LAGRANGE POLYNOMIAL INTERPOLATION METHOD APPLIED IN THE CALCULATION OF THE $J(\xi,\beta)$ FUNCTION

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Abstract. *The explicit dependence of the Doppler broadening function creates difficulties in the obtaining an analytical expression for J function . The objective of this paper is to present a method for the quick and accurate calculation of J function based on the recent advances in the calculation of the Doppler broadening function and on a systematic analysis of its integrand. The methodology proposed, of a semi-analytical nature, uses the Lagrange polynomial interpolation method and the Frobenius formulation in the calculation of Doppler broadening function . The results have proven satisfactory from the standpoint of accuracy and processing time.*

Keywords: *Doppler broadening function, Lagrange interpolation method, Frobenius method.*

1. INTRODUCTION

In the analysis of a nuclear reactor it is possible to find that the calculation of resonant absorption rates is not to be taken lightly. In order to determine reaction rates in a structure with few energy groups one needs to determine with precision the neutron flux in the regions where the absorbing isotopes are to be found. One way to calculate the neutrons flux is through approximations based on resonance integrals. These integrals are defined in a way that, when multiplied by the asymptotic flux to the resonance, they should produce the reaction rate inside it. Another important factor is that the movement of the nuclei should be taken into account in these calculations, which is accomplished by considering the Doppler broadening factor of the resonances (Duderstadt & Hamilton, 1976). Thus, in taking into account the thermal agitation movement of the nuclei in the reactor, the resonance integral is proportional to function $J(\xi , \beta)$, as defined by Dresner (1960):

$$J(\xi , \beta)=\int_0^{\infty} \frac{\psi(x,\xi)}{\psi(x,\xi)+\beta}dx, \tag{1}$$

where the Doppler broadening function $\psi(x,\xi)$ is written, according to the approximations of Bethe and Plackzec (Bethe & P1aczek, 1937) as:

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

being:

$$x=\frac{2(E-E_0)}{\Gamma} \tag{3}$$

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

All of the other parameters are well founded on literature (Duderstadt & Hamilton, 1976).

Function $J(\xi , \beta)$ is tabelated (Dresner, 1960) and different analytical approximations for the calculation of resonance integrals can be found in literature (Campos & Martinez, 1989), (Keshavamurthy & Harish, 1993). Based on recent advances in the analytical formulation of the Doppler broadening function $\psi(x,\xi)$, a semi-analytical method for the calculation of function $J(\xi , \beta)$ is proposed in this paper.

2. APPROXIMATION FOR FUNCTION $J(\xi,\beta)$

It is a fact that complex expressions for the Doppler broadening function lead to an impossibility in determining exact analytical expressions for function $J(\xi\,,\,\beta)$ and, as a result, for resonance integrals. The method proposed in this paper consists of applying the Lagrange method of polynomial interpolation (Alvim, 2007) to approximate the integrand of function $J(\xi\,,\,\beta)$, written by:

$$I(x,\xi,\beta) \equiv \frac{\psi(x,\xi)}{\psi(x,\xi)+\beta}, \tag{5}$$

so that an analytical integration is possible. For that, the integration interval in equation (1) will be divided into two intervals. As long as parameters x and ξ satisfy the $|x.\xi| \le 6$ relation, the expression for the Doppler broadening function will be calculated according to the Frobenius method (Palma et. al., 2006):

$$\psi_{Frob}(x,\xi) = \frac{\xi\sqrt{\pi}}{2}\exp\left[-\frac{1}{4}\xi^2\left(x^2-1\right)\right]\cos\left(\frac{\xi^2 x}{2}\right)\times$$
$$\left\{1+\mathrm{Re}\left[erf\left(\frac{i\xi x-\xi}{2}\right)\right]+\tan\left(\frac{\xi^2 x}{2}\right)\mathrm{Im}\left[erf\left(\frac{i\xi x-\xi}{2}\right)\right]\right\}. \tag{6}$$

For $|x.\xi| > 6$, one uses the asymptotic expansion $\psi_A(\mathrm{x},\xi)$ (Martinez et. al. , 2005):

$$\psi_A(x,\xi) \approx \frac{1}{1+x^2}, \tag{7}$$

Figure 1 shows the concordance of the asymptotic expression, Eq. (7), in comparison with the exact expression for the Doppler broadening function as obtained from the Frobenius method, Eq. (6), for large x values.

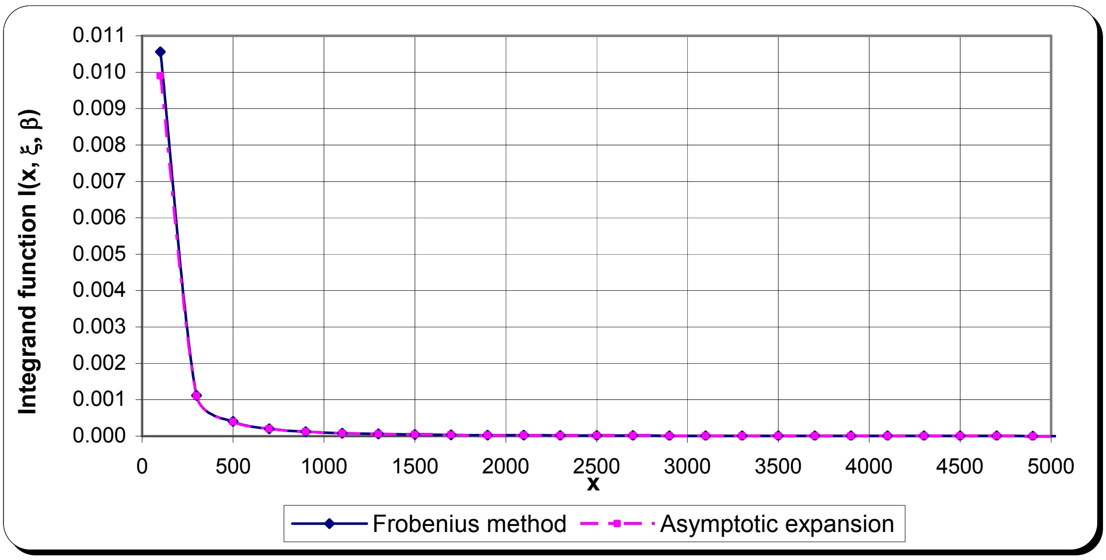

Figure 1. Comparison between the expressions of $\psi_{Frob}(\mathrm{x},\xi)$ and $\psi_A(\mathrm{x},\xi)$ for large x values in the calculation of function $I(x,\xi,\beta)$ for ξ=0.1 and $\beta = 1.0\times10^{-2}$.

In defining $X\max = 6/\xi$, function $J(\xi,\beta)$ will be calculated according to the expression:

$$J(\xi,\beta)=\int_0^{X\max=6/\xi}\frac{\psi_{Frob}(\mathrm{x},\xi)}{\psi_{Frob}(\mathrm{x},\xi)+\beta}dx+\int_{X\max=6/\xi}^{\infty}\frac{\psi_A(\mathrm{x},\xi)}{\psi_A(\mathrm{x},\xi)+\beta}dx. \tag{8}$$

2.1. The construction of inperpolating polynomials

Starting from an exact expression for the Doppler broadening function, Eq. (6), it is possible to obtain exact values for integrand $I(x,\xi,\beta)$. Having obtained $(n+1)$ x_i interpolation points, one can construct the n–degree Lagrange interpolating polynomial from the expression (Alvim, 2007):

$$P(x)=\sum_{k=0}^{n}f(x_k)l_k^n(x), \tag{9}$$

where

$$l_k^n(x)=\prod_{i=0,i\neq k}^{n}\frac{(x-x_i)}{(x_k-x_i)}. \tag{10}$$

In this paper, from four x_i interpolation points, a 3th order polynomial is constructed with the intent of approximating the integrand $I(x,\xi,\beta)$. In order not to overload the notation $I(x_k,\xi,\beta)=f(x_k)$ will be denoted by I_k. Thus, it is possible to construct the function $l_0^3(x)$ as follows:

$$l_0^3(x)=\frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}, \tag{11}$$

being that the other three polynomials $l_1^3(x)$, $l_2^3(x)$ and $l_3^3(x)$ are written in a similar fashion, using Eq. (10). From Eq. (11) one can write the following expression for $l_0^3(x)$:

$$l_0^3(x)=A_0x^3+B_0x^2+C_0x+D_0, \tag{12}$$

where the coefficients are defined as:

$$\begin{aligned}
A_0 &= \frac{1}{E_0}\\
B_0 &= -\frac{x_1+x_2+x_3}{E_0}\\
C_0 &= \frac{x_1x_2+x_2x_3+x_1x_3}{E_0}\\
D_0 &= -\frac{x_1x_2x_3}{E_0}\\
E_0 &= (x_0-x_1)(x_0-x_2)(x_0-x_3),
\end{aligned} \tag{13}$$

and all of the other three polynomials $l_k^3(x)$ are written similarly. As a result, from Eq. (9) it is possible to obtain the following Lagrange interpolating polynomial:

$$P(x) = P_0 x^3 + P_1 x^2 + P_2 x + P_3, \tag{14}$$

where the P_k coefficients are written by:

$$P_0 = \sum_{k=0}^{3} I_k A_k$$
$$P_1 = \sum_{k=0}^{3} I_k B_k$$
$$P_2 = \sum_{k=0}^{3} I_k C_k$$
$$P_3 = \sum_{k=0}^{3} I_k D_k. \tag{15}$$

Based on the methodology presented, the interval for integration $\left[0, X_{Max}\right]$ is divided into 4 equally spaced points, as 0, $\frac{2}{\xi}$, $\frac{4}{\xi}$, and X_{Max}, for the interpolation to be effected. Therefore, from the interpolating polynomial expressed by Eq. (14), it is possible to conclude that:

$$\int_0^{X_{\max}=6/\xi} \frac{\psi_{Frob}(\mathrm{x},\xi)}{\psi_{Frob}(\mathrm{x},\xi\,)+\beta} dx \approx \frac{P_0}{4} X_{\max}^4 + \frac{P_1}{3} X_{\max}^3 + \frac{P_2}{2} X_{\max}^2 + P_3 X_{\max} \tag{16}$$

The second term on the right side of Eq. (8) can be easily integrated by using the asymptotic expansion in the calculation of the Doppler broadening function $\psi_A(\mathrm{x},\xi)$, Eq. (7), being written by:

$$\int_{X_{\max}=6/\xi}^{\infty} \frac{\psi_A(\mathrm{x},\xi)}{\psi_A(\mathrm{x},\xi\,)+\beta} dx = \frac{1}{\beta} \int_{X_{\max}=6/\xi}^{\infty} \frac{1}{\mathrm{x}^2 + \left(\beta+1 \big/ \beta\right)} dx = \frac{1}{\sqrt{\beta(\beta+1)}} \left[\frac{\pi}{2} - \tan^{-1}\left(X_{\max} \sqrt{\frac{\beta}{\beta+1}} \right) \right] \tag{17}$$

As a result, from Eq. (16) and Eq. (17), the following approximation is written for the calculation of function $J(\xi\,,\beta)$:

$$J(\xi\,,\beta) = \frac{P_0}{4} X_{max}^4 + \frac{P_1}{3} X_{max}^3 + \frac{P_2}{2} X_{max}^2 + P_3 X_{max} + \frac{1}{\sqrt{\beta(\beta+1)}} \left[\frac{\pi}{2} - tan^{-1}\left(X_{max} \sqrt{\frac{\beta}{\beta+1}} \right) \right] \tag{18}$$

The Eq. (18) is a simple expression, of easy computational implementation. However, numerical studies have shown unsatisfactory results from taking only the single $\left[0, X_{Max}\right]$ interval. In order to attain adequate precision in the calculation of resonance integrals one needs to partition it. For the sake of simplicity, these sub-intervals can be equally divided and, in each one of them, 4 points $\left(x_i, I\left(x_i, \xi, \beta\right)\right)$ are calculated to have the interpolation of a grade 3 polynomial be carried out. With it, Eq. (18) can be re-written so to account for different intervals:

$$J(\xi\,,\beta) = \sum_{i=1}^{n} \left(\frac{P_{0i}}{4} X_{max}^4 + \frac{P_{1i}}{3} X_{max}^3 + \frac{P_{2i}}{2} X_{max}^2 + P_{3i} X_{max} \right) + \frac{1}{\sqrt{\beta(\beta+1)}} \left[\frac{\pi}{2} - tan^{-1}\left(X_{max} \sqrt{\frac{\beta}{\beta+1}} \right) \right] \tag{19}$$

In the present paper, we considered $n = 5$. Table 1 shows the interpolation points used.

Table 1. Interpolation points x_i .

	Interval 1	Interval 2	Interval 3	Interval 4	Interval 5
$\xi = 0.1$	0, 4, 8, 12	12, 16, 20, 24	24, 28, 32, 36	36, 40, 44, 48	48, 52, 56, 60
$\xi = 0.2$	0, 2, 4, 6	6, 8, 10, 12	12, 14, 16, 18	18, 20, 22, 24	24, 26, 28, 30
$\xi = 0.3$	$0, 4/3, 8/3, 4$	$4, 16/3, 20/3, 8$	$8, 28/3, 32/3, 12$	$12, 40/3, 44/3, 16$	$16, 52/3, 56/3, 20$
$\xi = 0.4$	0, 1, 2, 3	3, 4, 5, 6	6, 7, 8, 9	9, 10, 11, 12	12, 13, 14, 15
$\xi = 0.5$	$0, 4/5, 8/5, 12/5$	$12/5, 16/5, 4, 24/5$	$24/5, 28/5, 32/5, 36/5$	$36/5, 8, 44/5, 48/5$	$48/5, 52/5, 56/5, 12$
$\xi = 0.6$	$0, 2/3, 4/3, 2$	$2, 8/3, 10/3, 4$	$4, 14/3, 16/3, 6$	$6, 20/3, 22/3, 8$	$8, 26/3, 28/3, 10$
$\xi = 0.7$	$0, 4/7, 8/7, 12/7$	$12/7, 16/7, 20/7, 24/7$	$24/7, 28/7, 32/7, 36/7$	$36/7, 40/7, 44/7, 48/7$	$48/7, 52/7, 56/7, 60/7$
$\xi = 0.8$	$0, 1/2, 1, 3/2$	$3/2, 2, 5/2, 3$	$3, 7/2, 4, 9/2$	$9/2, 5, 11/2, 6$	$6, 13/2, 7, 15/2$
$\xi = 0.9$	$0, 4/9, 8/9, 4/3$	$4/3, 16/9, 20/9, 8/3$	$8/3, 28/9, 32/9, 12/3$	$12/3, 40/9, 44/9, 16/3$	$16/3, 52/9, 56/9, 20/3$
$\xi = 1.0$	$0, 2/5, 4/5, 6/5$	$6/5, 8/5, 2, 12/5$	$12/5, 14/5, 16/5, 18/5$	$18/5, 4, 22/5, 24/5$	$24/5, 26/5, 28/5, 6$

Table 2. Percentual desviation for the approximation proposed where $\beta = 2^j \times 10^{-5}$.

j	ξ=0.1	ξ=0.2	ξ=0.3	ξ=0.4	ξ=0.5	ξ=0.6	ξ=0.7	ξ=0.8	ξ=0.9	ξ=1.0
0	0.8	0.9	1.0	1.0	1.0	1.0	1.0	1.0	0.2	0.2
1	0.3	0.6	0.7	0.7	0.7	0.7	0.7	0.7	0.1	0.1
2	0.2	0.3	0.4	0.4	0.5	0.5	0.5	0.5	0.1	0.1
3	0.7	0.1	0.1	0.2	0.3	0.3	0.3	0.3	0.0	0.0
4	1.0	0.4	0.1	0.0	0.1	0.1	0.2	0.2	0.0	0.0
5	0.9	0.8	0.5	0.2	0.1	0.0	0.0	0.1	0.1	0.0
6	0.2	1.1	0.8	0.6	0.4	0.3	0.2	0.1	0.2	0.1
7	0.5	1.1	1.2	0.9	0.7	0.5	0.4	0.3	0.3	0.3
8	0.6	0.7	1.2	1.2	1.1	0.9	0.8	0.6	0.6	0.5
9	0.1	0.2	0.9	1.3	1.3	1.2	1.1	1.0	0.9	0.8
10	0.6	0.2	0.6	1.0	1.3	1.4	1.4	1.3	1.2	1.1
11	0.2	0.6	1.0	1.3	1.5	1.6	1.6	1.6	1.6	1.5
12	0.2	0.4	0.7	1.0	1.2	1.4	1.5	1.6	1.6	1.6
13	0.1	0.3	0.5	0.7	0.9	1.1	1.3	1.4	1.5	1.5
14	0.1	0.2	0.4	0.5	0.7	0.9	1.0	1.1	1.2	1.3
15	0.1	0.2	0.3	0.4	0.6	0.7	0.8	0.9	1.0	1.1
16	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.7	0.8	0.9
17	0.1	0.2	0.2	0.3	0.4	0.5	0.6	0.7	0.7	0.8
18	0.1	0.2	0.2	0.3	0.4	0.5	0.5	0.6	0.7	0.7
19	0.1	0.1	0.2	0.3	0.4	0.4	0.5	0.6	0.6	0.7
20	0.1	0.1	0.2	0.3	0.4	0.4	0.5	0.6	0.6	0.7
21	0.1	0.1	0.2	0.3	0.4	0.4	0.5	0.6	0.6	0.7
22	0.1	0.1	0.2	0.3	0.4	0.4	0.5	0.6	0.6	0.7
23	0.1	0.1	0.2	0.3	0.4	0.4	0.5	0.6	0.6	0.7
24	0.1	0.1	0.2	0.3	0.4	0.4	0.5	0.6	0.6	0.7
25	0.1	0.1	0.2	0.3	0.4	0.4	0.5	0.6	0.6	0.7
26	0.1	0.1	0.2	0.3	0.4	0.4	0.5	0.6	0.6	0.7
27	0.1	0.1	0.2	0.3	0.4	0.4	0.5	0.6	0.6	0.7
28	0.1	0.1	0.2	0.3	0.4	0.4	0.5	0.6	0.6	0.7
29	0.1	0.1	0.2	0.3	0.4	0.4	0.5	0.6	0.6	0.7
30	0.1	0.1	0.2	0.3	0.4	0.4	0.5	0.6	0.6	0.7
31	0.1	0.1	0.2	0.3	0.4	0.4	0.5	0.6	0.6	0.7

3. RESULTS

The section shows the results obtained with the method proposed in this paper for the calculation of function $J(\xi, \beta)$ at different values of parameters ξ and β. Table 2 shows the percentage deviations obtained from Eq. (19) through the use of the interpolation points found in Table 1. As a reference we used the Gauss-Legendre integration method (Alvim, 2007) both in the calculation of the Doppler broadening function as in the onedimensional integral that exists in the definition of the function $J(\xi, \beta)$, Eq. (1).

Table 3 shows processing times needed to calculated one value to the Dresner Table (Dresner, 1960) for the method used in the calculation of the function presented in this paper. The computer used was a PC with an Athlon XP, 1024 MB RAM, and running at 2.2GHz.

Table 3. Processing times needed to calculated one value to the Dresner table.

	Computation time
Reference method – Gaussian quadrature	44 min
Proposed method – Lagrange interpolation	0.0 s

From the percentage deviations found in Table 2 it is possible to conclude that the method is compatible with the reference values, presenting mean deviations below 1% and 1.6% of maximum deviation. These figures were obtained without the need for an excessive partitioning of the interval in which the Doppler broadening function is calculated according to the Frobenius method $\left[0, X_{Max}\right]$.

4. CONCLUSIONS

A simple and precise method for the calculation of the $J(\xi , \beta)$ function was proposed in this paper. This method is based on the coupling of an exact expression for the Doppler broadening function as obtained from the Frobenius method with an asymptotic expression that is well founded in literature. The Lagrange interpolation method was employed to approximate the integrand of the function $J(\xi , \beta)$ in the interval $\left[0, X_{Max}\right]$ through polynomials. The results obtained proved satisfactory from the accuracy standpoint as well as in terms of processing time.

5. ACKNOWLEDGEMENTS

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7. RESPONSIBILITY NOTICE