Programs for the R-Matrix Description of Neutron Cross-Section Structure

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Abstract

A study of neutron fission and non-fission cross sections, performed during many years in the Frank Laboratory of Neutron Physics, allowed to accumulate a significant experience in the analysis of resonance structure of the cross section as well as of correlation effects in fission using R-matrix formalism. We present a detailed description of the mathematical approach used for the analysis of experimental data with the help of least square method (FUMILI minimization) in order to extract the parameters of structure of cross section or correlation coefficients. The obtained results of the fits for the total, fission and capture cross sections of ^{235}U, in the energy range up to 10 eV, and for the total cross section of ^{181}Ta, in the energy range up to 50 eV, are presented.

The calculations were performed in Fortran-codes at JINR using the FLNP and LIT computer clusters.

In an initial stage of neutron cross-section investigations on a booster IBR-30+LUE-40 of Laboratory of neutron physics, JINR, in order to extract the neutron resonance parameters the experimental data was described in single-level Breit-Wigner approach using a program [1]. In a study of angular correlations of fragments at fission of the aligned nuclei of ^{235}U an attraction of *R*-matrix description of observable effects [2–4] is demanded, within the limits of the theoretical approach developed by A. Barabanov and W. Furman [5, 6]. This approach has been used also for analysis of P-even and P-odd effects in angular distributions of fission fragments of ^{235}U and ^{239}Pu [7, 8]. Results of long-term investigations are presented in the review [9], and information about used programs can be discovered in [10]. In these programs the mathematical apparatus provided that several channels of *K*-projections of spin *J* of compound nucleus to a nucleus axis are exhibited in fission.

Let's reduce the basic formulas used in the programs. Initial expression of a scattering matrix is of the form

$$S^J_{nc} = e^{-i(\phi_n+\phi_c)}\{2((I-K)^{-1})_{nc} - \delta_{nc}\},$$

where I is unit matrix, $K_{ij} = -\frac{1}{4}\sum_\lambda \frac{\Gamma_{\gamma\lambda}\sqrt{\Gamma_{i\lambda}\Gamma_{j\lambda}}}{d_\lambda} + \frac{i}{2}\sum_\lambda \frac{(E_\lambda - E)\sqrt{\Gamma_{i\lambda}\Gamma_{j\lambda}}}{d_\lambda}$, $d_\lambda = (E_\lambda - E)^2 + \Gamma^2_{\gamma\lambda}/4.$

Taking into account that $W^J_{nc} = ((I-K)^{-1})_{nc}$, cross sections can be written in the following way:

the total cross-section

$$\sigma_{tot} = \frac{4\pi}{k^2}\sum_J g_J [\sin^2\phi_n - \sin 2\phi_n \operatorname{Im} W_{nn}^J + \cos 2\phi_n (1 - \operatorname{Re} W_{nn}^J)],$$

the scattering cross section

$$\sigma_{nn} = \frac{4\pi}{k^2}\sum_J g_J [\cos^2\phi_n (1 - 2\operatorname{Re} W_{nn}^J) - \sin 2\phi_n \operatorname{Im} W_{nn}^J + \operatorname{Re}^2 W_{nn}^J + \operatorname{Im}^2 W_{nn}^J],$$

the absorption cross section

$$\sigma_{abs} = \frac{4\pi}{k^2}\sum_J g_J [\operatorname{Re} W_{nn}^J - \operatorname{Re}^2 W_{nn}^J - \operatorname{Im}^2 W_{nn}^J],$$

the fission cross section (here K - is the projection of a spin J to a nucleus axis)

$$\sigma_{fis} = \frac{4\pi}{k^2}\sum_J g_J \sum_K | W_{nfK}^J |^2,$$

and the capture cross-section

$$\sigma_{n\gamma} = \sigma_{abs} - \sigma_{fis}.$$

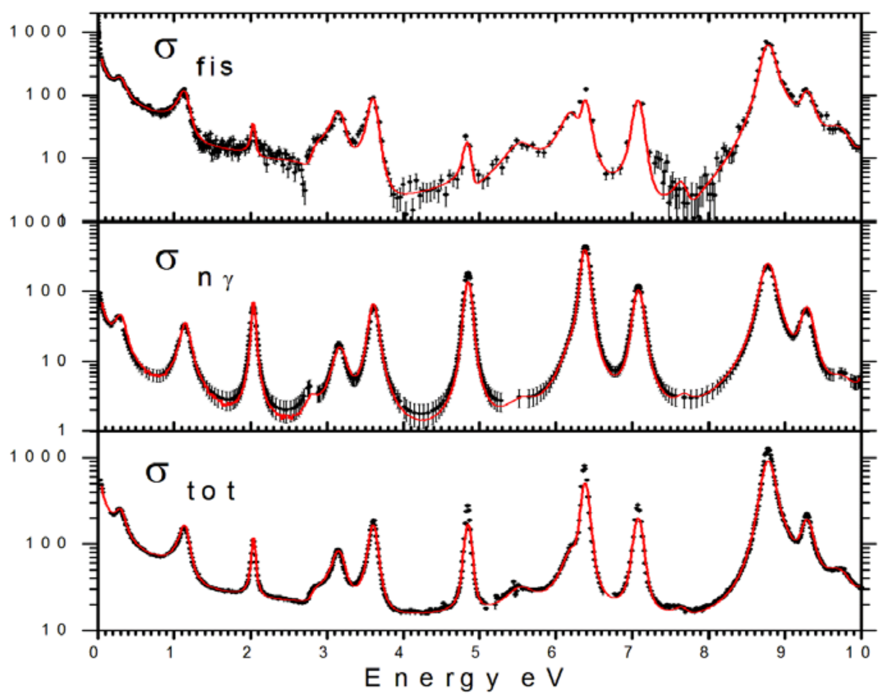

Fig. 1. Results of fitting for cross sections of ^{235}U: points – experimental data (in barn), curves – calculations.

The analysis of angular correlations of fragments at fission of the aligned ^{235}U nuclei was made with the use of FUMILI-code together with the known data on total neutron cross sections, total and spin-divided fission cross sections. In the present paper an adaptation of mentioned programs to the analysis of the cross-section data of fissionable and nonfissionable nuclei is made, without an attraction of data on the correlation effects. It would appear that for this aim it is quite enough to use, instead of four-rank matrix, a two-rank matrix, when only contributions of neutron and fission channels are taken into account. However, trying to describe the total neutron cross section, fission cross section and capture cross section of ^{235}U we ascertained again that these data are not fitted in a supposition of one (single) fission channel but, for a satisfactory description of the experimental data, it is required to introduce, at least, two fission channels. In fig. 1 the result of the fitting for cross-section data of ^{235}U taken from EXFOR-bank, in the range of 0 – 10 eV, is shown.

Note that in the calculations a correction for the Doppler broadening of resonances was made. There are no difficulties to take into account an influence of resolution function of a spectrometer used in measurements, as appropriate. There is also a certain ambiguity in values of fitted parameters caused by a number of introduced negative resonances.

For the analysis of cross section of nonfissionalbe nuclei the similar *R*-matrix parametrization looks simpler and it is possible to use formulas from the paper of A. Lukjanov and N. Janeva [11]:

$$\sigma_{tot} = \frac{4\pi}{k^2} \sum_J g_J \{\sin^2 \varphi_n + \mathrm{Re}[e^{-2i\varphi_n} \frac{-iK^J_{nn}}{1 - iK^J_{nn}}]\},$$

$$\sigma_{abs} = \frac{4\pi}{k^2} \sum_J g_J \,\mathrm{Re}\{\frac{-iK^J_{nn}}{|1 - iK^J_{nn}|^2}\}.$$

Here σ_{abs} is simply the capture cross section. We have tested the modified program for description of the total neutron cross section using the data ^{181}Ta from EXFOR. Results are presented in fig. 2.

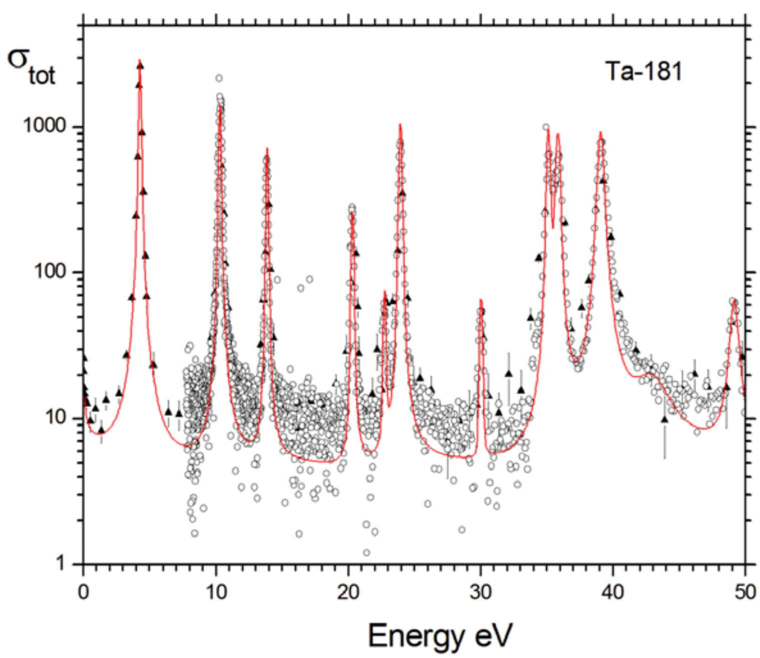

Fig. 2. The total neutron cross section of ^{181}Ta: points are experimental Belanova, etc. data, triangles are Pohan data (barn), curves are calculations with taking into account of the account Doppler-effect.

Singularity of our programs, unlike SAMMY-code used extensively, is a simultaneous fitting of different types of cross sections, in the same iteration. Despite a multi-parameter character of a problem and a numerical evaluation of fitted-parameters derivatives, using a modern computer cluster of LIT JINR a counting time, for example for ^{235}U, will be a few tens of minutes.

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