NEW APPROXIMATIONS FOR THE INTERFERENCE TERM APPLIED TO THE CALCULATION OF SCATTERING CROSS SECTION OF THE ISOTOPES ^{238}U

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Abstract. *The calculation of the Doppler broadening function and the interference term are very importante in the generation of nuclear data. Recent papers have proposed analytical formulations for both functions and, despite their being simple and precise, they contain the error function with a complex argument. With the intention of simplyfying the mathematical treatment two approximations are proposed in this paper. The first one consists of using an expansion in the form of series to treat the error function. The other approximation are based on simplifications in the differential equations that govern the Doppler broadening function. For of validation, pourpose the result obtained is compared to the one obtained in the calculation of the cross sections for isotope ^{238}U for different resonances. Results obtained have proved satisfactory from the standpoint of accuracy.*

Keywords*: Doppler broadening function, Interference term, Neutron cross section, Frobenius method.*

1. INTRODUCTION

The movement of thermal agitation of the nuclei is adequately represented in the microscopic cross sections of neutron-nucleus interaction through the Doppler broadening function and of the term of interference function (Duderstadt & Hamilton, 1976). This function is calculated numerically in modern systems for the calculation of the macro-group constants, needed to determine the power distribution of a nuclear reactor.

In a thermal balance medium in a temperature T the speed of the target nuclei is distributed by the distribution function of Maxwell-Boltzmann (Pathria, 1972) and the expressions for the mean scattering cross sections is written, after the formalism of Briet-Wigner (Duderstadt & Hamilton, 1976), by:

$$\bar{\sigma}_s\left(E,T\right)=\sigma_0\frac{\Gamma_n}{\Gamma}\psi\left(x,\xi\right)+\sigma_0\frac{2R}{\lambda\!\!\!^{-}}\chi\left(x,\xi\right)+\sigma_{pot.},\tag{1}$$

where the Doppler broadening function and the term of interference are written, according to the Bethe and Plackzec approximations, respectively by:

$$\psi\left(x,\xi\right)=\frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{+\infty}\frac{dy}{1+y^2}\exp\left[-\frac{\xi^2}{4}\left(x-y\right)^2\right],\tag{2}$$

$$\chi\left(x,\xi\right)=\frac{\xi}{\sqrt{\pi}}\int_{-\infty}^{+\infty}\frac{ydy}{1+y^2}\exp\left[-\frac{\xi^2}{4}\left(x-y\right)^2\right],\tag{3}$$

being:

$$x=\frac{2\left(E-E_0\right)}{\Gamma}\tag{4}$$

$$\xi=\frac{\Gamma}{\left(4E_0kT/A\right)^{1/2}},\tag{5}$$

where all the other parameters are well established in the literature (Duderstadt & Hamilton, 1976).

The expression of the mean scattering cross section, Equation (1), uses the Doppler broadening function and the term of interference function in an explicit manner. In the generation of nuclear data the accurate calculations of these functions are necessary and executing them from numerical integration methods such as the Gauss-Legendre or trapezoidal method (Alvim, 2007) makes this task costly from the computing standpoint, due to the number of times these calculations are repeated in practical applications. Aiming at reversing this scenario, analytical formulations for both functions $\psi(x,\xi)$ and $\chi(x,\xi)$ were proposed. In the present paper, approximations in the form of these functions are presented.

2. FUNCTIONS $\psi(x,\xi)$ and $\chi(x,\xi)$ ACCORDING TO THE FROBENIUS METHOD

The Doppler broadening function, Equation (2), can be written by the solution of the differential equation (Palma et. al., 2006)

$$\frac{\partial^2\psi(x,\xi)}{\partial x^2}+x\xi^2\frac{\partial\psi(x,\xi)}{\partial x}+\frac{\xi^2}{4}\left(x^2\xi^2+\xi^2+2\right)\psi(x,\xi)=\frac{\xi^4}{4} \tag{6}$$

subject to the initial conditions:

$$\psi(x,\xi)|_{x=0}\equiv\psi_0=\frac{\xi\sqrt{\pi}}{2}\exp\left(\frac{\xi^2}{4}\right)\left[1-erf\left(\frac{\xi}{2}\right)\right] \tag{7.a}$$

and

$$\frac{\partial\psi(x,\xi)}{\partial x}|_{x=0}=0. \tag{7.b}$$

The term of interference function, Equation (3), is the solution of the differential equation (Palma et. al., 2007)

$$\frac{d^2\chi(x,\xi)}{dx^2}+\xi^2x\frac{d\chi(x,\xi)}{dx}+\frac{\xi^2}{4}\left[\xi^2x^2+\xi^2+2\right]\chi(x,\xi)=\frac{\xi^4x}{2}, \tag{8}$$

subjected to the initial conditions:

$$\chi(x,\xi)|_{x=0}=\frac{\xi}{\sqrt{\pi}}\int_{-\infty}^{+\infty}\frac{ydy}{1+y^2}\exp\left(-\frac{\xi^2y^2}{4}\right)=0 \tag{9.a}$$

and

$$\frac{\partial\chi(x,\xi)}{\partial x}|_{x=0}=\xi^2\left\{1-\frac{\xi\sqrt{\pi}}{2}\exp\left(\frac{\xi^2}{4}\right)\left[1-erf\left(\frac{\xi}{2}\right)\right]\right\} \tag{9.b}$$

Equations (6) and (8) present identical homogeneous parts. The linearly independent solutions of this homogeneous equation can be obtained from the Frobenius Method (Arfken, 2007), being written by

$$\begin{Bmatrix}\psi_1\\ \chi_1\end{Bmatrix}(x,\xi)=\exp\left(-\frac{\xi^2x^2}{4}\right)\cos\left(\frac{\xi^2x}{2}\right) \tag{10.a}$$

and

$$\left\{\begin{matrix}\psi_2\\ \chi_2\end{matrix}\right\}(x,\xi)=\exp\left(-\frac{\xi^2x^2}{4}\right)\sin\left(\frac{\xi^2x}{2}\right) \tag{10.b}$$

Having obtained the linearly independent solutions expressed by Equations (10.a) and (10.b) it is possible to apply the parameter variation method to determine the respective particular solutions for the equations that govern the functions $\psi(x,\xi)$ and $\chi(x,\xi)$. After the imposition of the initial conditions it possible to obtain the following expressions for functions $\psi(x,\xi)$ and $\chi(x,\xi)$:

$$\psi(x,\xi)=\frac{\xi\sqrt{\pi}}{2}\exp\left[-\frac{1}{4}\xi^2\left(x^2-1\right)\right]\cos\left(\frac{\xi^2x}{2}\right)\left\{1+\operatorname{Re}E(x,\xi)+\tan\left(\frac{\xi^2x}{2}\right)\operatorname{Im}E(x,\xi)\right\} \tag{11}$$

$$\chi(x,\xi)=\xi\sqrt{\pi}\cos\left(\frac{\xi^2x}{2}\right)\exp\left[-\frac{\xi^2}{4}\left(x^2-1\right)\right]\left\{\operatorname{Im}E(x,\xi)-\tan\left(\frac{\xi^2x}{2}\right)\left(\operatorname{Re}E(x,\xi)+1\right)\right\}, \tag{12}$$

where $E(x,\xi)=erf\left(\frac{i\xi x-\xi}{2}\right)$. From Equations (11) and (12) it is possible to write the following expression for the mean scattering cross section (Fraga et. al., 2007)

$$\begin{aligned}\sigma_s(E)=\sigma_0\frac{\xi\sqrt{\pi}}{2}\cos\left(\frac{\xi^2x}{2}\right)\exp\left[-\frac{\xi^2}{4}\left(x^2-1\right)\right]\Bigg\{\frac{\Gamma_n}{\Gamma}\left[1+\operatorname{Re}E(x,\xi)+\tan\left(\frac{\xi^2x}{2}\right)\operatorname{Im}E(x,\xi)\right]\\ +\frac{4R}{\lambda_0}\left[\operatorname{Im}E(x,\xi)-\tan\left(\frac{\xi^2x}{2}\right)\left(\operatorname{Re}E(x,\xi)+1\right)\right]\Bigg\}+\sigma_{pot.},\end{aligned} \tag{13}$$

where σ_{pot} denote the potential scattering.

3. ANALYTICAL APPROXIMATIONS

3.1 Approximation 1: approximation in the equation that governs function $\chi(x,\xi)$

The first approximation proposed in the present paper consists of disregarding ξ^2 in the face of term ξ^2x^2+2 directly in Equation (8). Thus being, the approximated term of interference function should be solution of the equation:

$$\frac{d^2\chi_{Ap}(x,\xi)}{dx^2}+\xi^2x\frac{d\chi_{Ap}(x,\xi)}{dx}+\frac{\xi^2}{4}\left[\xi^2x^2+2\right]\chi_{Ap}(x,\xi)=\frac{\xi^4x}{2}, \tag{14}$$

subjected to the initial conditions expressed in Equations (9.a) and (9.b). By solving equation (14) in a manner similar to that presented in the previous section, it is possible to obtain the following approximation for function $\chi(x,\xi)$

$$\chi_{ap}(x,\xi)\cong-\frac{x\xi^3\sqrt{\pi}}{2}\exp\left[-\frac{1}{4}\xi^2\left(x^2+1\right)\right]\left[1-erf\left(\frac{\xi}{2}\right)\right]-i\xi\sqrt{\pi}\exp\left(-\frac{1}{4}\xi^2x^2\right)\left[erf\left(\frac{i\xi x}{2}\right)\right]. \tag{15}$$

The error function with a pure imaginary argument presents purely imaginary results. Thus, it is easy to verify that Equation (15) provides real approximations for the calculation of function $\chi(x,\xi)$. The results obtained from Equation (15) in the calculation of the scattering cross sections will be reported in the results section.

3.2 Approximation 2: approximation in the form of series of function $E(x,\xi)$

The error function with complex argument can be expanded in infinite series (Zukeran, 2004)

$$E(x,\xi) = erf\left(\frac{i\xi x - \xi}{2}\right) = E_{\mathrm{Re.}} + E_{\mathrm{Im.}} i, \tag{16}$$

where:

$$E_{\mathrm{Re.}} \cong -erf\left(\frac{\xi}{2}\right) + \exp\left(-\frac{\xi^2}{4}\right)\left\{\frac{1}{\pi\xi}\left[\cos\left(\frac{\xi^2 x}{2}\right) - 1\right] + \frac{2}{\pi}\sum_{n=1}^{n\max}\frac{\exp(-n^2/4)}{n^2+\xi^2} f_n(x,\xi)\right\}, \tag{17}$$

$$E_{\mathrm{Im.}} \cong \exp\left(-\frac{\xi^2}{4}\right)\left\{\frac{1}{\pi\xi}\sin\left(\frac{\xi^2 x}{2}\right) + \frac{2}{\pi}\sum_{n=1}^{n\max}\frac{\exp(-n^2/4)}{n^2+\xi^2} g_n(x,\xi)\right\}, \tag{18}$$

with the auxiliary functions being $f_n(x,\xi)$ and $g_n(x,\xi)$ written by:

$$f_n(x,\xi) = -\xi + \xi\cosh\left(\frac{n\xi x}{2}\right)\cos\left(\frac{\xi^2 x}{2}\right) - n\sinh\left(\frac{n\xi x}{2}\right)\sin\left(\frac{\xi^2 x}{2}\right), \tag{19}$$

$$g_n(x,\xi) = \xi\cosh\left(\frac{n\xi x}{2}\right)\sin\left(\frac{\xi^2 x}{2}\right) + n\sinh\left(\frac{n\xi x}{2}\right)\cos\left(\frac{\xi^2 x}{2}\right). \tag{20}$$

By replacing Equations (17) and (18) in Equation (13) it is possible to approximate the expression of the mean scattering cross section from expression

$$\begin{aligned}\sigma_s(E) = \sigma_{pot.} + \sigma_0\frac{\xi\sqrt{\pi}}{2}\cos\left(\frac{\xi^2 x}{2}\right)\exp\left[-\frac{\xi^2}{4}(x^2-1)\right]\left\{\frac{\Gamma_n}{\Gamma}\left[1 + E_{\mathrm{Re.}} + \tan\left(\frac{\xi^2 x}{2}\right)E_{\mathrm{Im.}}\right]\right.\\ \left.+\frac{4R}{\lambda_0}\left[E_{\mathrm{Im.}} - \tan\left(\frac{\xi^2 x}{2}\right)(E_{\mathrm{Re.}}+1)\right]\right\},\end{aligned} \tag{21}$$

In the present paper Nmax=20 and $\sigma_{pot.} = 10$ barn were used. The results obtained with this approximation will be presented in the next section.

4. RESULTS

This section presents the results obtained through the use of the methods proposed in the present paper in the calculation of the term of interference function and of the scattering cross sections for different resonances. Table 1 shows the percentage deviations in relation to the reference values of the term of interference function calculated from Equation (15). As a reference in the calculation of function $\chi(x,\xi)$ the values contained in tables found in the literature (Duderstadt & Hamilton, 1976) are considered.

Table 1. Percentage deviations in relation to the reference values in the calculation of $\chi(x,\xi)$ from Equation (15).

x/ξ	**0.10**	**0.20**	**0.30**	**0.40**	**0.50**
5	5.5x10^{-2}	4.9x10^{-1}	1.7x10^{0}	3.7x10^{0}	6.0x10^{0}
10	8.1x10^{-2}	7.3x10^{-1}	1.9x10^{0}	2.4x10^{0}	2.0x10^{0}
15	1.2x10^{-1}	8.1x10^{-1}	1.0x10^{1}	6.9x10^{-1}	5.5x10^{-1}
20	1.6x10^{-1}	6.0x10^{-1}	3.9x10^{-1}	3.0x10^{-1}	2.8x10^{-1}
30	1.9x10^{-1}	1.7x10^{-1}	1.3x10^{-1}	1.2x10^{-1}	1.2x10^{-1}
40	1.5x10^{-1}	7.6x10^{-2}	6.7x10^{-2}	6.5x10^{-2}	6.4x10^{-2}
50	8.3x10^{-2}	4.5 x10^{-2}	4.2x10^{-2}	4.1x10^{-2}	4.1x10^{-2}

From the data shown in Table 1 it is possible to conclude that the approximation proposed for the calculation of the function of the term of interference presents good results to describe the neutron-nucleus interaction for neutrons with incident energy not too close to resonance energy, that is, for large values for parameter x.

Table 2 shows the percentage deviations in relation to the reference values of the term of interference function calculated from Equation (16)

Table 2. Percentage deviations in relation to the reference values in the calculation of $\chi(x,\xi)$ from series approximation of function $E(x,\xi)$.

x/ξ	**0.10**	**0.20**	**0.30**	**0.40**	**0.50**
5	3.8x10^{-4}	7.2x10^{-4}	9.8x10^{-3}	5.9x10^{-3}	3.3x10^{-3}
10	1.8x10^{-3}	8.1x10^{-5}	8.6x10^{-3}	4.9x10^{-4}	8.9x10^{-3}
15	4.4x10^{-4}	6.2x10^{-4}	1.3x10^{-3}	2.9x10^{-2}	1.4x10^{-3}
20	8.6x10^{-4}	1.9x10^{-5}	1.9x10^{-3}	1.9x10^{-3}	2.0x10^{-3}
30	2.2x10^{-3}	2.8x10^{-3}	2.9x10^{-3}	4.1x10^{-2}	4.2x10^{-2}
40	7.9x10^{-4}	3.9x10^{-3}	3.9x10^{-3}	3.9x10^{-2}	4.0x10^{-3}
50	4.2x10^{-3}	9.8x10^{-3}	4.0x10^{-2}	1.5x10^{-3}	5.0x10^{-2}

Table 3 shows the nuclear parameters used to validate the approximation proposed in this article using isotope ^{238}U.

Table 3. Nuclear parameters related to the calculation of the cross sections at 1500K. Source: JENDL – 3.2.

Elemento	$E_0(eV)$	$\Gamma_n(eV)$	$\Gamma_\gamma(eV)$	ξ	$\lambda_0(m)$	$\sigma_0(b)$
^{238}U	6.67	0.0015	0.0230	0.20	177.14	2.4 . 10^{4}
	66.03	0.0246	0.0234	0.13	56.30	2.0 . 10^{4}

From this data the graphs shown in Figures 1 and 2 were constructed, containing the scattering cross sections calculated from two approximations proposed in the present article, Equations (15) and (16), taking as reference the numerical method in the calculation of functions $\psi(x,\xi)$ and $\chi(x,\xi)$.

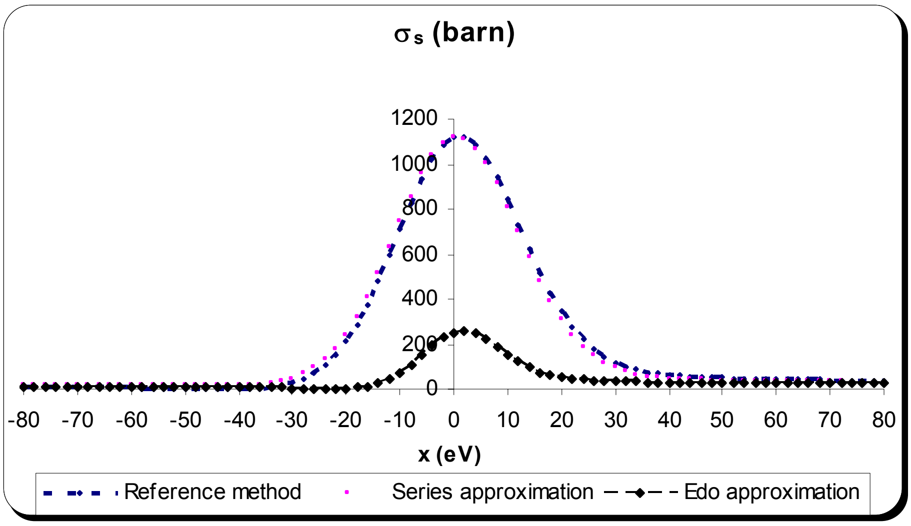

Figure 1. Mean scattering cross sections for resonance E_0 = 6.67eV of isotope ^{238}U at 1500K

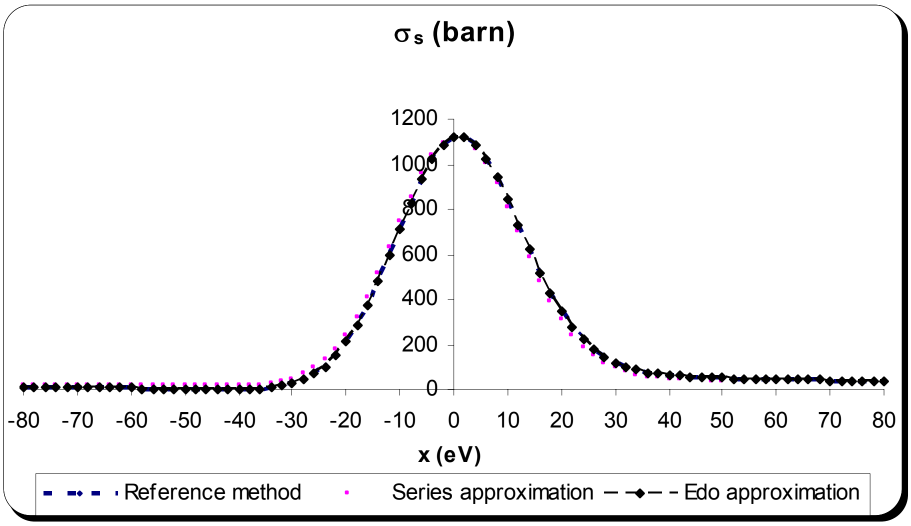

Figure 2. Mean scattering cross sections for resonance E_0 = 66.03eV of isotope ^{238}U at 1500K.

From the graphs contained in Figures (1) and (2) it is possible to see that the series approximation presents good results for the calculation of the term of interference function without distinction as to the absorbing or scattering character of the resonance. However, the same does not occur for the approximation based on the simplification of the differential equation that governs function $\chi(x,\xi)$.

5. CONCLUSIONS

Two approximations were proposed in this paper for the calculation of the term of interference function. Both the approximation based on the simplification of the differential equation that governs function $\chi(x,\xi)$, Equation (15), as the expansion in series of functions $E(x,\xi)$ presented small percentage deviations in relation to the values found in the literature. As a practical application, scattering cross sections of the isotope ^{238}U were calculated from approximations proposed in this work for low-energy resonances typical PWR reactor temperature. The graphs constructed demonstrate the advantage in the use of the series approximation for not distinguishing the type of resonance to be studied. The calculation of function $\chi(x,\xi)$ according to Equation (15) presents limitations related to the absorbing or scattering character of the resonance under study. For resonances with a predominantly scattering character Equation (15) presents accurate results, including the surroundings of the resonance, something that does not happen for predominantly absorbing resonances.

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