

An Approximation for the Doppler Broadening Function and Interference Term Using Fourier Series

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ABSTRACT

The calculation of the Doppler broadening function $\psi(x, \xi)$ and of the interference term $\chi(x, \xi)$ are important in the generation of nuclear data. In a recent paper, Goncalves and Martinez proposed an analytical approximation for the calculation of both functions based in sine and cosine Fourier transforms. This paper presents new approximations for these functions, $\psi(x, \xi)$ and $\chi(x, \xi)$, using expansions in Fourier series, generating expressions that are simple, fast and precise. Numerical tests applied to the calculation of scattering average cross section provided satisfactory accuracy.

Keywords: Doppler Broadening Function; Fourier Series; New Formulation for the Interference

1. Introduction

The phenomenon of thermal motion of the nuclei inside a nuclear reactor is well represented by the microscopic cross section of the neutron-nucleus interaction through the effect Doppler broadening. The precise determination of the Doppler broadening function and interference term are important for the calculation of the resonance integrals [1,2], self-shielding factors and for corrections of the measurements of the microscopic cross sections with the use of the activation technique [3].

The evaluation of the Doppler broadening function $\psi(x, \xi)$ and of the interference term $\chi(x, \xi)$ have a great importance in the generation of nuclear data and there are several methods for the calculation of both functions. This paper presents a new approximation for interference term applied to the calculation scattering average cross section [4] using expansions in Fourier series. The results have shown satisfactory accuracy and do not depend on the type of resonance considered. In thermally balanced medium at temperature T the velocity of the target nucleus is distributed by the Maxwell-Boltzmann distribution [5] and the expression for the average scattering cross sections is written, using to the one level formalism of Briet-Wigner, as:

$$\bar{\sigma}_s(E, T) = \sigma_0 \frac{\Gamma_n}{\Gamma} \psi(x, \xi) + \sigma_0 \frac{R}{\lambda} \chi(x, \xi) + \sigma_{pot} \quad (1)$$

where, the interference term and the Doppler broadening function are written, according with approximations pro-

posed by Goncalves *et al.* [6], by:

$$\chi(x, \xi) = 2 \int_0^{\infty} e^{-\frac{w^2}{\xi^2} - w} \sin(wx) dw \quad (2)$$

$$\psi(x, \xi) = \int_0^{\infty} e^{-\frac{w^2}{\xi^2} - w} \cos(wx) dw \quad (3)$$

The Equations (2) and (3) can be interpreted as sine and cosine Fourier transforms.

2. Mathematical Formulation

The integrals expressed by Equations (2) and (3) it is possible to find new representations for functions $\psi(x, \xi)$ and $\chi(x, \xi)$ using the Fourier series technique. In order to turn its use easily, Equations (2) and (3) can be re-written as:

$$\begin{cases} \psi \\ \chi \end{cases} (x, \xi) = \int_0^{\infty} G(w) e^{-w} \begin{cases} \cos(wx) \\ 2 \sin(wx) \end{cases} dw \quad (4)$$

where, $G(w) = e^{-\frac{w^2}{\xi^2}}$.

Analyzing the function $G(w)$ can be observed that it is a continuous and even function, which ensures it has a Fourier series representation. Thus, its Fourier series representation is given by:

$$G(w) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi w}{L}\right) \quad (5)$$

where

$$a_0 = \frac{\xi\sqrt{\pi}}{L} \operatorname{erf}\left(\frac{L}{\xi}\right) \tag{6}$$

$$a_n = \frac{\xi\sqrt{\pi}}{2L} e^{-\left(\frac{n\pi\xi}{2L}\right)^2} \operatorname{erf}\left(\frac{2L+n\pi\xi^2 i}{2\xi L}\right) + \frac{\xi\sqrt{\pi}}{2L} e^{-\left(\frac{n\pi\xi}{2L}\right)^2} \operatorname{erf}\left(\frac{2L-n\pi\xi^2 i}{2\xi L}\right) \tag{7}$$

Replacing the Equation (5) in the Equation (4) and applying the properties of the error functions with an imaginary argument [7], one can write the following expression for the functions $\psi(x, \xi)$ and $\chi(x, \xi)$:

$$\psi_{\text{Fourier}}(x, \xi) = \frac{\xi\sqrt{\pi}}{2L(1+x^2)} \operatorname{erf}\left(\frac{L}{\xi}\right) + \frac{\xi\sqrt{\pi}}{L} \sum_{n=1}^{\infty} F_n(x, \xi, L) \operatorname{Re}[Z(\xi, L)] \tag{8}$$

$$\chi_{\text{Fourier}}(x, \xi) = \frac{\xi\sqrt{\pi}}{L(1+x^2)} \operatorname{erf}\left(\frac{L}{\xi}\right) + \frac{2\xi\sqrt{\pi}}{L} \sum_{n=1}^{\infty} f_n(x, \xi, L) \operatorname{Re}[Z(\xi, L)] \tag{9}$$

where,

$$F_n(x, \xi, L) = \frac{\left[(n\pi)^2 + L^2(1+x^2)\right] e^{-\left(\frac{n\pi\xi}{2L}\right)^2}}{L^2(1+x^2)^2 + (n\pi)^2(2-2x^2 + (n\pi/L)^2)} \tag{10}$$

$$f_n(x, \xi, L) = \frac{x\left[L^2(1+x^2) - (n\pi)^2\right] e^{-\left(\frac{n\pi\xi}{2L}\right)^2}}{L^2(1+x^2)^2 + (n\pi)^2(2-2x^2 + (n\pi/L)^2)} \tag{11}$$

$$Z(n, \xi, L) = \operatorname{erf}\left(\frac{n\pi\xi^2 i + 2L^2}{2\xi L}\right) \tag{12}$$

Replacing Equations (8) and (9) in Equation (1) one obtains the following expression for the average scattering cross section:

$$\begin{aligned} \bar{\sigma}_s(E, T) = & \frac{\sigma_0 \xi \sqrt{\pi}}{2L(1+x^2)} \operatorname{erf}\left(\frac{L}{\xi}\right) \left(\frac{\Gamma_n}{\Gamma} + \frac{4Rx}{\lambda}\right) + \\ & + \frac{\sigma_0 \xi \sqrt{\pi}}{L} \left\{ \frac{\Gamma_n}{\Gamma} \sum_{n=1}^{N_{\max}} F_n(x, \xi, L) \operatorname{Re}[Z(n, \xi, L)] + \sigma_{\text{pot}} \right. \\ & \left. + \frac{4R}{\lambda} \sum_{n=1}^{N_{\max}} f_n(x, \xi, L) \operatorname{Re}[Z(n, \xi, L)] \right\} + \sigma_{\text{pot}} \end{aligned} \tag{13}$$

3. Numerical Test

This section contains the results obtained with Equations

(8) and (9) for the calculation interference term and of the Doppler broadening function with $L = \pi$ and $N_{\max} = 50$. In order to validate the obtained expression in this paper for $\chi(x, \xi)$ and $\psi(x, \xi)$, a systematic comparison was carried out with the comparison between the method presented in this paper and the 4-pole Padé approximation method, whose functional form is:

$$\psi_{\text{Padé}}(\xi, x) = \frac{a_0 + a_2(hx)^2 + a_4(hx)^4 + a_6(hx)^6}{b_0 + b_2(hx)^2 + b_4(hx)^4 + b_6(hx)^6 + b_8(hx)^8} \tag{14}$$

$$\chi_{\text{Padé}}(\xi, x) = \frac{2h(a_1(hx) + a_3(hx)^3 + a_5(hx)^5 + a_7(hx)^7)}{b_0 + b_2(hx)^2 + b_4(hx)^4 + b_6(hx)^6 + b_8(hx)^8} \tag{15}$$

The coefficients in Equations (14) and (15) are given by [8,9].

Figures 1 to 8 show the relative errors for the calculation of $\psi(x, \xi)$ and $\chi(x, \xi)$, using the proposed method paper, Equations (8) and (9), and the 4-pole Padé method, Equations (14) and (15), considering the benchmark results from Gauss-Legendre quadrature method that is well described in the literature [10].

From the Figures 1 and 2 is possible to see that when the variable ξ increases, keeping the variable x constant, the relative deviations of the Padé approximation increases and are systematically higher than those of the proposed method, Equation (8), in the calculation of the function $\psi(x, \xi)$.

From the Figures 3 and 4 it is possible to see that when the variable x increases, keeping the variable ξ constant, the relative deviations of the Padé approximation increases and are systematically higher than those of the proposed method, Equation (8), in the calculation of the function $\psi(x, \xi)$.

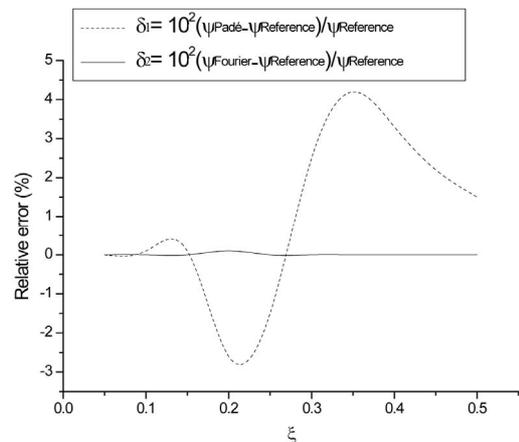


Figure 1. Relative error for the 4-pole Padé approximation, Equation (14), and for the proposed method, Equation (8), for $x = 20$.

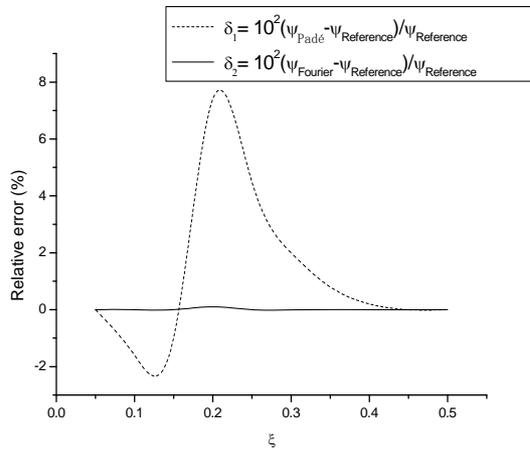


Figure 2. Relative error for the 4-pole Padé approximation, Equation (14), and for the proposed method, Equation (8), for $x = 35$.

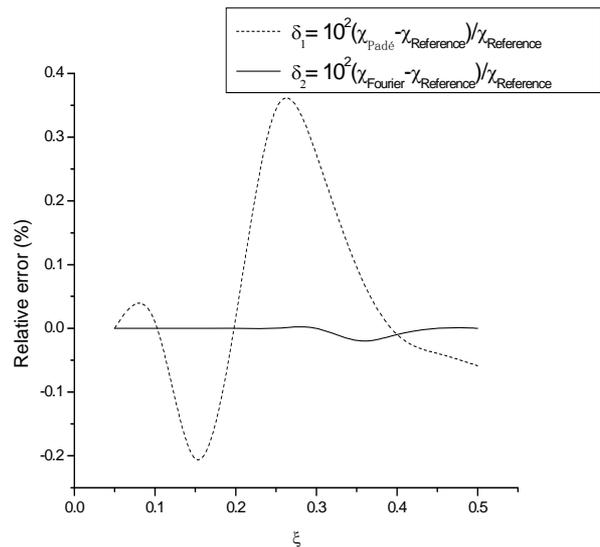


Figure 5. Relative error for the 4-pole Padé approximation, Equation (15), and for the proposed method, Equation (9), for $x = 20$.

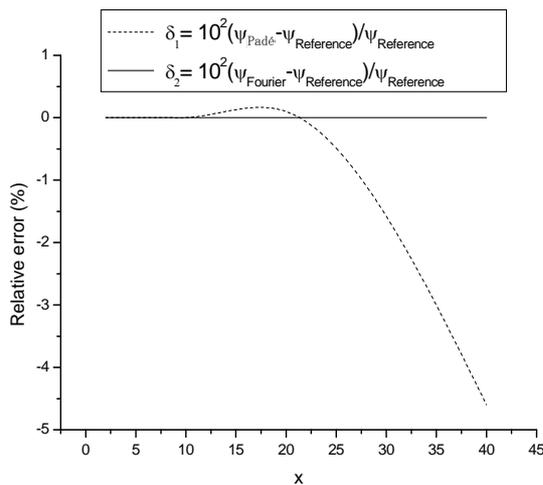


Figure 3. Relative error for the 4-pole Padé approximation, Equation (14), and for the proposed method, Equation (8), for $\xi = 0.10$.

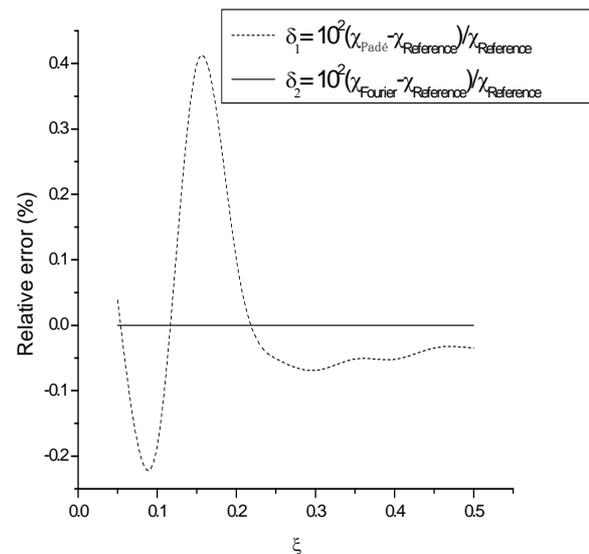


Figure 6. Relative error for the 4-pole Padé approximation, Equation (15), and for the proposed method, Equation (9), for $x = 35$.

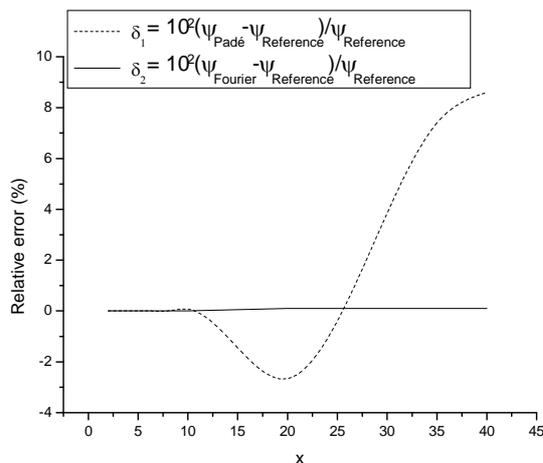


Figure 4. Relative error for the 4-pole Padé approximation, Equation (14), and for the proposed method, Equation (8), for $\xi = 0.20$.

From the Figures 5 and 6 it is possible to see that when the variable ξ increases, keeping the variable x constant, the relative deviations of the Padé approximation increases and are systematically higher than those of the proposed method, Equation (8), in the calculation of the function $\chi(x, \xi)$.

From the Figures 7 and 8 it is possible to see that when the variable x increases, keeping the variable ξ constant, the relative deviations of the Padé approximation increases and are systematically higher than those of the proposed method, Equation (8), in the calculation of the function $\chi(x, \xi)$.

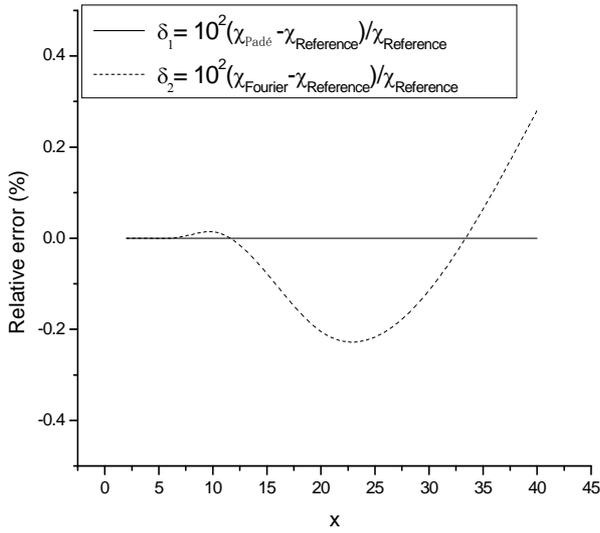


Figure 7. Relative error for the 4-pole Padé approximation, Equation (15), and for the proposed method, Equation (9), for $\xi = 0.15$.

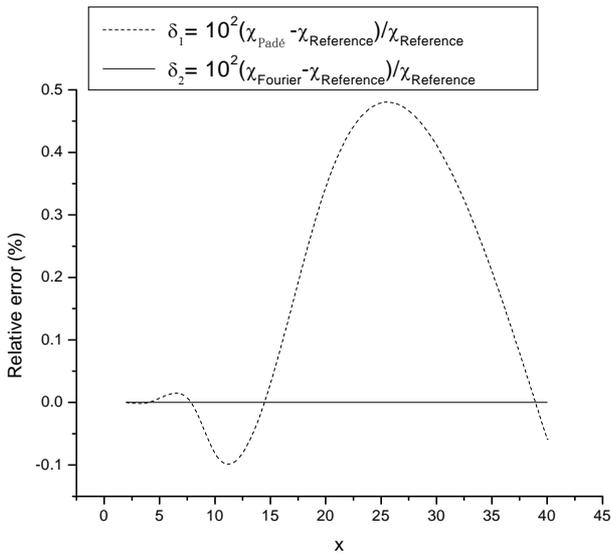


Figure 8. Relative error for the 4-pole Padé approximation, Equation (15), and for the proposed method, Equation (9), for $\xi = 0.25$.

The analysis of the results showed in **Figures 1-8** lead to the conclusion that the proposed method proved to be very precise and stable, having a 0.1% maximum relative error margin, when compared to reference values. From these results is possible to apply the approximate formalism presented in this paper in the calculation of the Doppler broadening function $\psi(x, \xi)$ and the Interference Term $\chi(x, \xi)$ in the determination of the microscopic average scattering cross sections.

4. Results

The average scattering cross section obtained from Equa-

tion (13) are found in **Figures 9-11** and **Figures 12-14** they shows their relative errors for the calculation of the average scattering cross section. The nuclear parameters used can be found in **Table 1** [2].

From the **Figures 9-11** it is possible to see that the results obtained with the method presented, Equation (13), overlapped those obtained from the numerical reference method, being compatible with the results obtained with the method proposed by Padé.

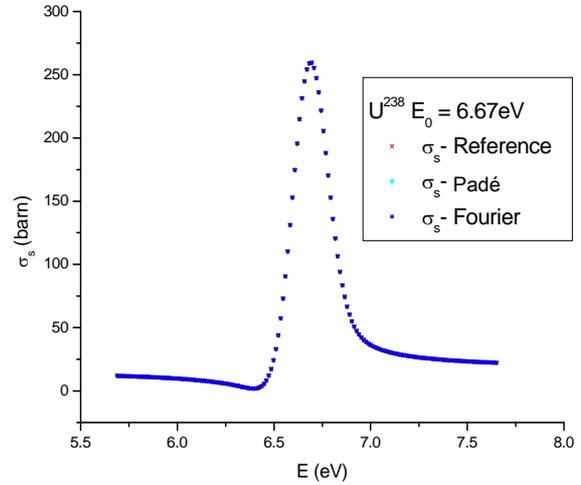


Figure 9. Average scattering cross sections of the $E_0 = 6.67$ eV resonance for the ^{238}U isotope and $T = 1500$ K.

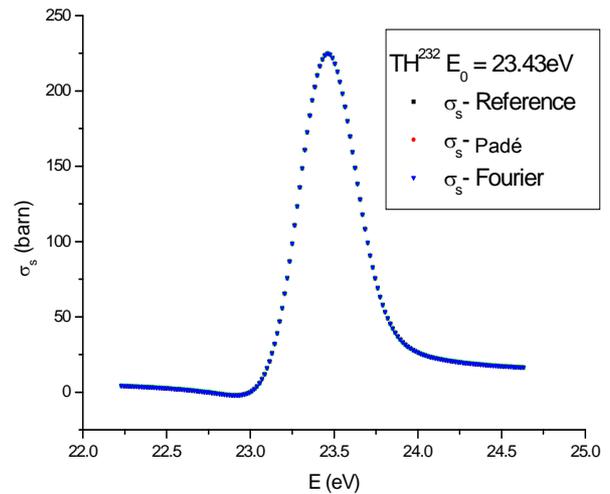


Figure 10. Average scattering cross sections of the $E_0 = 23.43$ eV resonance for the ^{232}Th isotope and $T = 1500$ K.

Table 1. Parameter used in the calculation of for average scattering cross sections for the ^{238}U , ^{232}Th and ^{240}Pu isotope, $\sigma = 10$ barn and $T = 1500$ K.

Isotope	E_0 (eV)	Γ_n (eV)	Γ_γ (eV)	ξ	λ_0 (m)	σ_0 (b)
^{238}U	6.67	0.0015	0.0230	0.20	177.14	2.4×10^4
^{232}Th	23.43	0.0039	0.0261	0.13	94.51	1.5×10^4
^{240}Pu	20.45	0.0027	0.0322	0.17	101.16	1.0×10^4

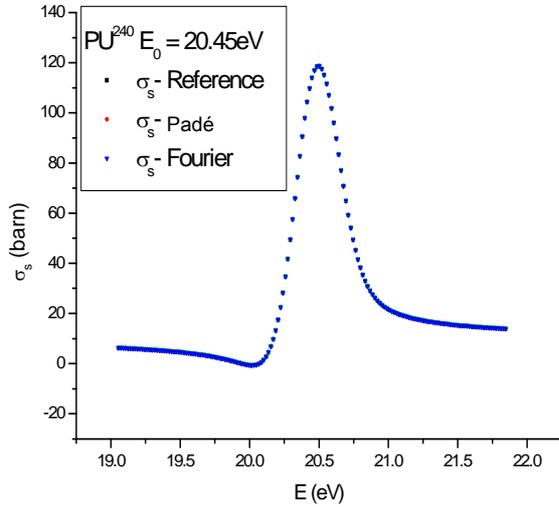


Figure 11. Average scattering cross sections of the $E_0 = 20.45$ eV resonance for the ^{240}Pu isotope and $T = 1500$ K.

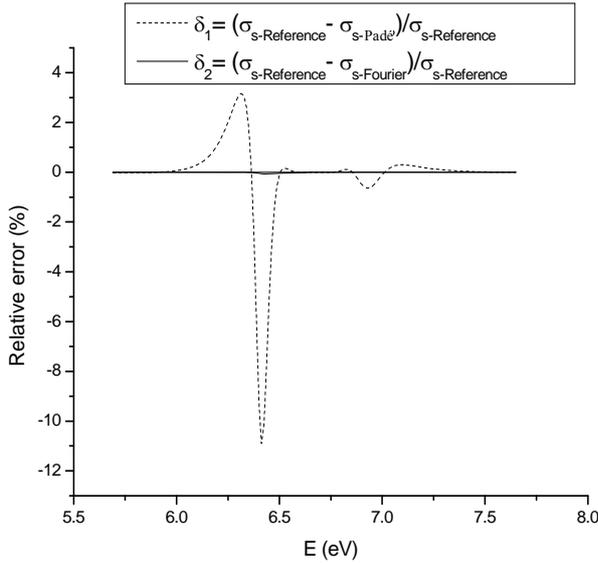


Figure 12. Relative error for average scattering cross sections of the $E_0 = 6.67$ eV resonance for the ^{238}U isotope and $T = 1500$ K.

From the **Figures 12 to 14** it is possible to conclude that the expression proposed in this paper presents results that overlap the numerical reference method.

5. Conclusion

This paper presents a simple and precise formulation for the Doppler broadening function $\psi(x, \xi)$ and of the interference term $\chi(x, \xi)$ based in sine and cosine Fourier transforms proposed by Goncalves *et al.* Expanding the function $G(w)$ in Fourier Series was possible to obtain an accurate analytical expression for the average scattering cross section, Equation (13), that can be an alternative to other methods existing in the literature.

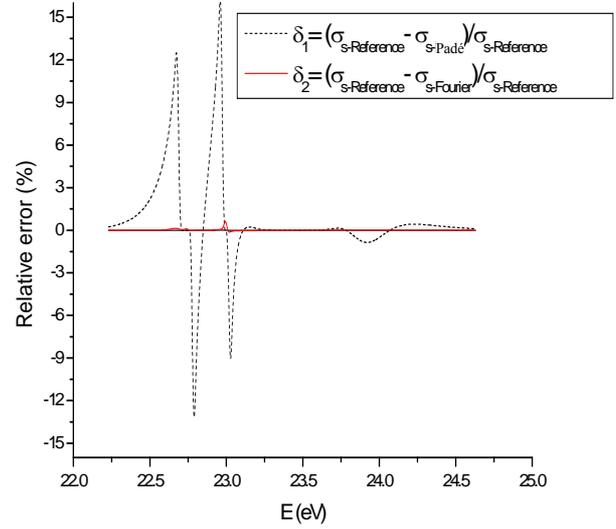


Figure 13. Relative error for average scattering cross sections of the $E_0 = 23.43$ eV resonance for the ^{232}Th isotope and $T = 1500$ K.

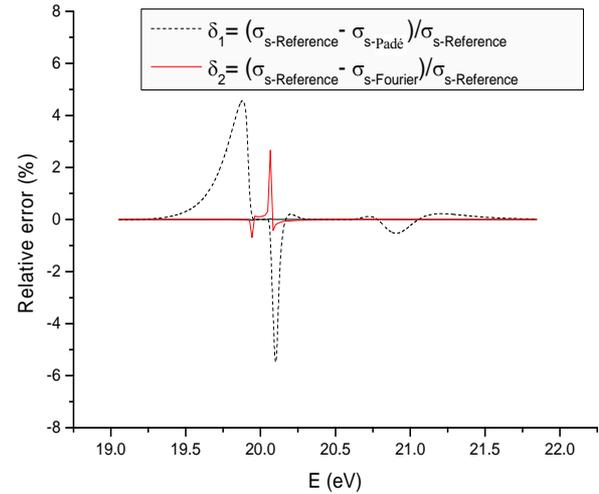


Figure 14. Relative error for average scattering cross sections of the $E_0 = 20.45$ eV resonance for the ^{240}Pu isotope and $T = 1500$ K.

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