of this paper is to show how the exact Doppler-broadening method can also be applied to resonances specified by the three formalisms mentioned above. Like the case of Reich-Moore, this can also be accomplished via conversion of the set of parameters in question into the pole parameters, so that the subsequent Doppler-broadening procedure can follow the same route. For the Adler-Adler formalism, the computation of pole parameters is quite trivial: it only requires the partial fraction of its cross section expressions in the energy domain at zero temperature. Therefore, it will not be included in the following discussions. Instead, the discussions to follow will be focused on the case of SLBW and MLBW. Two pertinent features of these two formalisms are particularly note-worthy. First, the energy dependence of the cross sections is explicitly specified. Like the Reich-Moore formalism, it is manifest not only through the traditional Lorentzian shape but also through the penetration, level shift and hard-sphere scattering factors. Detailed accounting for all these factors is required when the respective parameters are converted into the pole parameters in the k-plane. Secondly, the resonance cross sections so specified are usually accompanied by additional 'smooth' cross sections to remedy the inadequacy of the approximations. One complication is that these 'smooth' cross sections must also be Doppler-broadened when the cross sections at a given temperature are subsequently computed. These issues will be addressed.

2 Review of pole representation

The generalized pole representations are alternatives to the R-matrix theory (Lynn, 1968), the well-known formal nuclear reaction theory that is widely used to describe cross sections in the resolved resonance region. This recently developed formalism originates from the rationale suggested by de

Saussure and Perez (Saussure, 1969) for s-wave resonances. The rationale of this approach is based on the property that the collision matrix must be single-valued and meromorphic in the momentum domain ($\sqrt{E}$ -domain). This property makes it possible to rationalize the collision matrix.

For the radiative capture or fission channel ($x = \gamma, f$), the cross section can be expressed in terms of poles $p^*_{\ell,J,j}$ and residues $R^{(x)}_{\ell,J,j}$ at zero temperature:

$$\sigma_x = \frac{1}{E}\sum_{\ell,J}\sum_{j=1}^{M} \mathrm{Re}\left\{\frac{-iR^{(x)}_{\ell,J,j}}{p^*_{\ell,J,j} - u}\right\}, \tag{1}$$

where $u = \sqrt{E}$ and M is the number of poles for a given pair of ℓ- and J-states (* refers to the complex conjugate). In that representation, the poles play a role similar to energy levels and half widths. The residues characterize a specific channel x and the poles are simple and non-real because of the discrete, real and non-degenerate nature of the resonance energy levels.

For the scattering or total cross section, the factor $\exp(-i2\phi_\ell)$ has to be taken into account. That energy-dependent factor, which is responsible for a second order Doppler effect, signifies the interference between the potential scattering cross section and the resonance component. In Refs. (Hwang, 1998a) and (Hwang, 1998b), it is shown how the rationalization of that exponential function for all ℓ-states can be performed. In the present work, it is sufficient to consider only the following rational terms that appear in the pole expansion of the scattering or total cross section ($x = s, t$ respectively):

$$L(u) = \frac{-ie^{-i2\phi_\ell}\, R^{(x)}_{\ell,J,j}}{p^*_{\ell,J,j} - u} \tag{2}$$

where the poles $p^*_{\ell,J,j}$ are common to any resonant cross sections. Equation (8) can be viewed as a generalized form of Lorentzian in the momentum domain. It retains the general features of the traditional Doppler-broadened line shape function upon broadening except for the minor shift resulting from the presence of the exponential factor. Thus, the most two important characteristics of the pole representation is that all parameters are genuine energy-independent and the Lorentzian form of the rational terms allows an exact Doppler-broadening (Hwang, 1987). Conceptually, it provides the vehicle to preserve the widely used resonance integral concept independent of how the resonance cross sections are specified.

3 Derivation of pole parameters from Breit-Wigner formalisms

The poles $p^*_{\ell,J,j}$ and residues $R^{(x)}_{\ell,J,j}$ defined in Eqs. (1) and (2) are called resonance pole parameters. In the case of Breit-Wigner formalisms, they can be derived from Eqs. (A.1), (A.2) and (A.3) given in appendix A.

3.1 Poles

According to the expression of any cross section in the Breit-Wigner representations, it can be seen that all resonant poles are solutions of a polynomial equation of order $2(\ell+1)$:

$$q_\ell(u)A_\lambda(u) = \sum_{m=0}^{2(\ell+1)} a_{\lambda,m}^{(\ell)} u^m = 0, \tag{3}$$

where the ℓ–dependent function q_ℓ and coefficients $a_{\lambda,m}$ are defined in Ref. (Hwang, 1987). Those coefficients have been calculated for different ℓ-values up to 2 (*d*-wave). That algebraic equation, which can be solved by an usual root solver for polynomials with complex coefficients, reveals that a set of $2(\ell+1)$ poles $p^*_{\ell,J,\lambda,j}$ is associated with each energy level E_λ. Then, the polynomial of Eq. (3) can be thus rewritten in a factorized form:

$$q_\ell(u)A_\lambda(u) = -\rho_0^{2\ell} \prod_{j=1}^{2(\ell+1)} \left(p^*_{\ell,J,\lambda,j} - u\right), \tag{4}$$

where $\rho_0 = \left(0.002196771 \times \frac{A}{A+1}\right) \times a$, a and A being the channel radius and the isotopic mass, respectively. It can be shown that always two out of the $2(\ell+1)$ poles are almost symmetric with respect to the imaginary axis, while the 2ℓ other poles are close to the roots of the equation $q_\ell(u) = 0$ (q_ℓ being a polynomial of order 2ℓ), not to sensitive to the Breit-Wigner resonance parameters.

3.2 Residues corresponding to the single level case

For the SLBW representation, the line-shape functions exhibited in Eqs. (1) and (2) lead to the following pole expansions of the radiative capture or fission cross sections σ_x ($x = \gamma, f$) and the total cross section σ_t in the momentum domain:

$$\sigma_x = \frac{1}{E} \sum_{\ell,J} \sum_{\lambda=1}^{N} \sum_{j=1}^{2(\ell+1)} \mathrm{Re}\left\{ \frac{-iR^{(x)}_{\ell,J,\lambda,j}}{p^*_{\ell,J,\lambda,j} - u} \right\} \text{ and } \sigma_t = \frac{1}{E} \sum_{\ell,J} \sum_{\lambda=1}^{N} \sum_{j=1}^{2(\ell+1)} \mathrm{Re}\left\{ \frac{-ie^{-i2\phi_\ell} R^{(t)}_{\ell,J,\lambda,j}}{p^*_{\ell,J,\lambda,j} - u} \right\}. \tag{5}$$

The scattering cross section is then directly deduced from Eq. (6).

All residues relative to a channel *x* are directly obtained from the expressions of the cross section for the same channel with the use of Eq. (4) and the well-known relation

$$R^{(x)}_{\ell,J,\lambda,j} = \lim_{u \to p^*_{\ell,J,\lambda,j}} \left(p^*_{\ell,J,\lambda,j} - u\right) \times f^{(x)}_{\ell,J,\lambda}(u), \tag{6}$$

where $f^{(x)}_{\ell,J,\lambda}$ is a meromorphic function defined in appendix A for the different channels in question. Thus, the residues relative to the total cross section are equal to

$$R^{(t)}_{\ell,J,\lambda,j} = \frac{2\pi}{k_0^2} g_J \times \frac{q_\ell(p^*_{\ell,J,\lambda,j}) \times \Gamma^{(\ell)}_{\lambda n}(p^*_{\ell,J,\lambda,j})}{-\rho_0^{2\ell} \prod_{\substack{k=1 \\ k\neq j}}^{2(\ell+1)} \left(p^*_{\ell,J,\lambda,j} - p^*_{\ell,J,\lambda,k}\right)}, \tag{7}$$

and the ones relative to the radiative capture or fission cross sections ($x = \gamma, f$) are given by

$$R^{(x)}_{\ell,J,\lambda,j} = R^{(t)}_{\ell,J,\lambda,j} \times \frac{\Gamma_{\lambda x}}{\Gamma^{(\ell)}_{\lambda n}(p^*_{\ell,J,\lambda,j}) + \Gamma_{\lambda\gamma} + \Gamma_{\lambda f}}. \tag{8}$$

3.3 Residues corresponding to the multilevel case

In the case of the MLBW formalism, the radiative capture and fission cross sections are identical in the two Breit-Wigner representations, while an interference cross section σ_{int} must be added to the total cross section of the SLBW representation:

$$\sigma_t^{MLBW} = \sigma_t^{SLBW} + \sigma_{int}, \tag{9}$$

where the interference cross section is recalled to be defined as

$$\sigma_{int} = \sum_{\ell,J} \frac{\pi}{k_0^2 E} g_J \,\mathrm{Re}\left\{ \sum_{\lambda=1}^{N} \sum_{\substack{\mu=1 \\ \mu\neq\lambda}}^{N} \frac{\Gamma^{(\ell)}_{\lambda n}(u)\, \Gamma^{(\ell)}_{\mu n}(u)}{A_\lambda(u)\, A^*_\mu(u)} \right\} \tag{10}$$

Then, the scattering cross section can be directly computed as the difference between the total and absorption cross sections. That interference cross section exhibits cross terms that expresses the interference between the energy levels of a given $(\ell, J)-$state. Since there is no exponential factor $\exp(-i2\phi_\ell)$ in its expression, the interference cross section can be obviously expanded in terms of pole parameters.

One first considers the rationalization of the following generic cross term that appears in the expression of the interference cross section:

$$\begin{aligned} \frac{\pi}{k_0^2} g_J \,\mathrm{Re}\left\{ \frac{\Gamma^{(\ell)}_{\lambda n}(u)\, \Gamma^{(\ell)}_{\mu n}(u)}{A_\lambda(u)\, A^*_\mu(u)} \right\} &= \frac{\pi}{k_0^2} g_J \,\mathrm{Re}\left\{ \frac{\Gamma^{(\ell)}_{\lambda n}(u)\, \Gamma^{(\ell)}_{\mu n}(u)}{A^*_\lambda(u)\, A_\mu(u)} \right\} \\ &= \mathrm{Re}\left\{ \sum_j \frac{-i r^{\mu}_{\ell,J,\lambda,j}}{p^*_{\ell,J,\lambda,j} - u} \right\} + \mathrm{Re}\left\{ \sum_j \frac{-i r^{\lambda}_{\ell,J,\mu,j}}{p^*_{\ell,J,\mu,j} - u} \right\}. \end{aligned} \tag{11}$$

Each residue $r^{\mu}_{\ell,J,\lambda,j}$ can be obtained in the same way described in Eq. (6) and with the use of:

$$\begin{aligned} r^{\mu}_{\ell,J,\lambda,j} &= \lim_{u \to p^*_{\ell,J,\lambda,j}} \left(p^*_{\ell,J,\lambda,j} - u\right) \times f^{\mu}_{\ell,J,\lambda}(u) \\ &= R^{(t)}_{\ell,J,\lambda,j} \times \frac{i}{2} \left[\frac{\Gamma^{(\ell)}_{\mu n}(p^*_{\ell,J,\lambda,j})}{A^r_\mu(p^*_{\ell,J,\lambda,j}) + i A^i_\mu(p^*_{\ell,J,\lambda,j})} \right], \end{aligned} \tag{12}$$

where the meromorphic function $f^{\mu}_{\ell,J,\lambda}$, the two components A^{r}_{λ} and A^{i}_{λ} of the level matrix are given in appendix A. From Eq. (9), it is directly shown that each residue $r^{\mu}_{\ell,J,\lambda,j}$, relative to a generic cross term, appears exactly two times in the full pole expansion of the interference cross section. Thus, the residue $R^{(int)}_{\ell,J,\lambda,j}$ relative to that interference cross section is given by:

$$R^{(int)}_{\ell,J,\lambda,j} = 2\sum_{\substack{\mu=1 \\ \mu\neq\lambda}}^{N} r^{\mu}_{\ell,J,\lambda,j} = R^{(t)}_{\ell,J,\lambda,j} \times i\left[\sum_{\substack{\mu=1 \\ \mu\neq\lambda}}^{N} \frac{\Gamma^{(\ell)}_{\mu n}(p^{*}_{\ell,J,\lambda,j})}{A^{r}_{\mu}(p^{*}_{\ell,J,\lambda,j}) + iA^{i}_{\mu}(p^{*}_{\ell,J,\lambda,j})}\right]. \tag{13}$$

4 Results and discussions

According to the previous section, the proposed method based on the pole representation, which makes possible an exact Doppler-broadening, clearly allows preserving the information contained in a given set of Breit-Wigner resonance parameters since the deduced poles and residues directly depend on them.

4.1 The developed Code BW2PR

A code named BW2PR has been developed to implement the conversion of Breit-Wigner resonance parameters to pole parameters. The code accomplishes several tasks that are described as follows.

i) Breit-Wigner resonance parameters for a given isotope are extracted from an ENDF-format based file.

ii) Smooth cross section components are re-processed in order to force the tabulated data to follow a linear-linear interpolation law consistent with a piecewise Doppler-broadening scheme. It will be recalled that smooth cross section components provide the remedy for the lack of rigor in Breit-Wigner formalisms.

iii) Resonant poles and residues are computed in extended precision using Eqs. (3), (7), (8) and (13). All those parameters are displayed in an output file.

iv) The code generates a binary file storing the computed pole parameters and other relevant data to be passed to the code POLEBRD (Hwang, 1998a) that performs an analytical and exact Doppler-broadening of any cross section described by the pole representation.

v) The code produces an output of pointwise cross sections at zero temperature obtained using the generalized pole representation, and relative errors to compare the results with the directly computed Breit-Wigner cross sections.

4.2 Comparison tests for few isotopes of interest

Because the cross section computation using the generalized pole representation involves a large number of parameters that cause inevitable numerical errors, some comparisons of results with the directly computed Breit-Wigner cross sections are required. Thus, relative errors of the resulting cross sections are examined for the isotopes listed in Table 1. There are two fission products (^{109}Ag, ^{99}Tc), one minor actinide (^{241}Am) and one structural isotope (^{23}Na). The four selected nuclides allow testing the BW2PR code for very different cases covering all situations of practical interest.

Table 1. Features of Tested Isotopes

Isotope	Library	Formalism	Highest ℓ-state	Number of Poles
^{241}Am	ENDF/B-VI	SLBW	0	390
^{109}Ag	ENDF/B-VI	MLBW	0	166
^{99}Tc	ENDF/B-VI	SLBW	1	186
^{23}Na	JEF-2.2	MLBW	2	74

Before examining the results of the comparison between the proposed method and the Breit-Wigner one, two important points are worth noting. The first is that all cross sections are computed for several thousands of energy mesh points throughout the resolved energy region. The second is that the results are expected to be totally self-consistent because the input data and all necessary constants are the same for whatever formalism.

Table 2. Comparison Between the Proposed Method and the SLBW Method for ^{241}Am

^{241}Am	Relative Errors (%)	
	Average	Maximum
σ_t	< 1.00E-9	< 1.00E-9 at 7.95E+01 eV
σ_n	2.15E-06	5.84E-06 at 3.62E+01 eV
σ_a	< 1.00E-9	< 1.00E-9 at 7.95E+01 eV
σ_f	< 1.00E-9	< 1.00E-9 at 7.95E+01 eV

Table 3. Comparison Between the Proposed Method and the MLBW Method for ^{109}Ag

^{109}Ag	Relative Errors (%)	
	Average	Maximum
σ_t	< 1.00E-9	< 1.00E-9 at 1.06E+03 eV
σ_{int}	3E-09	1.76E-07 at 1.00E-05 eV
σ_n	2.49E-06	5.86E-06 at 7.01E-01 eV
σ_a	< 1.00E-9	< 1.00E-9 at 1.06E+03 eV

Table 4. Comparison Between the Proposed Method and the SLBW Method for ^{99}Tc

^{99}Tc	Relative Errors (%)	
	Average	Maximum
σ_t	< 1.00E-9	4E-09 at 1.17E-05 eV
σ_n	1.85E-06	5.9E-06 at 4.95E+02 eV
σ_a	< 1.00E-9	< 1.00E-9 at 3.86E+02eV

Table 5. Comparison Between the Proposed Method and the MLBW Method for ^{23}Na

^{23}Na	Relative Errors (%)	
	Average	Maximum
σ_t	2.02E-06	8.62E-05 at 1.04E-05 eV
σ_{int}	0.000266	0.020785 at 1.04E-05 eV
σ_n	1.37E-05	0.000836 at 1.04E-05 eV
σ_a	< 1.00E-9	< 1.00E-9 at 3.54E+04 eV

The comparison results for ^{241}Am, ^{109}Ag and ^{99}Tc are summarized in Tables 2 through 4. The absolute relative errors are below or around 10^{-9}% for the absorption, fission, total and interference cross sections and close to 10^{-6}% for the scattering cross section. The reason for the slight deterioration in the accuracy of the scattering cross section comes from the fact that it is calculated as the difference between the total and absorption cross sections, which causes inevitable round-off problems. The majority of the corresponding absolute relative errors are uniformly located throughout the energy range inside a band between 6×10^{-6}% and 10^{-7}%. However, the observed discrepancies remain insignificant for all cross sections.

Table 5 summarizes the comparison results for ^{23}Na. It is noticeable that the magnitude of the relative errors is more important for the interference, scattering and total cross sections at very low energy. The absolute relative errors in question decrease rapidly as energy increases. This lack of accuracy in the low energy region is accounted for the difficult numerical estimation of the small contribution of Lorentzian tails corresponding to very high-energy resonances. Table 6 shows that using an enhanced version of the BW2PR code completely written in extended precision can alleviate this numerical issue. However, for practical applications, the standard version of the BW2PR code using the extended precision only for computing pole parameters offers a sufficient accuracy.

Table 6. Results for ^{24}Na Obtained with a Fully Extended-Precision Version of BW2PR

^{23}Na	Relative Errors (%)	
	Average	Maximum
σ_t	< 1.00E-9	< 1.00E-9 at 1.00E-05 eV
σ_{int}	< 1.00E-9	< 1.00E-9 at 1.00E-05 eV
σ_n	1.97E-06	5.93E-06 at 2.96E+04 eV
σ_a	< 1.00E-9	< 1.00E-9 at 1.00E-05 eV

5 Conclusions

The goal of the present work was to develop an algorithm to convert the Breit-Wigner resonance parameters to the pole parameters, in order to supplement the capability of converting the Reich-Moore parameters to the pole parameters already in place. As mentioned earlier, conversion of the Adler-Adler parameters to pole parameters can be easily added if the need arises. Completion of this work makes possible utilization of the generalized pole representation for all isotopes, independent of how the resonance parameters are specified. Thus, a high degree of accuracy in the point-wise cross section at any temperature can be assured without question via the same analytical approach previously described. The results obtained by the code BW2PR developed for this purpose and applied to four selected nuclides demonstrate that the generalized pole representation is not only analytically rigorous but also numerically exact. The code has been successfully and extensively tested for the SLBW and MLBW formalisms as well as for all angular momentum states up to d-wave. Thus the use of the pole parameters to compute the cross sections originally described in an ENDF-format file by Breit-Wigner resonance parameters preserves all the accuracy that is required in reactor applications. The code is being incorporated into the existing POLEBRD (Hwang, 1998a) code which provides the exact Doppler-broadening of the point-wise cross sections readily

applicable to generation of the base libraries for the VIM Monte Carlo code. Finally, it is worth noting that the proposed method is easily adaptable to any existing neutronic code because of its compatibility with the resonance integral concepts.

A Appendix

As previously mentioned, the Breit-Wigner formalisms assume that the level matrix is diagonal. The diagonal elements are equal to

$$A_\lambda(u) = A_\lambda^r(u) + i\,A_\lambda^i(u) = \left[E_\lambda - \Delta_\lambda^{(\ell)}(u) - u^2\right] - \frac{i}{2}\left[\Gamma_{\lambda n}^{(\ell)}(u) + \Gamma_{\lambda\gamma} + \Gamma_{\lambda f}\right]. \tag{A.1}$$

where A_λ^r and A_λ^i are, respectively, the real and imaginary components of the level matrix when considering u as real. $\Gamma_{\lambda n}^{(\ell)}$, $\Gamma_{\lambda\gamma}$, $\Gamma_{\lambda f}$ denote the neutron, capture and fission widths, respectively. In the case of the SLBW representation, the expression of the capture or fission cross sections ($x = \gamma, f$) are given by

$$\begin{aligned}\sigma_x &= \sum_{\lambda=1}^{N}\sum_{\ell,J}\frac{\pi}{k_0^2 E}\,g_J\left|\frac{\Gamma_{\lambda n}^{(\ell)}(u)^{1/2}\,\Gamma_{\lambda x}^{1/2}}{A_\lambda(u)}\right|^2 = \sum_{\lambda=1}^{N}\sum_{\ell,J}\frac{2\pi}{k_0^2 E}\,g_J\,\mathrm{Re}\left\{-i\frac{\Gamma_{\lambda n}^{(\ell)}(u)^{1/2}\,\Gamma_{\lambda x}^{1/2}}{\Gamma_{\lambda n}^{(\ell)}(u) + \Gamma_{\lambda\gamma} + \Gamma_{\lambda n}} \times \frac{1}{A_\lambda(u)}\right\} \\ &= \frac{1}{E}\sum_{\ell,J}\sum_{\lambda=1}^{N}\mathrm{Re}\left\{-i\,f_{\ell,J,\lambda}^{(x)}(u)\right\},\end{aligned} \tag{A.2}$$

and the total cross section

$$\sigma_t = \sigma_p + \sum_{\lambda=1}^{N}\sum_{\ell,J}\frac{2\pi}{k_0^2 E}\,g_J\,\mathrm{Re}\left\{e^{-i2\phi_\ell}\,\frac{-i\Gamma_{\lambda n}^{(\ell)}(u)}{A_\lambda(u)}\right\} = \sigma_p + \frac{1}{E}\sum_{\ell,J}\sum_{\lambda=1}^{N}\mathrm{Re}\left\{-ie^{-i2\phi_\ell}\,f_{\ell,J,\lambda}^{(t)}(u)\right\}, \tag{A.3}$$

where σ_p is the potential cross section given by

$$\sigma_p = \frac{2\pi}{k_0^2 E}\sum_{\ell,J} g_J\,\mathrm{Re}\left\{1 - e^{-i2\phi_\ell}\right\}.$$

In the case of the MLBW representation, the following interference cross section must be added to the SLBW scattering or total cross section:

$$\sigma_{int} = \sum_{\ell,J}\frac{\pi}{k_0^2 E}\,g_J\,\mathrm{Re}\left\{\sum_{\lambda=1}^{N}\sum_{\substack{\mu=1\\ \mu\neq\lambda}}^{N}\frac{\Gamma_{\lambda n}^{(\ell)}(u)\,\Gamma_{\mu n}^{(\ell)}(u)}{A_\lambda(u)\,A_\mu^*(u)}\right\} = \frac{1}{E}\sum_{\ell,J}\sum_{\lambda=1}^{N}\sum_{\substack{\mu=1\\ \mu\neq\lambda}}^{N}\mathrm{Re}\left\{f_{\ell,J,\lambda}^{\mu}\right\} \tag{A.4}$$

where A_μ^* is the complex conjugate.

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