International Conference on Nuclear Data for Science and Technology 2007
DOI: 10.1051/ndata:07706

Generalization of the SPRT method: application to ^{242}Pu cross sections in the Unresolved Resonance Range

E. Rich[1], G. Noguere[1], C. De Saint Jean[1], O. Sérot[1], and A. Tudora[2]

[1] Commissariat à l'Énergie Atomique (CEN-Cadarache), 13108 Saint-Paul-lez-Durance, France
[2] Bucarest University, Bucarest Mägurele P.O. Box MG-11, 76900 Bucarest, Romania

Abstract. The modelling of the neutron cross sections consists in their interpretation in three different energy ranges: the first one is the Resolved Resonance Range (RRR) at low energy, the second is the Unresolved Resonance Range (URR), and the third one concerns the high energies. For this, we generally use the Reich-Moore approximation of the R-Matrix formalism, the average R-Matrix formalism and optical model calculations. One of the main challenges of such a work is to study the consistency of the average parameters obtained by these different calculations. With the ESTIMA and SPRT methods, we provide a set of parameters for partial s and p waves (strength functions, effective potential scattering radius, mean-level spacing and reduced neutron width). But, in order to analyse accurately the URR domain, we need more information than the parameters associated to the orbital moments $L = 0$ and $L = 1$. This work describes the link between the average R-Matrix formalism and the optical model, especially concerning the transmission coefficients, total and shape elastic cross sections. Based on these two models, we propose a generalization of the SPRT method for L > 1, and we obtain a new set of parameters for the URR domain in terms of S_{LJ} and R^{∞}_{JL}.

1 Introduction

The work presented in this paper was realized in the frame of the ^{242}Pu evaluation. Several results, coming from integral and microscopic measurement campaigns carried out on different reactors and accelerators shined lacks in the capture and fission cross section modelling of JEFF-3.1.

Two of these experiments (PROFIL and PROFIL-2 [1]) took place at the reactor PHENIX (CEA Marcoule) and were interpreted with the ERANOS code. They show an overestimation of the ^{242}Pu capture cross section of about 14 ± 3%. This tendency is also confirmed by microscopic measurements obtained at Karlsruhe [2].

To evaluate the neutron cross sections of an isotope like ^{242}Pu, the energy range is generally divided in three parts, each one being treated with a different formalism. At low energy, the Resolved Resonance Range is analysed with the Reich-Moore approximation of the R-Matrix formalism. For intermediary domain, where resonances become to overlap, we use the average R-Matrix formalism, and at high energy (i.e., for the continuum region), the optical model (phenomenologic or microscopic) is the most appropriated one.

One systematic challenge for this kind of evaluation is the overlap between these three regions and their formalisms. The link between RRR and URR domains is treated with statistical tests based on the resonance parameters distributions. But concerning the step between the URR and the continuum, we must use another method, which is called the SPRT method [3]. It consists to compare the average resonance parameters obtained by the Resolved Resonance Range analysis with those coming from the optical model calculations. Parameters which are used for this control are the effective potential scattering radius R′ and the strength functions for s and p waves. This document describes the link between the average R-Matrix formalism and the optical model. Relationships between these two models will be used in order to generalize the SPRT method to the higher order L-values ($L > 1$).

2 SPRT method

2.1 Presentation of the method

The SPRT method is used to study the consistency between the average R-Matrix parameters adjusted on experimental data and those given by optical model calculations. This method is applied to the strength functions S_0 and S_1 and to the effective scattering radius value R' [3]. The method calculates the strength functions using the "low energy" approximation of the transmission coefficients $T_L(E)$:

$$T_L(E) \approx 4\pi P_L(E) S_L. \tag{1}$$

Replacing the s_L parameter by the following expression:

$$s_L = \frac{S_L \sqrt{E}}{2ka_c} \tag{2}$$

the strength function is then given by:

$$S_L \approx \frac{1}{2\pi} \frac{ka_c \sqrt{E}}{P_L(E)} T_L(E) \tag{3}$$

where k is the wave number, a_c the channel radius, and $P_L(E)$ the penetrability factor.

In the optical model frame:

$$T_L(E) = \sum_j \sum_J g_{LJ} T_{Lj}(E). \tag{4}$$

In the case of the "low energy" approximation, the transmission coefficients involved in equation (5) could be calculated from this equation based on the C Collision Matrix knowledge:

$$T_{Lj}(E) = 4\mathrm{Im}\left[C^J_{Lj}(E)\right] - 4\left|C^J_{Lj}(E)\right|^2. \quad (5)$$

This last approximation consists in neglecting the coupled channel calculations.

The third parameter involved in SPRT method is the scattering radius R'. In practice, it could be simply deduced from the shape elastic cross section and then, allows an easy comparison between R' and the values reported in the literature. Its application domain is limited because it supposes a low variation of the shape elastic cross section with the neutron incident energy.

This method is included in the TALYS code [4]. This code gives S_0, S_1 and R' up to 100 keV. The interest of such a process is to obtain the energy dependence of each parameter and to extrapolate if necessary their value at B_n (i.e., $E = 0$). However, this method is limited, because it is restricted to $L \leq 1$ and gives an R' value which is not present in the R-Matrix formalism. The use of the Average Collision Matrix will be the starting point to generalize the SPRT method in order and to deduce average parameters useful in the Unresolved Resonance Range [5].

2.2 Generalization of the method

The generalization of the SPRT method could not be only supported by neutron transmission coefficients. Actually, R-Matrix formalism doesn't reproduce the direct contribution of inelastic reactions which is, on the other hand, correctly taken into account by coupled-channel calculations. Then, in order to generalize the SPRT approach, we decided to use the expressions of the total and shape elastic cross sections. In the URR domain, the exercise consists in determining the parameters s_{LJ} and R^{∞}_{LJ} as:

$$\begin{cases} \sigma_t\left(s_{LJ}, R^{\infty}_{LJ}, E\right) = \sigma_t\left(\mathrm{Im}[C^J_{Lj}(E)]\right) \\ \sigma_e\left(s_{LJ}, R^{\infty}_{LJ}, E\right) = \sigma_{et}\left(|C^J_{Lj}(E)|]\right). \end{cases} \quad (6)$$

Then, solving the above equation system leads directly to the following analytical expressions. For a couple (L, J), we obtain:

$$R^{\infty}_{LJ} = \frac{2a_{LJ}(E)\cos\left[2\phi_L(E)\right] + (1 - 2b_{LJ}(E))\sin\left[2\phi_L(E)\right]}{P_L(E)\left(1 + 2c^2_{LJ}(E) - 2b_{LJ}(E) + (1 - 2b_{LJ}(E))\cos\left[2\phi_L(E)\right] - 2a_{LJ}(E)\sin\left[2\phi_L(E)\right]\right)} \quad (7)$$

$$s_{LJ} = \frac{2\left(b_{LJ}(E) - c^2_{LJ}(E)\right)}{\pi P_L(E)\left(1 + 2c^2_{LJ}(E) - 2b_{LJ}(E) + (1 - 2b_{LJ}(E))\cos\left[2\phi_L(E)\right]\right) - 2a_{LJ}\sin\left[2\phi_L(E)\right]} \quad (8)$$

For a ground state spin $I = 0$, the parameters $a_{LJ}(E)$, $b_{LJ}(E)$ and $c_{LJ}(E)$are defined as :

$$\begin{cases} a_{LJ}(E) = \mathrm{Re}\left[C^J_{Lj=J}(E)\right] \\ b_{LJ}(E) = \mathrm{Im}\left[C^J_{Lj=J}(E)\right] \\ c_{LJ}(E) = \left|C^J_{Lj=J}(E)\right|. \end{cases} \quad (9)$$

Expressions above are very close to those coming from the ref. [5]. Generalization to target nuclei having a spin different from zero consists in combining the Real and Imaginary parts and the module of the Collision Matrix elements, and to calculate the average value of following quantities:

$$a^2_{LJ}(E) = c^2_{LJ}(E) - b^2_{LJ}(E) \quad (10)$$

$$b_{LJ}(E) = \left\langle \sum_j \mathrm{Im}\left[C^J_{Lj}(E)\right] \right\rangle \quad (11)$$

$$c^2_{LJ}(E) = \left\langle \sum_j \left|C^J_{Lj}(E)\right|^2 \right\rangle. \quad (12)$$

Equations (7), (8), (10) and (11) constitute a system of expressions which will be used to generalize the SPRT method.

In practice, the treatment of the URR domain with the average R-Matrix formalism implies the knowledge of average parameters for a given orbital momentum L. The system to be solved is now:

$$\begin{cases} \sigma^L_t\left(s_L, R^{\infty}_L, E\right) = \sum_J \sum_j g_{LJ}\sigma^{Lj}_t\left(\mathrm{Im}[C^J_{Lj}(E)]\right) \\ \sigma^L_t\left(s_L, R^{\infty}_L, E\right) = \sum_J \sum_j g_{LJ}\sigma^{Lj}_{et}\left(|C^J_{Lj}(E)]|\right). \end{cases} \quad (13)$$

Expressions of parameters s_{LJ} and R^{∞}_{LJ} satisfying the conditions up above are formally identical to the eqs. (7) and (8). The parameters $a_{LJ}(E)$, $b_{LJ}(E)$ and $c_{LJ}(E)$ are replaced by $a_L(E)$, $b_L(E)$ and $c_L(E)$ which are defined as:

$$a^2_L(E) = c^2_L(E) - b^2_L(E) \quad (14)$$

$$b_L(E) = \sum_J \sum_j g_{LJ}\mathrm{Im}\left[C^J_{Lj}(E)\right] \quad (15)$$

$$c^2_L(E) = \sum_J \sum_j g_{LJ}\left|C^J_{Lj}(E)\right|^2. \quad (16)$$

This formalism becomes very powerful because the total and shape elastic cross sections are defined by a restricted set of parameters. Two parameters are sufficient to calculate each partial wave contribution for a given L.

However, as we want to build a consistent modelling of neutron induced reactions cross sections from few meV to hundreds of MeV, combining s_{LJ} and R^{∞}_{LJ} parameters is a priority. Actually, in the R-Matrix frame, only the distant level parameter for a given (L, J) couple have a physical sense that we want to maintain over the Unresolved Resonance Range. For the strength function, the parameterization in terms of L is sufficient as it is generally difficult to extract realistic information for the average reduced neutron width for a given J. Then, the generalization of the SPRT method consists in determining the R^{∞}_{LJ} parameters with equation (7) by using equations (10)–(12). The s_L parameter is determined by minimisation of the following conditions:

$$\begin{cases} \sigma^L_t\left(s_L, R^{\infty}_{LJ}, E\right) = \sigma^L_t\left(s_{LJ}, R^{\infty}_{LJ}, E\right) \\ \sigma^L_e\left(s_L, R^{\infty}_{LJ}, E\right) = \sigma^L_e\left(s_{LJ}, R^{\infty}_{LJ}, E\right). \end{cases} \quad (17)$$

For analysing the Resonance Range, the author of the REFIT code chose the parameterization in terms of R^{∞}_{LJ}. To satisfy the coherence criteria, this choice was also included in the CONRAD code [6], dedicated to the neutron cross section analysis in the Resolved and Unresolved Resonance Range.

Table 1. Strength functions (S_L,S_{LJ}) and distant level parameters (R_L^∞, R_{LJ}^∞) for the reaction ^{242}Pu+n. Average parameters were obtained with the generalized SPRT method, using ECIS results with the Soukhovitsky potential [8].

Neutronic Strength functions ($\times 10^{-4}$)		
$S_0 = 0.882$	$S_{0,1/2} = 0.882$	
$S_1 = 2.298$	$S_{1,1/2} = 1.957$	$S_{1,3/2} = 2.469$
$S_2 = 1.181$	$S_{2,3/2} = 1.479$	$S_{2,5/2} = 0.982$
$S_3 = 2.000$	$S_{3,5/2} = 2.020$	$S_{3,7/2} = 1.985$

Distant level parameters		
$R_0^\infty = -0.1308$		
$R_1^\infty = 0.1189$	$R_{1,1/2}^\infty = 0.0678$	$R_{1,3/2}^\infty = 0.1515$
$R_2^\infty = -0.0569$	$R_{2,3/2}^\infty = -0.1053$	$R_{2,5/2}^\infty = -0.0171$
$R_3^\infty = 0.2391$	$R_{3,5/2}^\infty = 0.2358$	$R_{3,7/2}^\infty = 0.2414$

3 ^{242}Pu Analysis with SPRT method

We applied the generalized SPRT method to the ECIS03 code results [7] in order to model the ^{242}Pu cross sections. The ECIS code, written by J. Raynal, is dedicated to the optical model calculations. We used the RIPL library furnished by AIEA, and injected recovered potential parameters in the ECIS03 code.

3.1 E. Soukhovitsky potential

For this study, we realized coupled channel calculations with the Soukhovitsky potential parameters [8] which is relativistic, but non dispersive. The advantage of such a potential is that it has been adjusted for the actinide region, in particular for the ^{242}Pu. Strength functions and distant level parameters for s, pd and f waves are given in table 1. These results represent the extrapolated values to the binding energy B_n ($E = 0$). To describe the energy dependence of each parameter, we used a relatively simple representation in Lagrange polynomials.

Introducing the values $a_c = 8.42$ fm and $R_0^\infty = -0.1308$ in the following expression [9, 10]:

$$R'_L \approx a_c[1 - (2L + 1)R_L^\infty]^{1/(2L+1)}. \quad (18)$$

We obtain $R' = 9.53$ fm. Then, using the expression

$$\sigma_{pot} = 4\pi R'^2 \quad (19)$$

we deduce a potential scattering cross section of 11.4 barns which is a value in excellent agreement with the optical model calculation result.

These parameters could also be used in analysis code like CONRAD [6] and FITACS [11]. They allow the modelling of the total, capture, fission and scattering cross sections. Strength functions, distant level parameters and average reduced widths (for gamma rays and fission) for a given orbital momentum L are adjusted on experimental data. The total cross section is defined with the average R-Matrix formalism. Partial cross sections are modelled with the Moldauer [12] prescription associated with the Hauser-Feschbach formulae [13]

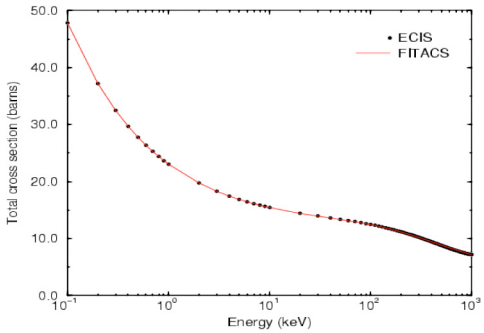

Fig. 1. Total cross section of ^{242}Pu calculated with ECIS (performed with the Soukhovitsky potential) and FITACS codes.

with width fluctuation. The energy dependence of the average radiation width is described by the GDR formalism. For the mean level spacing, we use the Gilbert-Cameron formulae and the fission barriers transmission coefficients are based on the Hill-Wheeler treatment.

Figure 1 compares the total cross section of the reaction ^{242}Pu+n obtained with ECIS and FITACS. ECIS calculations were done using the Soukhovitsky potential parameters available in RIPL.

The FITACS calculation uses average parameters coming from table 1. At low energy, results are in excellent agreement. Between 100 keV and 1 MeV, the discrepancy remains lower than 4%.

Above 1 MeV, the average R-Matrix formalism not allows a reliable modelling of the total cross section because of the wrong energy dependence of the parameters. Agreement between ECIS and FITACS calculations could be improved by introducing the energy dependences provided by ECIS. That is the reason why we decided to study this variation, which we will introduce as a development in the new CONRAD code [6].

3.2 R. Capote potential

This dispersive and relativistic potential [14] is one of the most recent proposed in the RIPL Library. It is a coupled channel potential, dedicated to the actinides and built for incident neutron energies from 1 keV to 200 MeV. The OPTMAN code [15] must be used as geometry is different for Hartree-Fock real potential V_{hf} and imaginary potential W_v. The different average parameters obtained with generalized SPRT method and extrapolated to the binding energy B_n (table 2) are very close, even sometimes identical to those presented in ref. [14]. For example, the value given by R. Capote for S_0 is 0.88 and for S_1 is 1.97. Moreover, considering the channel radius $a_c = 8.42$ fm, we evaluate the scattering radius R' to 9.54 fm, which corresponds exactly to the value given by R. Capote [14].

Figure 2 shows the EXFOR experimental data compared with the ECIS calculations performed with the R. Capote potential and the FITACS result obtained with the SPRT average parameters. The high energy part of the data is well reproduced by the optical model calculation, (which is quite logical because this potential was adjusted for ^{242}Pu). But at lower energy, discrepancies are observable and we should ask the question of the normalisation of the data.

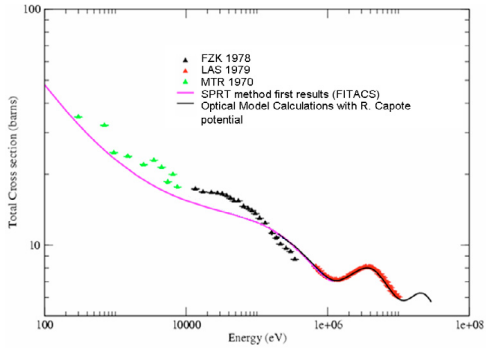

Fig. 2. ^{242}Pu total cross section calculated with ECIS (performed with the Capote potential) and FITACS codes, and compared to the experimental data available in the EXFOR data base.

Table 2. Average parameters obtained for the reaction ^{242}Pu+n with the generalized SPRT method, using ECIS results with the Capote potential [14].

Neutronic Strength functions	Distant level parameters
$S_0 = 0.886\ (\times 10^{-4})$	$R_0^{\infty} = -0.1359$
$S_1 = 1.988\ (\times 10^{-4})$	$R_1^{\infty} = 0.1403$
$S_2 = 1.200\ (\times 10^{-4})$	$R_2^{\infty} = -0.0497$
$S_3 = 2.107\ (\times 10^{-4})$	$R_3^{\infty} = 0.3796$

4 Conclusion

The comparison between the average parameters extracted from high energy calculations and those adjusted on experimental data with the average R-Matrix formalism is crucial. The generalization of the SPRT method, applied to the ^{242}Pu, allows us to obtain a consistent set of average parameters, even if a question still remains on the renormalization of some data points. This method, associated to the Capote potential gives good results. Its study should be continued with other optical potentials. For example, the global and spherical potential of P. Romain and B. Morillon [16,17] also attracts our attention. This global potential was originally adjusted on a large range of isotopes (A = 24 to 209) for neutron incident energies from 1 keV to 200 MeV. It could be very interesting to explore this potential as it takes into account the dispersion relation, but we need to extend it to the actinide region to extract all the power of this new potential.

We want to thank P. Romain for the fruitful discussions about ECIS, and I. Sirakov for his useful comments.

References

1. J. Tommasi, Technical Note NT-DER/SPRC/LEPh **04/217** (2005).
2. K. Wisshak, F. Kaeppeler, Nucl. Sci. Eng. **69**, 1 (1979).
3. J.-P. Delaroche et al., Rapport IAEA-**190**, 251 (1976).
4. A.J. Koning, S. Hilaire, M.C. Duijvestijn, *Proceeding International Conference on Nuclear Data for Science and Technology*, *26 Sep.–1st Oct.*, *Santa Fe*, *USA*, *2004*.
5. A. Courcelle (2004) (private communication).
6. C. De Saint Jean, G. Noguere, B. Iooss, Proceeding *American Nuclear Society's Topical Meeting on Reactor Physics PHYSOR, 10–14 Sept., Vancouver, Canada*, *2006*.
7. J. Raynal, Technical Note CEA N-2772.
8. E. Soukhovitsky et al., Phys. Rev. C **72**, 024604 (2005).
9. I. Sirakov, *Proceeding Worshop on nuclear data and evaluation for reactor applications, 9–11 Oct.*, *Château de Cadarache*, *Saint-Paul-lez-Durance, France, 2006*.
10. F.H. Fröhner, *Proceeding Computation and analysis of Nuclear Data Relevant to Nuclear Energy and Safety*, *10 Feb.–13 March*, *Trieste*, *Italie, (1992)*; see also the report Karlsruhe, KFK-5073 (1992).
11. F. Fröhner, NSE **103**, 119 (1989).
12. P.A. Moldauer, Phys. Rev. C **11**, 426 (1975).
13. W. Hauser, H. Feshbach, Phys. Rev. **87**, 366 (1952).
14. R. Capote et al., *Dispersive coupled-channel neutron OMP for incident energies between 1 keV to 200 MeV for actinides*. *Perspectives of Nuclear Data for the next decade P_ND^2, Paris* (2005).
15. E. Soukhovitsky et al., J. Phys. G Nucl. Part. Phys. **30**, 905 (2004).
16. B. Morillon, P. Romain, Phys. Rev. C **70**, 014601 (2004).
17. B. Morillon, P. Romain, Phys. Rev. C **74**, 014601 (2006).