On the use of the generalized SPRT method in the equivalent hard sphere approximation for nuclear data evaluation

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Abstract. A consistent description of the neutron cross sections from thermal energy up to the MeV region is challenging. One of the first steps consists in optimizing the optical model parameters using average resonance parameters, such as the neutron strength functions. They can be derived from a statistical analysis of the resolved resonance parameters, or calculated with the generalized form of the SPRT method by using scattering matrix elements provided by optical model calculations. One of the difficulties is to establish the contributions of the direct and compound nucleus reactions. This problem was solved by using a slightly modified average R-Matrix formula with an equivalent hard sphere radius deduced from the phase shift originating from the potential. The performances of the proposed formalism are illustrated with results obtained for the ^{238}U+n nuclear systems.

1. Introduction

Experimentally we can observe that there is a continuous transition from the extreme situation of well-isolated resonances to complete overlap. This transition was first described by Feshbach et al. [1], explaining how the R-Matrix and optical models may coexist between the "resonance region" and the "continuum region".

The main ingredients of the theory of average cross section are given in this document. Equations are then slightly modified to account for direct reactions by introducing complex background terms in the Reich-Moore approximation of the R-Matrix theory [2]. Consequences on the neutron strength functions calculated in the hard sphere approximation are discussed with results provided by the OPTMAN code.

2. Theory of average cross section

For the sake of clarity, we define U_c, $\overline{U}_c$ and $\mathcal{S}_c$ the elements of the scattering matrix respectively used in the Resolved Resonance Range, in the Unresolved Resonance Range and in the "continuum" for $c = c'$. Historically, $\overline{U}_c$ is called the average collision function by analogy with the collision matrix U_c involved in the R-Matrix theory.

In the resonance region, the elements of U_c exhibit rapid fluctuations coming from the numerous close-spaced resonances of the compound nucleus. An average value of U_c can be defined over an interval ΔE containing many overlapping levels. This condition is written as:

$$\Delta E \gg D_c, \tag{1}$$

where D_c stands for the average spacing of the compound levels. If the interval ΔE is small enough to assume constant the phase shift ϕ_c, the penetration factor P_c and the reduced R-function R_c, it follows that the analytical averaging of the collision matrix U in terms of average resonance parameters yields a diagonal collision matrix $\overline{U}$ with elements [3,4]:

$$\overline{U}_c \simeq e^{-2i\phi_c} \frac{\mathcal{B}_c + i\,P_c\overline{R}_c}{\mathcal{B}_c - i\,P_c\overline{R}_c}. \tag{2}$$

The factor $\mathcal{B}_c$ depends on boundary condition parameters, which choice is often a matter of convenience [5]. In the present work a "standard" formulation is used, for which $\mathcal{B}_c = 1$ [6]. Under these conditions, Eq. (2) becomes:

$$\overline{U}_c \simeq e^{-2i\phi_c} \frac{1 + i\,P_c\overline{R}_c}{1 - i\,P_c\overline{R}_c}. \tag{3}$$

In that case, the average value of the total and shape elastic cross sections can be evaluated as follow:

$$\overline{\sigma}_{t_c} \simeq g_J \frac{2\pi}{k^2} (1 - Re[\overline{U}_c]), \tag{4}$$

$$\overline{\sigma}_{e_c} \simeq g_J \frac{\pi}{k^2} |1 - \overline{U}_c|^2. \tag{5}$$

The neutron transmission coefficients are given by:

$$\mathcal{T}_c = 1 - |\overline{U_c}|^2. \tag{6}$$

3. Average reduced R-function

In this work, the average reduced R-function $\overline{R}_c$ has been determined from the reduced R-function given by the

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Reich-Moore approximation of the R-Matrix theory [2]:

$$R_c(E) = \sum_\lambda \frac{\gamma_{\lambda n_c}^2}{E_\lambda - E - i\Gamma_{\lambda\gamma_c}/2} + \mathcal{R}_c(E), \qquad (7)$$

in which E_λ is the resonance energy, $\gamma_{\lambda n_c}$ is the reduced neutron width amplitude and $\Gamma_{\lambda\gamma_c}$ is the partial radiation width of the compound state λ. Lynn derived an expression in which the background term $\mathcal{R}_c$ is complex [7]:

$$R_c(E) = \sum_\lambda \frac{\gamma_{\lambda n_c}^2}{E_\lambda - E - i\Gamma_{\lambda\gamma_c}/2} + R_c^\infty(E)$$
$$+ R_c^{\text{loc}}(E) + i\pi s_c^{\text{loc}}(E). \qquad (8)$$

The real part of $\mathcal{R}_c$ can be split into the contributions of neighboring (R_c^{loc}) and far-off levels (R_c^∞). Feshbach [1] assumes that only the immediate-neighbor resonances R_c^{loc} contribute appreciably. He suggests that such a contribution may formally be replaced by a sum over an infinite number of external levels μ, having negative or positive energies. As the consequence, the contribution of these "fictitious" resonances can be included in the sum over levels λ of the reduced R-matrix (Eq. (7)):

$$R_c(E) \simeq \sum_{\eta=\lambda,\mu} \frac{\gamma_{\eta n_c}^2}{E_\eta - E - i\Gamma_{\eta\gamma_c}/2} + R_c^\infty(E) + i\pi s_c^{\text{loc}}(E). \qquad (9)$$

Throughout the R-matrix theory, R_c^∞ is called the distant level parameter. Its value is lower than unity. Lynn indicates that the far away contribution R_c^∞ modifies the channel radius a_c to give the effective hard-sphere potential scattering radius R_c' [8]. Denoting $R' = R_c'$ for the s-wave channel, one obtains:

$$R' = a_0(1 - R_0^\infty). \qquad (10)$$

The imaginary part $\text{Im}[\mathcal{R}_c] = \pi s_c^{\text{loc}}$ modifies the absorption cross section and adds a contribution that is inversely proportional to the velocity.

In the uniform level approximation, where the amplitude $\gamma_{\eta n_c}^2$ are all equal and the levels η are uniformly spaced by an amount D_c, the average value of the reduced R-function R_c is:

$$\overline{R}_c \simeq \int_a^b \frac{s_c}{E' - z}\mathrm{d}E' + \frac{1}{\Delta E}\int_a^b R_c^\infty(E')\mathrm{d}E'$$
$$+ \frac{i\pi}{\Delta E}\int_a^b s_c^{\text{loc}}(E')\mathrm{d}E', \qquad (11)$$

with

$$z = E + i\frac{\Gamma_\gamma}{2}, \qquad (12)$$

in which Γ_γ represents the average radiation width. The first integral of Eq. (11) is called the Stieltjes transform of the pole strength function s_c, where s_c is a probability density function defined as the ratio of the average reduced width to level spacings:

$$s_c = \frac{\langle \gamma_{n_c}^2 \rangle}{D_c}. \qquad (13)$$

The method used by Thomas [3] for assigning a value to the Stieltjes transform of the pole strength function

relies on the Sokhotsky's formula. The latter state that:

$$\lim_{x\to 0} \frac{1}{x \mp i\varepsilon} = \mathcal{P}\left(\frac{1}{x}\right) \pm i\pi\delta(x), \qquad (14)$$

where $\delta(x)$ is the delta function and $\mathcal{P}$ is the Cauchy principal value of the inverse function $1/x$. According to the expression (11), we have $\varepsilon = \Gamma_\gamma/2$ and $x = E' - E$. The Sokhotsky's formula can be applied if Γ_γ is small. This condition is satisfied in the unresolved resonance range of many isotopes, such as actinides, for which the average radiation widths is lower than $50\,\text{meV}$. As a consequence, the identity (14) can be introduced in Eq. (11) to give:

$$\overline{R}_c \simeq i\pi s_c + \underbrace{\mathcal{P}\int_a^b \frac{s_c}{E' - E}\mathrm{d}E' + \frac{1}{\Delta E}\int_a^b R_c^\infty(E')\mathrm{d}E'}_{\overline{R}_c^\infty}$$
$$+ i\pi \underbrace{\frac{1}{\Delta E}\int_a^b s_c^{\text{loc}}(E')\mathrm{d}E'}_{\overline{s}_c^{\text{loc}}}. \qquad (15)$$

This mathematical trick allows to distinguish, without much complication, the "statistical R-function" $i\pi s_c$ and the background contribution $\overline{R}_c^\infty + i\pi\overline{s}_c^{\text{loc}}$:

$$\overline{R}_c \simeq \overline{R}_c^\infty + i\pi\left(s_c + \overline{s}_c^{\text{loc}}\right). \qquad (16)$$

In the framework of the average R-Matrix approximation, the parameter $\overline{R}_c^\infty$, the pole strength function s_c and the background term $\overline{s}_c^{\text{loc}}$ are free parameters. Prior values can be deduced from optical model parameters by using the SPRT method.

4. Average R-Matrix parameters

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. The standard SPRT method [9] was developed for s- and p-wave parameters ($l = 0, 1$). The method was generalized in order to provide pole strength functions and parameter $\overline{R}_c^\infty$ for higher order partial wave ($l \geq 1$) [10]. In practice, the analytically averaged collision matrix (3) can be equated to the optical model S-Matrix $\mathcal{S}_c$ expressed for further convenience through the diagonal C-matrix:

$$\mathcal{S}_c = 1 + 2iC_c. \qquad (17)$$

Thus, from Eqs. (3) and (17) one obtains the pole strength functions and distant level parameter $\overline{R}_c^\infty$:

$$P_c\overline{R}_c^\infty = \frac{2\alpha_c\cos[2\phi_c] + (1 - 2\beta_c)\sin[2\phi_c]}{1 + 2\theta_c^2 - 2\beta_c + (1 - 2\beta_c)\cos[2\phi_c] - 2\alpha_c\sin[2\phi_c]}, \qquad (18)$$

$$\pi P_c(s_c + \overline{s}_c^{\text{loc}}) =$$
$$\frac{2(\beta_c - \theta_c^2)}{1 + 2\theta_c^2 - 2\beta_c + (1 - 2\beta_c)\cos[2\phi_c] - 2\alpha_c\sin[2\phi_c]}. \qquad (19)$$

in which α_c, β_c and θ_c are free parameters. In the ground state channel, for target nucleus with $I = 0$, they represent

the real part, the imaginary part and the absolute value of C_c:

$$\begin{cases} \alpha_c = \mathrm{Re}[C_c] \\ \beta_c = \mathrm{Im}[C_c] \\ \theta_c = |C_c| \end{cases} \quad (20)$$

An explicit separation of the pole strength function s_c and of the background term $\overline{s}_c^{\mathrm{loc}}$ can be achieved by using the neutron transmission coefficients. By introducing Eq. (3) in Eq. (6), the neutron transmission coefficients can be written as follow:

$$\mathcal{T}_c = \frac{4\pi P_c(s_c + \overline{s}_c^{\mathrm{loc}})}{[1 + \pi P_c(s_c + \overline{s}_c^{\mathrm{loc}})]^2 + P_c^2 \overline{R}_c^{\infty^2}}. \quad (21)$$

The latter expression can be split in two contributions:

$$\mathcal{T}_c = \underbrace{\frac{4\pi P_c s_c}{[1 + \pi P_c(s_c + \overline{s}_c^{\mathrm{loc}})]^2 + P_c^2 \overline{R}_c^{\infty^2}}}_{T_c}$$

$$+ \underbrace{\frac{4\pi P_c \overline{s}_c^{\mathrm{loc}}}{[1 + \pi P_c(s_c + \overline{s}_c^{\mathrm{loc}})]^2 + P_c^2 \overline{R}_c^{\infty^2}}}_{T_{D_c}}. \quad (22)$$

For spherical or weakly deformed nuclei, the contribution of the direct reactions T_{D_c} disappears ($\overline{s}_c^{\mathrm{loc}} = 0$), and the expression of the neutron transmission coefficient becomes:

$$\mathcal{T}_c = T_c = \frac{4\pi P_c s_c}{(1 + \pi P_c s_c)^2 + P_c^2 \overline{R}_c^{\infty^2}} \quad (23)$$

By using the notation

$$f = \frac{1}{(1 + \pi P_c s_c)^2 + P_c^2 \overline{R}_c^{\infty^2}}, \quad (24)$$

the expression (23) can be rewritten as:

$$T_c = 4\pi P_c s_c f. \quad (25)$$

The latter result indicates that the neutron transmission coefficient and the penetration factor differ by a factor equal to $4\pi s_c f$. In Ref. [11], f was also introduced to account for the difference in reflexion between a diffuse-edge optical potential and its equivalent square-well. The latter study mainly suggests to replace the channel radius a_c involved in the R-Matrix formalism by an equivalent hard-sphere radius deduced from the phase shift originating from the potential.

5. Hard-sphere approximation

The channel radius is one of the boundary conditions introduced in the R-matrix and Optical Model reaction formalisms to match the solution of the Schrodinger equation with its corresponding expression valid outside the region of nuclear forces. Such an abrupt separation of the configuration space by an imaginary closed surface of radius a_c leads to the notions of "internal" and "external" regions [12]. The complex mean-field potential $V(r)$ vanishes in the external region. The size of the internal
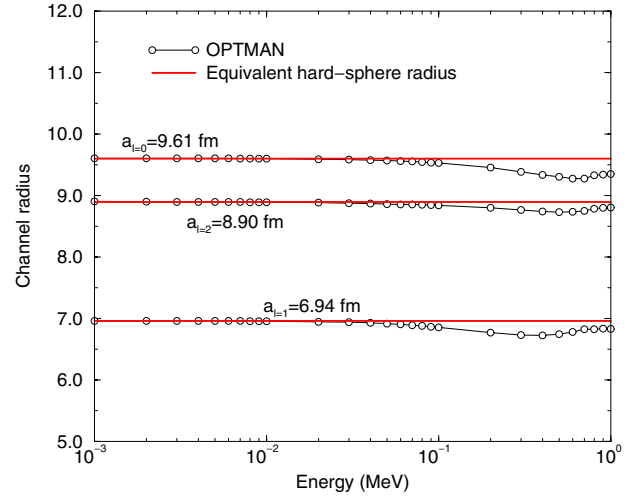

Figure 1. Channel radii for ^{238}U+n calculated with the OPTMAN code by using Eq. (26) with optical model parameters of Ref. [13].

region is not defined. Therefore, the channel radii are more or less chosen arbitrarily. In this work, this ambiguity is solved by choosing a_c such that the optical model and its equivalent square-well provide the same phase shifts at the common channel radii. The resonance theory determines the hard-sphere phase shifts ϕ_l from the precisely known radial wave functions at the channel radius a_c. Denoting $\rho = ka_c$, one obtains:

$$\begin{cases} \phi_0(\rho) = \rho, \\ \phi_1(\rho) = \rho - \tan^{-1}(\rho), \\ \phi_2(\rho) = \rho - \tan^{-1}\left(\frac{3\rho}{3-\rho^2}\right), \end{cases} \quad (26)$$

Figure 1 shows the channel radii calculated with Eq. (26) by using the phase shifts provided by the OPTMAN code with a set of optical model parameters recently established for the nuclear system ^{238}U+n [13]. A good agreement is observed with the equivalent hard-sphere radii up to 150 keV, which is a satifactory upper energy limit for the analysis of the Unresolved Resonance Range of the neutron cross sections.

Equations (18), (19) and (22) were implemented in the OPTMAN code for calculating the neutron strength functions and distant level parameters for $l = 0, 1, 2$. Results obtained for ^{238}U+n are reported in Fig. 2. They were obtained by using the same set of optical model parameters as used in Fig. 1 together with the equivalent hard-sphere radii $a_0 = 9.61$ fm, $a_1 = 6.94$ fm and $a_2 = 8.90$ fm. Similar calculations were repeated by replacing the l-dependent equivalent hard-sphere radii by a single channel radius calculated with the ENDF convention [14]:

$$a_c = 1.23\, A^{1/3} + 0.8\ (\text{in fm}). \quad (27)$$

For the nuclear system ^{238}U+n, the channel radius in the ENDF convention is $a_c = 8.42$ fm. In Fig. 2, we can observe that the distant levels parameters vanish ($\overline{R}_c^\infty \simeq 0$) when the equivalent hard sphere radii are used. Consequently, Eq. (10) indicates that the channel radius a_c becomes strictly equivalent to the potential scattering radius R'. As stated by Vogt in the 90s, the equivalent hard-sphere radius becomes the "natural" choice of a_c for each
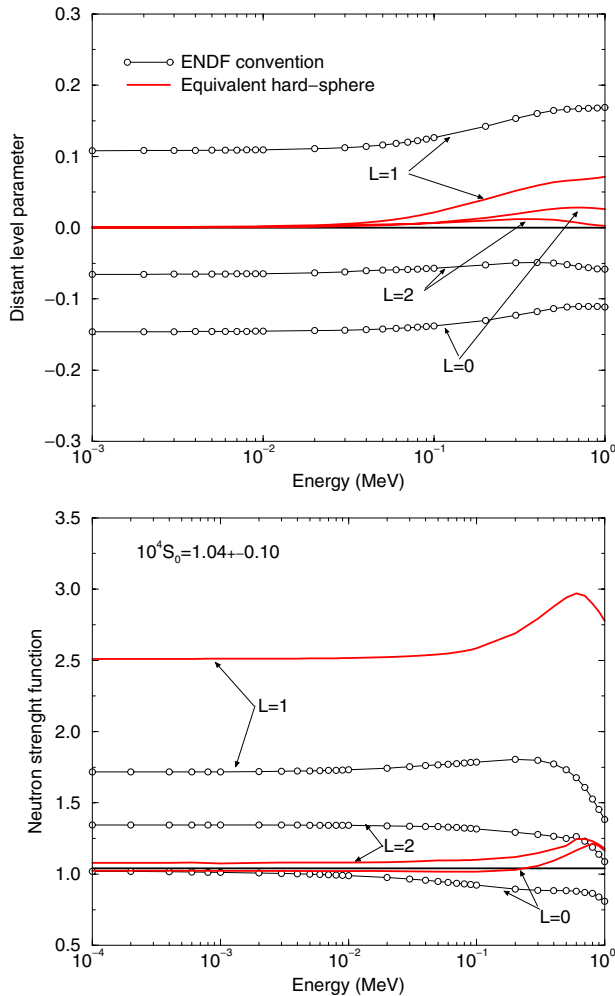
Figure 2. Distant level parameters and neutron strength functions for ^{238}U+n calculated with the OPTMAN code by using Eqs. (18), (19) and (22) with optical model parameters of Ref. [13]. The solid-dot lines were obtained with the channel radius calculated with Eq. (27), and the solid lines with the channel radii of Fig. 1.

reaction channel [15]. For s-wave channels, it represents the "effective" radius R' of the target at zero energy:

$$R' = a_{l=0} \tag{28}$$

The main conclusion of this work is that the SPRT method yields s-wave and d-wave neutron strength functions of similar magnitude and nearly independent of the neutron energy:

$$S_0 \simeq S_2 \simeq \text{cst},$$

if and only if the optical model and its equivalent square-well provide the same phase shifts at the common channel radii a_c. These results provide a mathematical framework for the "rule of thumb" often used by Fröhner and Bouland [16], which defines the behavior of the neutron strength functions for odd and even angular momentum l. For higher-order partial waves, this empirical rule says

that the strength functions for $l = 0, 2, 4, ...$ are similar, and those for $l = 1, 3, 5, ...$ are likewise similar.

6. Conclusions

Average R-Matrix parameters (neutron strength function and distant level parameter) were determined by focusing our analysis on the conspicuous role of the channel radius a_c. This parameter is one of the boundary condition introduced in the R-matrix theory assuming an abrupt division of the configuration space. The resonance theory has some undesirable features of the square-well potential for which a_c is chosen more or less arbitrarily. The use of equivalent hard sphere radii, deduced from phase shifts provided by optical model calculations, shows that the contribution of the distant level parameters vanishes in the average R-Matrix formalism. As a consequence, the effective radius R' and the channel radius a_0 for resonances having zero neutron orbital angular momentum ($l = 0$) are the same quantity. It must be emphasized that, for ^{238}U+n, this property leads to s- and d-wave neutron strength functions of similar magnitude ($S_0 \simeq S_2$). The OPTMAN results confirm that such low-energy neutron spectroscopic information could be a strong constraint in the optimization procedure of the optical model parameters.

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