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Resonance data for self-shielding problems

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Abstract. The investigation of resonance self-shielding effects in macroscopic medium is important for the physics of nuclear reactors and shielding. The degree of consistency of evaluated resonance cross sections data and the requirements to the accurate presentation of self-shielding effects can be estimated by using the simplest benchmark data for resonance averaged functions of neutron transmission and self-indication cross section at arbitrary filter thickness n. We report the developed (for nonfissile nuclei) methods for description of cross sections and their functionals in the unresolved resonance range that aim to estimate properly the self-shielding effects and reveal the resonance structure in averaging intervals (groups).

1 Introduction

The analysis of self-shielding effects in reactor medium related to the energy structure of neutron spectrum in resonance region is important part of reactor physics [1–4]. The recent simulations of these effects are of high level, so that the possible uncertainties could arise mainly from the inaccurate input information about cross section full energy structure of reactor materials. The qualitative criteria for that are requirements to proper description by evaluated files the simplest macroscopic characteristics like resonance averaged neutron transmission for relatively thick samples $\langle \exp(-n\sigma)\rangle$, reaction cross sections on filtered beams $\langle \sigma_c \exp(-n\sigma)\rangle$, effective integrals of the type $\langle \sigma_c/\sigma\rangle$ and average flux $\sim \langle 1/\sigma\rangle$ in medium, etc.

1.1 Resonant structure

In the resolved range the only problem is to make more precise total cross section near interferential minima that are essential to a great extent for macroscopic characteristics. The test of evaluated files against thick filter transmission data apparently is important for that [5].

For partly resolved and unresolved resonances the evaluated data files contain only averaged (over energy intervals, groups) values presenting smoothly the energy structure. At the same time the general consideration about this structure and accessible data for thick filter neutron transmission, where $\langle \exp(-n\sigma)\rangle \neq \exp(-n\langle\sigma\rangle)$, (see fig. 1), prove the need to take into account the resonance effects in this region (up to ~100 keV for heavy nuclei and ~MeV for medium ones) [6–9].

Considering self-shielding problems more natural approach seems to be the modeling of resonance structure in energy intervals so that the average cross section values are in agreement with the corresponding ENDF data. We report here some algorithms and results of such modeling for nonfissile nuclei.

Table 1. Boundaries of ABBN [4] energy groups in MeV.

Group No	lower boundary	upper boundary
10	0.0215	0.0465
11	0.01	0.0215
12	0.00465	0.01
13	0.00215	0.00465
14	0.001	0.00215
15	0.000465	0.001
16	0.000215	0.000465

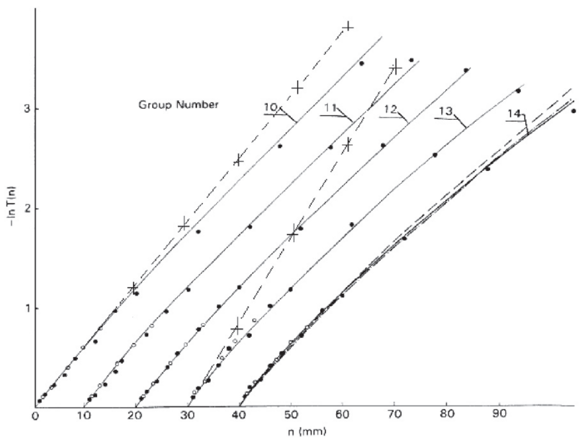

Fig. 1. The disagreement of the transmission values calculated through evaluated data files with the experimental results [8].

2 Modeling the resonance averaged cross sections

The methodical base is R-matrix formalism, where the cross section are expressed via collision matrix U elements chosen in the form applied in SAMMY [5, 10]

$$\mathbf{U}(E) = e^{-i\varphi}\left(\frac{2}{1 - iK(E)} - 1\right)e^{-i\varphi}$$

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where K(E) is an analogue of R-matrix in Reich-Moore approach with the elements

$$K_{cn}(E) = \frac{1}{2}\sum_{\lambda} \Gamma_{\lambda c}^{1/2}\Gamma_{\lambda n}^{1/2} / (E_\lambda - E - i\Gamma_{\lambda c}/2). \qquad (1)$$

It is obvious that with this presentation of U(E) the problem of creation the cross section model in unresolved range is reduced methodically to the corresponding modeling of $K_{cn}(E)$ elements equation (1). Here the evaluated data are limited to average resonance parameters of Hauser-Feshbach formalism and statistical distribution functions of the widths $\Gamma_{\lambda c}$ and level spacing $|E_\lambda - E_{\lambda-1}|$ (distributions of Porter-Thomas and Wigner) [5,10] in averaging interval. Is something more necessary for application to self-shielding problems, to the estimation, e.g., of thick filter neutron transmission data $\langle \exp(-n\sigma)\rangle$.

2.1 Equidistant equal resonances

Let us consider the simplest model of equal equidistant resonances. Here in one neutron channel case the periodical function corresponds to the element $K_{nn}(E)$ [11]

$$\tilde{K} = s_n \,\mathrm{ctg}(x - iy), \qquad (2)$$

with $s_n = \pi\bar{\Gamma}_n/2D$, $y = \pi\Gamma_c/2D$, $x = \pi(E_0 - E/D$. Then $\tilde{U}_{nn}(x)$ and model cross sections $\tilde{\sigma}(x) \sim 1 - \mathrm{Re}\tilde{U}_{nn}(x)$, $\tilde{\sigma}_c(x) \sim 1 - |\tilde{U}_{nn}(x)|^2$ as well are periodical functions of the energy (x), and the important for self-shielding problem functionals are determined as corresponding average value over the period $-\pi/2 \le x \le \pi/2$. So, $\langle\tilde{K}\rangle = is_n$, that is in agreement with the averaging of R_{nn} in the general scheme of Wigner formalism [1] and this confirms that our model reproduces properly average total cross section. For average cross section of neutron absorption the model gives Hauser-Feshbach formula, which does not account the effect of resonance parameters fluctuations. The analytical expressions are obtained for the following functionals as well:

$$\langle \exp(-n\sigma)\rangle \sim \frac{1}{\sqrt{\pi n\sigma_0}} e^{-n\sigma_m} \qquad (n\sigma_0 > 10)$$
$$\langle \sigma_c \exp(-n\sigma)\rangle = \langle\sigma_c\rangle I_0(n\sigma_0/2)\, \exp[-n(\sigma_m + \sigma_0/2)]$$
$$\langle \sigma_c/\sigma\rangle = \langle\sigma_c\rangle / \sqrt{\sigma_m(\sigma_0 + \sigma_m)} \qquad \text{and so on,}$$

where σ_0 and σ_m are the values of model cross section in minimum and maximum. These values can be calculated through evaluated strength functions and phases, however it is more comfortable to adopt them as free parameters for energy intervals (groups in multigroup schemes). The application of our model to the analysis of transmission data dependence on filter thickness for iron and chromium present the data properly with σ_0 and σ_m rather close to estimated values. For ^{238}U Doppler broadening should be taken into account and our parameters became more phenomenological being dependent on the temperature [12,13].

2.2 Generalized statistical approach

The fluctuations of resonance parameters in $K_{nn}(E)$ equation (1) could be accounted by using the resonance ladder method and our model [11]:

$$\tilde{K}(x) = s_n \frac{1}{N}\sum_{\lambda=0}^{N-1} \xi_\lambda \,\mathrm{ctg}\left[(x - iy + \delta_\lambda)/N\right]$$
$$\xi_\lambda = \Gamma_{\lambda n}/\bar{\Gamma}_n, \quad \delta_\lambda = \pi(E_\lambda - E_0)/D \qquad (3)$$
$$\left(\sum \xi_\lambda = 1, \quad \sum \delta_\lambda = 0\right).$$

Here is supposed that N levels ladder is repeated periodically and this permits to avoid the complications in assessment the contribution of distant levels. Traditionally the parameters for such ladder $\xi_\lambda, \delta_\lambda$ are chosen independently in accordance with the Porter-Thomas and Wigner statistical distributions.

Our approach utilizes the idea of twofold statistical distribution function directly for real and imaginary parts of $K_{nn}(E)$. The characteristic function of that distribution is the following:

$$F(t, t') = \langle \exp[i(Kt - K^* t')]\rangle \qquad (4)$$

and has been computed for a wide diapason of parameters t and t' ($s_n t$ and $s_n t'$) [14]. An analogous function was determined for the model $\tilde{K}(x)$ equation (3) and the optimal set of $\xi_\lambda, \delta_\lambda$ for our ladder equation (3) was found by comparison of the both functions in wide range of t and t'. Thereby it is possible to affirm that the composed in this way resonance ladder suits not only for description of resonance averaged cross sections but for receiving as well the average functionals for self-shielding problems. This idea is applied in the code HARFOR for computing in the unresolved range the both-averaged in energy group cross sections and the corresponding self-shielding coefficients for our functionals [15].

The results of HARFOR agree in general with these obtained by the codes GRUCON [16], NJOY [17] and by resonance sampling Monte Carlo method [8]. The version of our scheme for two neutron channels case was developed as well [18]. In principle it is possible to think about the resonance cross section modeling for bigger number of channels, considering the case of fissile nuclei. It seems to be not as important for practice because the existing resolved resonances data for these nuclei overlap the energy range where the resonance self-shielding is considerable; in addition the admixture of other isotopes always diminishes here this effect.

However for nonfissile isotopes of heavy nuclei and mainly for those of structural elements the problem of an adequate to the nuclear technology requirements modeling of resonance structure in unresolved range remains open in the context of self shielding analysis. The reason for that is usage by nearly all calculating schemes the statistical approach concentrated on Hauser-Feshbach results for average cross sections parameterization. However following the thick filter neutron transmission data the dependence on cross sections values in the interferential minima occurring in the averaging interval is obvious. In several cases these fluctuate considerably from the statistical modeling results and it seems necessary to add the data about minimal cross sections to

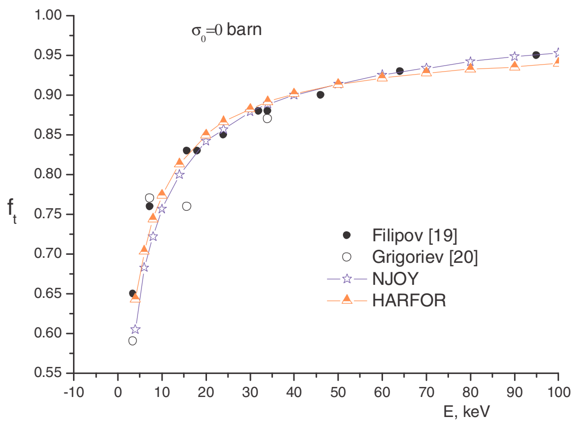

Fig. 2. Self-shielding factors for ^{232}Th (4–100) keV.

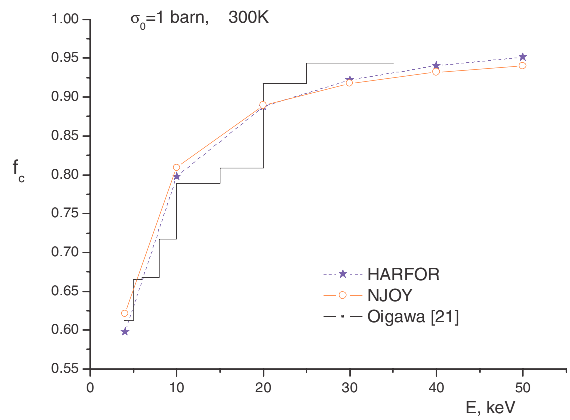

Fig. 3. Self-indication in neutron capture for ^{232}Th (4–50 keV).

the average parameters table in some groups surely if these differ significantly from potential cross section σ_p. In our simplest model of identical resonances these are σ_m and σ_0 with regard to their temperature dependence. It seems that for the resonance ladder schemes the parameters $\xi_\lambda, \delta_\lambda$ should be derived with accounting of the transmission function asymptotic in several groups. Evidently the optimal approach is connected here with the extension of data base with thick samples transmission functions.

3 Some practical applications

3.1 Self-shielding factors

The self-shielding factors are determined mainly through the evaluated average resonance parameters from the Evaluated Nuclear Data Files. Also they can be determined experimentally. In these experiments the self-shielding factors are obtained from sets of neutron transmission ratio measurements and self-indication ratio measurements with several transmission samples of different thicknesses n (atom/barn).

$$f_x(\sigma_0) = \int_0^\infty T_x(n)e^{-n\sigma_0}dn \Big/ \int_0^\infty T(n)e^{-n\sigma_0}dn.$$

Consequently two functions T(n) and Tx(n) must be measured together. In figures 2 and 3 we show the calculated self-shielding factors for ^{232}Th with HARFOR and NJOY and using the average resonance parameters from ref. [19]. The results are compared with the available experimental data [19–21].

In table 2 we show the calculated self-shielding and self-indication factors for neutron capture for ^{238}U at $E_n = 4$ keV. The calculations are performed with HARFOR and GRUCON for some values of the dilution cross section σ_0 and different temperature of the medium.

3.2 Thick filters transmission data

The total cross section energy dependence and self-shielding effects in the energy region of unresolved levels reveal strong resonance structure, which is presented properly by statistical modelling. The average parameters characterizing resonance structure–mean level spacing; average partial widths and potential scattering phases could be derived from thick sample transmission or self-indication data through the comparison with simulated cross sections and functionals. Consequently these average parameters became an important part of modern evaluated data files.

Table 2. Self-shielding factors for ^{238}U at 4 keV – upper line GRUCON, down line – HARFOR.

σ_0	300 K		1000 K		2000 K	
barn	f	f_c	f	f_c	f	f_c
1	.57 ± .01	.51 ± .01	.63 ± .01	.61 ± .01	.67 ± .01	.68 ± .01
	.56 ± .01	.51 ± .01	.63 ± .01	.63 ± .01	.67 ± .01	.68 ± .01
10	.65 ± .01	.60 ± .01	.70 ± .01	.70 ± .01	.72 ± .01	.75 ± .01
	.64 ± .01	.60 ± .01	.69 ± .01	.71 ± .01	.72 ± .01	.76 ± .01
100	.79 ± .01	.83 ± .01	.84 ± .01	89 ± .01	.87 ± .01	.92 ± .01
	.80 ± .02	.82 ± .02	.85 ± .02	89 ± .02	.88 ± .02	.92 ± .02

The measured cross section value in the minimum between resonances diminishes with the growth of the filter thickness reaching the minimal value σ_m. This value contains interference minima, contributions of other isotopes, higher spin states and radiative capture.

The thick samples transmission measurements can be treated as simplest benchmark experiments. These are the only integral measurements easily reproduced by evaluated files and can be used for validation and improvements of the evaluated libraries. The energy region of overlapping and unresolved resonances is quite large rather more than resolved resonance range and very important for modern nuclear technologies. The fluctuations of cross sections and functionals observable here could be described properly by accurate investigation of the resonance structure and especially thick filter transmission measurements.

The main advantage of using such measurements is the possibility of achieving high accuracy in experiment and measuring the dependence of neutron transmission on filter thickness. The asymptotical value of the transmission function corresponds to the value of $n\sigma_0 > 10$.

This shows the vision of possible advance in the investigation of hidden resonance structure in the unresolved range on new high intensity neutron sources with promising extent of neutron yield of 2–3 orders of magnitude.

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