Chapter 2

New Methods in Doppler Broadening Function Calculation

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1. Introduction

In all nuclear reactors some neutrons can be absorbed in the resonance region and, in the design of these reactors, an accurate treatment of the resonant absorptions is essential. Apart from that, the resonant absorption varies with fuel temperature, due to the Doppler broadening of the resonances (Stacey, 2001). The thermal agitation movement of the reactor core is adequately represented in microscopic cross-section of the neutron-core interaction through the Doppler Broadening function. This function is calculated numerically in modern systems for the calculation of macro-group constants, necessary to determine the power distribution in a nuclear reactor. This function has also been used for the approximate calculations of the resonance integrals in heterogeneous fuel cells (Campos and Martinez, 1989). It can also be applied to the calculation of self-shielding factors to correct the measurements of the microscopic cross-sections through the activation technique (Shcherbakov and Harada, 2002). In these types of application we can point out the need to develop precise analytical approximations for the Doppler broadening function to be used in the codes that calculates the values of this function. Tables generated from such codes are not convenient for some applications and experimental data processing.

This chapter will present a brief retrospective look at the calculation methodologies for the Doppler broadening function as well as the recent advances in the development of simple and precise analytical expressions based on the approximations of Beth-Plackzec according to the formalism of Briet-Wigner.

2. The Doppler broadening function

Let us consider a medium with a temperature where the target nuclei are in thermal movement. In a state of thermal equilibrium for a temperature T, the velocities are distributed according to Maxwell-Boltzmann distribution (Duderstadt and Hamilton, 1976),

$$f(V) = N\left(\frac{M}{2\pi kT}\right)^{\frac{3}{2}} e^{-MV^2/2kT}, \tag{1}$$

where N is the total number of nucleus, M is the mass of the nucleus and k is Boltzmann's constant.

Considering the neutrons as an ideal gas in thermal equilibrium, it is possible to write the average cross-section for neutron-nucleus interaction taking into consideration the movement of the neutrons and of the nucleus as:

$$\bar{\sigma}(v,T) = \frac{1}{vN}\int d^3V(|\vec{v}-\vec{V}|)\sigma(|\vec{v}-\vec{V}|)f(\vec{V}), \tag{2}$$

where $f(\vec{V})$ is the distribution function of Maxwell-Boltzmann as given by equation (1) and $\vec{V}=V\hat{\Omega}$ is the velocity of the target nuclei. Denoting $\vec{v}_r=\vec{v}-\vec{V}$ the relative velocity between the movement of the neutron and the movement of the target nucleus and considering the isotropic case, that is, with no privileged direction, it is possible to separate the integration contained in equation (2) in the double integral:

$$\bar{\sigma}(v,T) = \frac{1}{vN}\int_0^\infty dVV^2 f\left(\vec{V}\right)\int_{4\pi} v_r\sigma(v_r)\,d\hat{\Omega}. \tag{3}$$

It is possible to see clearly in equation (3) that the cross-section depends of the relative velocity between the neutrons and the target nuclei. As the nuclei are in thermal movement, the relative velocity can increase or decrease. This difference between relative velocities rises to the Doppler deviation effect in cross-section behaviour. After integrating equation (3) in relation to the azimuthal angle (ϕ) the average cross-section for neutron-nucleus interaction can be written thus:

$$\bar{\sigma}(v,T) = \frac{2\pi}{vN}\int_0^\infty dVV^2 f(\vec{V})\int_0^\pi v_r\sigma(v_r)\sin\theta d\theta. \tag{4}$$

Denoting $\mu=\cos\theta$ so that $d\mu=-\sin\theta d\theta$, equation (4) takes the form of:

$$\bar{\sigma}(v,T) = \frac{2\pi}{vN}\int_0^\infty dVV^2 f(\vec{V})\int_{-1}^1 v_r\sigma(v_r)d\mu. \tag{5}$$

From the definition of the relative velocity one has the relation,

$$v_r^2 = v^2 + V^2 - 2vV\mu, \tag{6}$$

and, as a result,

$$d\mu = -\frac{v_r dv_r}{vV}. \tag{7}$$

With the aid of a simple substitution, using relations (6) and (27), equation (5) is thus written as:

$$\bar{\sigma}(v,T) = \frac{2\pi}{v^2 N}\int_0^\infty dVVf(\vec{V})\int_{|v-V|}^{|v+V|} v_r^2\sigma(v_r)dv_r. \tag{8}$$

In equation (8), the limits of integration are always positive due to the presence of the module. As a result, one should separate the integral found in equation (8) into two separate integrals, as follows,

$$\bar{\sigma}(v,T) = \frac{2\pi}{v^2 N}\left[\int_0^v dVVf(\vec{V})\int_{v-V}^{v+V} v_r^2\sigma(v_r)dv_r + \int_v^\infty dVVf(\vec{V})\int_{V-v}^{v+V} v_r^2\sigma(v_r)dv_r\right]. \tag{9}$$

It is possible to modify the limits of integration for equation (9) taking into account that the mass of the target nucleus is much larger than the mass of the incident neutron. In terms of relative velocity, equation (9) can be written as:

$$\bar{\sigma}(v,T) = \frac{2\pi}{v^2 N}\left[\int_{v-v_r}^{v+v_r} v_r^2\sigma(v_r)dv_r\int_0^v dVVf(\vec{V}) + \int_{v_r-v}^{v+v_r} v_r^2\sigma(v_r)dv_r\int_v^\infty dVVf(\vec{V})\right]. \tag{10}$$

In replacing the expression of the Boltzmann distribution function, equation (1), in equation (10) one has:

$$\bar{\sigma}(v,T) = \frac{2\beta^3}{v^2\sqrt{\pi}}\left[\int_{v-v_r}^{v+v_r} v_r^2\sigma(v_r)dv_r\int_0^v dVVe^{-\beta^2V^2} + \int_{v_r-v}^{v+v_r} v_r^2\sigma(v_r)dv_r\int_v^\infty dVVe^{-\beta^2V^2}\right], \tag{11}$$

where it was defined $\beta^2 \equiv \frac{M}{2kT}$. Introducing the variables for reduced velocities $\varpi_r = \beta v_r$ and $\varpi = \beta v$, equation (11) is written by:

$$\bar{\sigma}(v,T) = \frac{2\beta^2}{\varpi^2\sqrt{\pi}}\times \left[\int_0^{\varpi/\beta} \varpi_r^2\sigma(\varpi_r)d\varpi_r\int_{(\varpi-\varpi_r)/\beta}^{(\varpi+\varpi_r)/\beta} dVVe^{-\beta^2V^2} + \int_{\varpi/\beta}^\infty \varpi_r^2\sigma(\varpi_r)d\varpi_r\int_{(\varpi_r-\varpi)/\beta}^{(\varpi+\varpi_r)/\beta} dVVe^{-\beta^2V^2}\right]. \tag{12}$$

Integrating equation (12) in relation to V one gets to the expression:

$$\bar{\sigma}(v,T) = \frac{1}{\varpi^2\sqrt{\pi}}\int_0^\infty \varpi_r^2\sigma(\varpi_r)\left[e^{-(\varpi-\varpi_r)^2} - e^{-(\varpi+\varpi_r)^2}\right]d\varpi_r. \qquad (13)$$

For resonances (that is, for the energy levels of the composed nucleus) it is possible to describe the energy dependence of the absorption cross-section by a simple formula, valid for $T = 0K$, known as Breit-Wigner formula for resonant capture, expressed in function of the energy of the centre-of-mass by,

$$\sigma_\gamma(E_{CM}) = \sigma_0 \frac{\Gamma\gamma}{\Gamma}\left(\frac{E_0}{E_{CM}}\right)^{1/2} \frac{1}{1+\frac{4}{\Gamma^2}(E_{CM}-E_0)^2}, \qquad (14)$$

where E_0 is the energy where the resonance occurs and E_{CM} is the energy of the centre-of-mass of the neutron–nucleus system. Apart from that, we find in equation (14) the term σ_0, that is the value of the total cross-section $\sigma_{total}(E)$ in resonance energy E_0 that can be written in terms of the reduced wavelength λ_0 by:

$$\sigma_0 = 4\pi\lambda_0^2\frac{\Gamma_n}{\Gamma}g = 2.608\times10^6\frac{(A+1)^2}{A^2E(eV)}\frac{\Gamma_n}{\Gamma}g, \qquad (15)$$

where the statistical spin factor g is given by the expression:

$$g = \frac{2J+1}{2(2I+1)}, \qquad (16)$$

where I is the nuclear spin and J is the total spin (Bell and Glasstone, 1970).

In replacing the expression (14) in equation (13) one finds an exact expression for the average cross-section, valid for any temperature:

$$\bar{\sigma}_\gamma(v,T) = \sigma_0\frac{\Gamma_\gamma}{\Gamma}\frac{\beta^2}{\sqrt{\pi}v^2}\times$$
$$\int_0^\infty dv_r\left(\frac{E_0}{E_{CM}}\right)^{1/2}\frac{v_r^2}{1+\frac{4}{\Gamma^2}(E_{CM}-E_0)^2}\left[e^{-\beta^2(v-v_r)^2} - e^{-\beta^2(v+v_r)^2}\right], \qquad (17)$$

In a system with two bodies it is possible to write the kinetic energy in the centre-of-mass system, by

$$E_{CM} = \frac{M_R v_r^2}{2}, \tag{18}$$

where $M_R = \frac{mM}{m+M}$ is the reduced mass of the system.

For the problem at hand, of a neutron that is incident in a thermal equilibrium system with a temperature T, it is a good approximation to assume that $v \approx v_r$. Thus, the ratio between the kinetic energy of the incident neutron and the kinetic energy of the centre-of-mass system is thus written

$$\frac{E_{CM}}{E_0} = \frac{A+1}{A}, \tag{19}$$

where A is the atomic mass of the target core. Resulting:

$$\begin{aligned} y &= \frac{2}{\Gamma}\left(E_{CM} - E_0\right) \text{ (a)} \\ x &= \frac{2}{\Gamma}\left(E - E_0\right), \quad \text{(b)} \end{aligned} \tag{20}$$

and denoting $\beta^2 = \frac{1}{2v_{th}^2}$ one finally obtains the expression for the cross-section of radioactive capture near any isolated resonance with an energy peak E_0, as written by:

$$\bar{\sigma}_\gamma\left(E,T\right) = \sigma_0 \frac{\Gamma_\gamma}{\Gamma}\left(\frac{E_0}{E}\right)^{1/2} \Psi\left(x,\xi\right), \tag{21}$$

where

$$\Psi\left(x,\xi\right) = \frac{\xi}{2}\int_{-2E/\Gamma}^{+\infty} \frac{dy}{1+y^2}\left[\exp\left(-\frac{\left(v-v_r\right)^2}{2v^2_{th}}\right) - \exp\left(-\frac{\left(v+v_r\right)^2}{2v^2_{th}}\right)\right], \tag{22}$$

where v_r is the module for relative neutron-nucleus velocity, v is the module for neutron velocity, and

$$\xi \equiv \frac{\Gamma}{\Gamma_D}. \tag{23}$$

The Doppler width for resonance Γ_D is expressed by:

$$\Gamma_D = \left(4E_0 kT / A\right)^{1/2}. \quad (24)$$

All the other nuclear parameters listed below are well established in the literature,

- A= mass number;
- T= absolute temperature;
- E= energy of incident neutron;
- E_{CM}= energy of centre-of-mass;
- E_0= energy where the resonance occurs;
- Γ= total width of the resonance as measured in the lab coordinates;
- $\Gamma_D = (4E_0 kT / A)^{1/2}$= Doppler width of resonance;
- v= neutron velocity module;
- $v_r = |v - V|$= module of the relative velocity between neutron movement and nucleus movement;
- $v_{th} = \sqrt{\frac{2kT}{M}}$= module of the velocity for each target nucleus.

3. The Bethe and Placzek approximations

The expression proposed by Bethe and Placzek for the Doppler broadening function $\psi(x, \xi)$ is obtained from some approximations, as follows:

1. one neglects the second exponential in equation (22), given that it decreases exponentially and is negligible in relation to first integral in equation (22) given that $(v + v_r)^2 >> (v - v_r)^2$.
2. it is a good approximation to extend the lower limit for integration down to $-\infty$ in equation (22), given that the ratio between the energy of neutron incidence and the practical width is big.
3. being E_{CM} the energy of the system in the centre-of-mass system and E the energy of the incident neutron, the following relation is always met:

$$E_{CM}^{1/2} = E^{1/2}\left(1 + \frac{E_{CM} - E}{E}\right)^{1/2} = E^{1/2}\left(1 + \eta\right)^{1/2}, \quad (25)$$

where it was denoted that $\eta = \dfrac{E_{CM} - E}{E}$. Equation (25) can be expanded in a Taylor series and, to the first order, is written by

$$E_{CM}^{1/2} = E^{1/2}\left(1 + \frac{\eta}{2} - \frac{\eta^2}{4} + \ldots\right) \approx E^{1/2}\left(1 + \frac{E_{CM} - E}{2E}\right) \tag{26}$$

In terms of the masses and velocities, equation (26) is written as follows:

$$\left(\frac{M_R v_r^2}{2}\right)^{1/2} = \left(\frac{mv^2}{2}\right)^{1/2}\left(1 + \frac{\frac{M_R v_r^2}{2} - \frac{mv^2}{2}}{mv^2}\right), \tag{27}$$

where M_R is the reduced mass of the system. For heavy nucleus $M_R \approx m$ and equation (27) can be written as:

$$v_r = \frac{v_r^2 + v^2}{2v}, \tag{28}$$

so that,

$$v - v_r = v - \frac{v_r^2 + v^2}{2v} = \frac{v^2 - v_r^2}{2v}. \tag{29}$$

In replacing approximation equation (29) in the remaining exponential of equation (22) one finally obtains the Doppler broadening function that will be approached in this chapter,

$$\psi(x,\xi) \approx \frac{\xi}{2\sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{dy}{1+y^2} \exp\left[-\frac{\xi^2}{4}(x-y)^2\right]. \tag{30}$$

The approximations made in this section apply in almost all the practical cases, and are not applicable only in situations of low resonance energies ($E < 1eV$) and very high temperatures.

4. Properties of the Doppler broadening function $\psi(x, \xi)$

The function $\psi(x, \xi)$ as proposed by the approximation of Bethe and Placzek has an even parity, is strictly positive and undergoes a broadening as that variable ξ diminishes, that is, varies inversely with the absolute temperature of the medium. For low temperatures, that is, when temperature in the medium tend to zero, the Doppler broadening function can be represented as shown below:

$$\lim_{T\to 0}\psi(x,\xi)=\frac{\xi}{2\sqrt{\pi}}\lim_{T\to 0}\int_{-\infty}^{+\infty}\frac{dy}{1+y^2}\exp\left[-\frac{\xi^2}{4}(x-y)^2\right]=\frac{1}{1+x^2} \tag{31}$$

Equation (31) is known as an asymptotic approximation of the Doppler broadening function. For high temperatures, that is, when the temperature of the medium tends to infinite, the Doppler broadening function can be represented through the Gaussian Function, given that:

$$\lim_{T\to\infty}\psi(x,\xi)=\frac{\xi}{2\sqrt{\pi}}\lim_{T\to\infty}\int_{-\infty}^{+\infty}\frac{dy}{1+y^2}\exp\left[-\frac{\xi^2}{4}(x-y)^2\right]=\frac{\xi}{2\sqrt{\pi}}\exp\left(-\frac{\xi^2}{4}x^2\right). \tag{32}$$

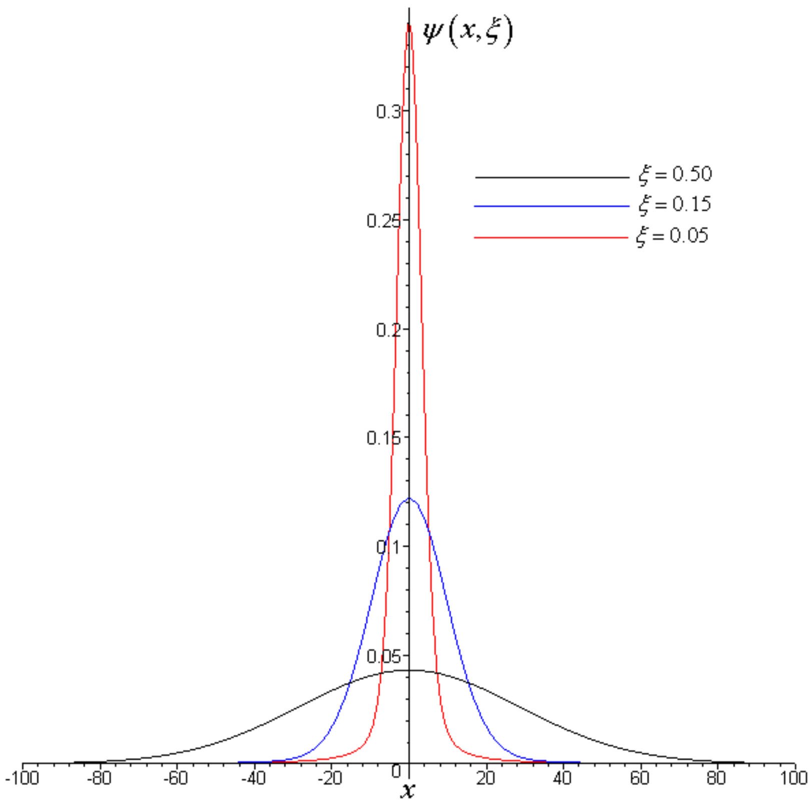

Figure 1. The Doppler broadening function for ξ=0.05, 0.15 and 0.5.

The area over the curve of the Doppler Broadening function is written as below and, as it consists of separable and known integers it is possible to write:

$$\int_{-\infty}^{+\infty}\psi(x,\xi)dx=\frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{+\infty}\frac{dy}{1+y^2}\int_{-\infty}^{+\infty}e^{-\frac{\xi^2}{4}(x-y)^2}dx=\frac{\xi}{2\sqrt{\pi}}(\pi)\left(\sqrt{\pi}\frac{2}{\xi}\right)=\pi. \tag{33}$$

From equation (33) once concludes that the area over the curve of the Doppler Broadening function is constant for the intervals of temperature and energy of interest in thermal reactors. This property is valid even for broadened resonances as shown in Figure 1, considering the different values of variable ξ.

5. Analytical approximations for the Doppler broadening function

This section describes the main approximation methods for the Doppler broadening function, according to the approximation of Bethe and Placzek, equation (30).

5.1. Asymptotic expansion

A practical choice to calculate the Doppler broadening function is its asymptotic expression resulting from the expansion of the term $\frac{1}{1+y^2}$ in equation (30) in a Taylor series around $y = x$.

$$\frac{1}{1+y^2} = \frac{1}{1+x^2} - \frac{2x}{\left(1+x^2\right)^2}(y-x) + \frac{-1+3x^2}{\left(1+x^2\right)^2}(y-x)^2 - \frac{4x\left(-1+x^2\right)}{\left(1+x^2\right)^4}(y-x)^3 + \ldots \tag{34}$$

In replacing equation (34) in equation (30) and integrating term by term, one obtains the following the asymptotic expansion:

$$\psi(x,\xi) = \frac{1}{1+x^2}\left\{\begin{array}{l} 1 + \frac{2}{\xi^2}\frac{\left(3x^2-1\right)}{\left(1+x^2\right)^2} + \\ \frac{12}{\xi^4}\frac{\left(5x^4-10x^2-1\right)}{\left(1+x^2\right)^4} + \ldots \end{array}\right\}. \tag{35}$$

Despite equation (35) being valid only for $|x.\xi| > 6$, it is quite useful to determine the behaviour of the Doppler Broadening function in specific conditions. For high values of x, it is possible to observe that function $\psi(x, \xi)$ presents the following asymptotic form:

$$\psi(x,\xi) \approx \frac{1}{1+x^2} \tag{36}$$

5.2. Method of Beynon and Grant

Beynon and Grant (Beynon and Grant, 1963) proposed a calculation method for the Doppler broadening function that consists of expanding the exponential part of the integrand of the Doppler broadening function $\psi(x, \xi)$ in the Chebyshev polynomials and integrate, term by term, the resulting expression, which allows writing:

$$\psi(a,\ b)=\frac{1}{a}\left\{\sqrt{\pi}\cos(ab)[1-\ E_2(a)]e^{a^2}+J(a,b)\right\}e^{-\frac{1}{4}b^2}, \tag{37}$$

where $a=\dfrac{1}{2}\xi$ and $b=\xi\cdot x$ and still,

$$\begin{aligned} J(a,b)=&\frac{1}{a}\left\{\frac{1}{2!}(ab)^2-\frac{1}{4!}(ab)^4+\frac{1}{6!}(ab)^6\cdots\right\}\\ &+\frac{1}{2a^3}\left\{\frac{1}{4!}(ab)^4-\frac{1}{6!}(ab)^6\cdots\right\}+\\ &\cdots+\frac{1}{\sqrt{\pi}a^{2n+1}}\Gamma\left(\frac{2n+1}{2}\right)\cdot\left\{\frac{1}{(2n+2)!}(ab)^{2(n+1)}\cdots\right\}+ \end{aligned} \tag{38}$$

and,

$$E_2(a)=\frac{2}{\sqrt{\pi}}\int_0^a e^{-y^2}\ dy. \tag{39}$$

For values where the condition $|x.\xi|>6$ was met (Beynon and Grant, 1963) is recommended the use of the asymptotic expression of the function $\psi(x,\ \xi)$, equation (36). It should be pointed that the results obtained by this method have become a reference in several works on the Doppler broadening function.

5.3. Method of Campos and Martinez

The core idea of the method proposed by (Campos and Martinez, 1987) is to transform the Doppler broadening function from its integral form into a differential partial equation subjected to the initial conditions. Differentiating equation (30) in relation to x one obtains:

$$\begin{aligned} \frac{\partial\psi(x,\xi)}{\partial x}=&\frac{\xi^2}{2}\times\\ &\left\{-\frac{\xi x}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{dy}{1+y^2}\exp\left[-\frac{\xi^2}{4}(x-y)^2\right]+\frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{ydy}{1+y^2}\exp\left[-\frac{\xi^2}{4}(x-y)^2\right]\right\}. \end{aligned} \tag{40}$$

Acknowledging in equation (40) the very Doppler broadening function and the term of interference as defined by the integral:

$$\chi(x,\xi)=\frac{\xi}{\sqrt{\pi}}\int_{-\infty}^{+\infty}\frac{ydy}{1+y^2}\exp\left[-\frac{\xi^2}{4}(x-y)^2\right], \tag{41}$$

it is possible to write:

$$\frac{\partial\psi(x,\xi)}{\partial x}=\frac{\xi^2}{2}\left[-x\psi(x,\xi)+\frac{\chi(x,\xi)}{2}\right]. \tag{42}$$

Deriving equation (42) again in relation to x, after expliciting function $\chi(x, \xi)$ in the same equation, one has:

$$\begin{aligned}&\frac{\partial^2\psi(x,\xi)}{\partial x^2}+x\xi^2\frac{\partial\psi(x,\xi)}{\partial x}+\frac{\xi^2}{4}\left(x^2\xi^2+2\right)\psi(x,\xi)\\&=\frac{\xi^5}{8\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{y^2dy}{1+y^2}\exp\left[-\frac{\xi^2}{4}(x-y)^2\right].\end{aligned} \tag{43}$$

The right side of equation (43) can be written in another way, given that $\frac{y^2}{1+y^2}=1-\frac{1}{1+y^2}$,

$$\int_{-\infty}^{\infty}\frac{y^2dy}{1+y^2}\exp\left[-\frac{\xi^2}{4}(x-y)^2\right]=\frac{2\sqrt{\pi}}{\xi}\left[1-\psi(x,\xi)\right]. \tag{44}$$

In replacing the result obtained in (44) in equation (43) one obtains the differential equation where Campos and Martinez based themselves to obtain an analytical approximation for the broadening function $\psi(x, \xi)$:

$$\frac{4}{\xi^2}\frac{\partial^2\psi(x,\xi)}{\partial x^2}+4x\frac{\partial\psi(x,\xi)}{\partial x}+\left(\xi^2x^2+\xi^2+2\right)\psi(x,\xi)=\xi^2, \tag{45}$$

subjected to the initial conditions:

$$\begin{aligned}&\psi(x,\xi)|_{x=0}\equiv\psi_0=\frac{\xi\sqrt{\pi}}{2}\exp\left(\frac{\xi^2}{4}\right)\left[1-erf\left(\frac{\xi}{2}\right)\right] \quad \text{(a)}\\&\frac{\partial\psi(x,\xi)}{\partial x}|_{x=0}=0. \quad \text{(b)}\end{aligned} \tag{46}$$

Admitting that function $\psi(x, \xi)$ may be expanded in series,

$$\psi(x,\xi)=\sum_{n=0}^{\infty}c_n(\xi)\,x^n \tag{47}$$

and in replacing-se equation (47) in the differential equation as given by equation (45), one obtains after some algebraic manipulation the following polynomial equation:

$$\begin{aligned}&\left[\frac{8}{\xi^2}c_2+\left(\xi^2+2\right)c_0\right]+\left[\frac{24}{\xi^2}c_3+\left(\xi^2+6\right)c_1\right]x+\\&+\sum_{n=2}^{\infty}\left[\frac{4}{\xi^2}(n+2)(n+1)c_{n+2}+\left(4n+\xi^2+2\right)c_n+\xi^2c_{n-2}\right]x^n=\xi^2,\end{aligned} \tag{48}$$

where:

$c_0 = \psi_0,$

$c_1 = \frac{\xi^2}{8}\left[\xi^2 - \left(\xi^2 + 2\right)\psi_0\right],$

and all the other terms are calculated from the following relation of recurrence:

$$c_{n+1} = -\frac{\xi^2}{4}\frac{\left(4n + \xi^2 + 2\right)c_n + \xi^2 c_{n-1}}{(n+2)(n+1)}$$

The representation in series for the Doppler broadening function, as given by equation (47), is valid only for $|x.\xi| < 6$. For the cases where $|x.\xi| > 6$, (Campos and Martinez, 1987) used the asymptotic form as given by equation (35), as well as proposed by Beynon and Grant.

5.4. Four order method of Padé

The Padé approximation is one of the most frequently used approximations for the calculation of the Doppler broadening function and its applications and can efficiently represent functions, through a rational approximation, that is, a ratio between polynomials. For the four-order Padé approximation (Keshavamurthy& Harish, 1993) they proposed the following polynomial ratio:

$$\psi(x,\xi) = h\frac{a_0 + a_2(hx)^2 + a_4(hx)^4 + a_6(hx)^6}{b_0 + b_2(hx)^2 + b_4(hx)^4 + b_6(hx)^6 + b_8(hx)^8}, \quad (49)$$

whose coefficients are given in Tables 1 and 2.

$p_0 = \sqrt{\pi}$	$q_1 = \frac{\sqrt{\pi}(-9\pi + 28)}{2\left(6\pi^2 - 29\pi + 32\right)}$
$p_1 = \frac{-15\pi^2 + 88\pi - 128}{2\left(6\pi^2 - 29\pi + 32\right)}$	$q_2 = \frac{36\pi^2 - 195\pi + 256}{6\left(6\pi^2 - 29\pi + 32\right)}$
$p_2 = \frac{\sqrt{\pi}(33\pi - 104)}{6\left(6\pi^2 - 29\pi + 32\right)}$	$q_3 = \frac{\sqrt{\pi}(-33\pi + 104)}{6\left(6\pi^2 - 29\pi + 32\right)}$
$p_3 = \frac{-9\pi^2 + 69\pi - 128}{3\left(6\pi^2 - 29\pi + 32\right)}$	$q_4 = \frac{9\pi^2 - 69\pi + 128}{3\left(6\pi^2 - 29\pi + 32\right)}$

Table 1. Coefficients *p* and *q* of the four-order Padé Approximation

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$h = {}^{\xi}\!/_{2}$
$a_0 = \left(p_0 + p_1 h - p_2 h^{2} - p_3 h^{3}\right)\left(1 - q_1 h - q_2 h^{2} + q_3 h^{3} + q_4 h^{4}\right)$
$a_2 = \left(p_2 + 3p_3 h\right)\left(1 - q_1 h - q_2 h^{2} + q_3 h^{3} + q_4 h^{4}\right) + \left(p_0 + p_1 h - p_2 h^{2} - p_3 h^{3}\right)\left(q_2 - 3q_3 h - 6q_4 h^{2}\right) + \left(-p_1 + 2p_2 h + 3p_3 h^{2}\right)\left(q_1 + 2q_2 h - 3q_3 h^{2} - 4q_4 h^{3}\right)$
$a_4 = q_4\left(p_0 + p_1 h - p_2 h^{2} - p_3 h^{3}\right) + \left(p_2 + 3p_3 h\right)\left(q_2 - 3q_3 h - 6q_4 h^{2}\right) - p_3\left(q_1 + 2q_2 h - 3q_3 h^{2} - 4q_4 h^{3}\right) + \left(-p_1 + 2p_2 h + 3p_3 h^{2}\right)\left(q_3 + 4q_4 h\right)$
$a_6 = q_4\left(p_2 + 3p_3 h\right) - p_3\left(q_3 + 4q_4 h\right)$
$b_0 = \left(1 - q_1 h - q_2 h^{2} + q_3 h^{3} + q_4 h^{4}\right)^2$
$b_2 = 2\left(1 - q_1 h - q_2 h^{2} + q_3 h^{3} + q_4 h^{4}\right)\left(q_2 - 3q_3 h - 6q_4 h^{2}\right) + \left(q_1 + 2q_2 h - 3q_3 h^{2} - 4q_4 h^{3}\right)^2$
$b_4 = \left(q_2 - 3q_3 h - 6q_4 h^{2}\right)^2 + 2q_4\left(1 - q_1 h - q_2 h^{2} + q_3 h^{3} + q_4 h^{4}\right) + 2\left(q_1 + 2q_2 h - 3q_3 h^{2} - 4q_4 h^{3}\right)\left(q_3 + 4q_4 h\right)$
$b_6 = 2q_4\left(q_2 - 3q_3 h - 6q_4 h^{2}\right) + \left(q_3 + 4q_4 h\right)^2$
$b_8 = q_4^2$

Table 2. Coefficients h , a and b of the four-order Padé Approximation

From the coefficients of Tables 1 and 2, and of equation (49), one obtains in the end the following analytical approximation for function $\psi(x,\ \xi)$, according to the four-order Padé approximation:

$$\psi\left(x,\xi\right) = \frac{\eta\left(x,\xi\right)}{\omega\left(x,\xi\right)}, \tag{50}$$

where $\eta(x,\ \xi)$ and $\omega(x,\ \xi)$ are the following polynomials:

$$\begin{aligned}\eta\left(x,\xi\right) = 2\xi\cdot\Big(&7,089815404\cdot10^{22} + 1,146750844\cdot10^{23}\,\xi + 8,399725059\cdot10^{22}\,\xi^{2}\\ &+3,622207053\cdot10^{22}\,\xi^{3} + 9,957751740\cdot10^{21}\,\xi^{4} + 1,749067258\cdot10^{21}\,\xi^{5}\\ &+1,835165213\cdot10^{20}\,\xi^{6} + 8,940072699\cdot10^{18}\,\xi^{7} - 2,539736657\cdot10^{21}\,\xi^{2}x^{2}\\ &+2,069483991\cdot10^{21}\,\xi^{3}x^{2} + 3,972393548\cdot10^{21}\,\xi^{4}x^{2} + 1,919319560\cdot10^{21}\,\xi^{5}x^{2}\\ &+3,670330426\cdot10^{20}\,\xi^{6}x^{2} + 2,682021808\cdot10^{19}\,\xi^{7}x^{2} + 1,048748026\cdot10^{19}\,\xi^{4}x^{4}\\ &+1,702523008\cdot10^{20}\,\xi^{5}x^{4} + 1,835165209\cdot10^{20}\,\xi^{6}x^{4} + 2,682021806\cdot10^{19}\,\xi^{7}x^{4}\\ &+8,940072688\cdot10^{18}\,\xi^{7}x^{6}\Big),\end{aligned} \tag{51}$$

and

$$\begin{aligned}\eta(x,\xi) = \Big(&3{,}490642925\cdot 10^{23}\xi + 3{,}464999381\cdot 10^{23}\xi^2 + 2{,}050150991\cdot 10^{23}\xi^3\\
&+7{,}933771118\cdot 10^{22}\xi^4 + 3{,}670330427\cdot 10^{20}\xi^7x^6 + 1{,}788014539\cdot 10^{19}\xi^8x^8\\
&+3{,}670330426\cdot 10^{20}\xi^7 + 3{,}533894806\cdot 10^{21}\xi^6 + 1{,}788014541\cdot 10^{19}\xi^8\\
&+2{,}062859460\cdot 10^{22}\xi^5 + 3{,}426843796\cdot 10^{22}\xi^2x^2 + 5{,}586613630\cdot 10^{22}\xi^4x^2\\
&+2{,}649703323\cdot 10^{22}\xi^5x^2 + 6{,}613512625\cdot 10^{22}\xi^3x^2 + 1{,}101099129\cdot 10^{21}\xi^7x^2\\
&+7{,}301013353\cdot 10^{21}\xi^6x^2 + 3{,}590774413\cdot 10^{21}\xi^4x^4 + 1{,}101099125\cdot 10^{21}\xi^7x^4\\
&+5{,}868438581\cdot 10^{21}\xi^5x^4 + 4{,}000342261\cdot 10^{21}\xi^6x^4 + 7{,}152058156\cdot 10^{19}\xi^8x^2\\
&+2{,}332237305\cdot 10^{20}\xi^6x^6 + 1{,}072808721\cdot 10^{20}\xi^8x^4 + 7{,}152058152\cdot 10^{19}\xi^8x^6.\end{aligned} \tag{52}$$

5.5. Frobenius method

In this method the homogeneous part of the differential equation that rules the Doppler broadening function, equation (45), is solved using the Frobenius Method (Palma et. al., 2005) that consists fundamentally of seeking a solution of the differential equation in the form of series around the point $x = x_0$, with a free parameter, that is, as follows:

$$\psi(x,\xi) = x^s \sum_{n=0}^{\infty} c_n(\xi)\, x^n = \sum_{n=0}^{\infty} c_n(\xi)\, x^{n+s}, \tag{53}$$

with $c_0 \neq 0$ and where s is the parameter that grants the method flexibility.

Deriving equation (53) and replacing it in the homogeneous equation associated to equation (45) one obtains, after grouping the similar terms:

$$\begin{aligned}&\sum_{n=0}^{\infty} c_n (n+s)(n+s-1)\, x^{n+s-2} + \sum_{n=0}^{\infty} c_n \xi^2 \left[(n+s) + \frac{\xi^2+2}{4}\right] x^{n+s}\\
&+\frac{\xi^2}{4}\sum_{n=0}^{\infty} c_n\, x^{n+s-2} = 0.\end{aligned} \tag{54}$$

The initial equation of the problem, obtained when $n = 0$, remembering that $c_0 \neq 0$ is

$$c_0 s(s-1) = 0. \tag{55}$$

From equation (55), as $c_0 \neq 0$, one obtains that $s = 0$ or $s = 1$. Using first $s = 0$ and $c_0 \neq 0$ one obtains the following relations of recurrence:

$$c_n = -\frac{\xi^2\left(4n + \xi^2 - 6\right)}{4n(n+1)} c_{n-2}, \text{ valid for } n = 2 \text{ or } n = 3 \tag{56}$$

$$c_n = -\frac{\xi^2\left[c_{n-2}\left(4n + \xi^2 - 6\right) + c_{n-4}\xi^2\right]}{4n(n+1)}, \text{valid for } n \geq 4. \tag{57}$$

Considering the case where $s = 1$, one obtains the other series linearly independent with the first term, not null, denoted by $\tilde{c}_0$:

$$c_n = -\frac{\xi^2\left(4n+\xi^2-2\right)}{4n\left(n+1\right)}c_{n-2}, \text{ valid for } n \geq 4 \tag{58}$$

$$c_n = -\frac{\xi^2\left[c_{n-2}\left(4n+\xi^2-2\right)+c_{n-4}\xi^2\right]}{4n\left(n+1\right)}, \text{ valid for } n \geq 4 \tag{59}$$

With this the homogeneous solution assumes the following form:

$$\psi_h\left(x,\xi\right) = \left(c_0 + c_2x^2 + c_4x^4 + \ldots\right) + \left(\tilde{c}_0x + \tilde{c}_2x^3 + \tilde{c}_4x^5 + \ldots\right), \tag{60}$$

where the coefficients are all known from the relations of recurrence, equations (56) to (59). In writing function $\psi_h(x, \xi)$ as:

$$\begin{aligned}\psi_h\left(x,\xi\right) &= \exp\left(-\frac{\xi^2x^2}{4}\right)\sum_{n=0}^{\infty}A_nx^n = \left(1-\frac{\xi^2x^2}{4}+\frac{\xi^4x^4}{32}+\ldots\right)\sum_{n=0}^{\infty}A_nx^n \\ &= A_0 + A_1x + \left(A_2 - \frac{\xi^2}{4}A_0\right)x^2 + \left(A_3 - \frac{\xi^2}{4}A_1\right)x^3 + \left(A_4 - \frac{\xi^2}{4}A_2 + \frac{\xi^4}{32}A_0\right)x^4 + \\ &\left(A_5 - \frac{\xi^2}{4}A_3 + \frac{\xi^4}{32}A_1\right)x^5 + \left(A_6 - \frac{\xi^2}{4}A_4 + \frac{\xi^4}{32}A_2 - \frac{\xi^6}{384}A_0\right) + \left(A_7 - \frac{\xi^2}{4}A_5 + \frac{\xi^4}{32}A_3 - \frac{\xi^6}{384}A_1\right) + \ldots\end{aligned} \tag{61}$$

it is possible to determine all the coefficients A_n equalling, term by term, equations (60) and (61) so to write:

$$\begin{aligned}\psi_h\left(x,\xi\right) &= k_1\exp\left(-\frac{\xi^2x^2}{4}\right)\left[1-\frac{1}{2}\left(\frac{\xi^2x}{2}\right)^2+\frac{1}{24}\left(\frac{\xi^2x}{2}\right)^4+\frac{1}{720}\left(\frac{\xi^2x}{2}\right)^6+\ldots\right] \\ &+k_2\exp\left(-\frac{\xi^2x^2}{4}\right)\left[\frac{\xi^2x}{2}-\frac{1}{6}\left(\frac{\xi^2x}{2}\right)^3+\frac{1}{120}\left(\frac{\xi^2x}{2}\right)^5+\frac{1}{5040}\left(\frac{\xi^2x}{2}\right)^7+\ldots\right],\end{aligned} \tag{62}$$

Acknowledging the expansion of the cosine and sine functions, one obtains an analytical form to solve the homogeneous part of the differential equations that rule the Doppler broadening function:

$$\psi_h\left(x,\xi\right) = \exp\left(-\frac{\xi^2x^2}{4}\right)\left[k_1\cos\left(\frac{\xi^2x}{2}\right)+k_2\sin\left(\frac{\xi^2x}{2}\right)\right]. \tag{63}$$

In order to obtain the particular solutions of equation (45), and consequently its general solution, it is possible to apply the method of parameter variation from the linearly independent solutions:

$$\psi_1(x,\xi) = \exp\left(-\frac{\xi^2 x^2}{4}\right)\cos\left(\frac{\xi^2 x}{2}\right) \tag{64}$$

$$\psi_2(x,\xi) = \exp\left(-\frac{\xi^2 x^2}{4}\right)\sin\left(\frac{\xi^2 x}{2}\right), \tag{65}$$

Supposing a solution thus,

$$\psi_p(x,\xi) = u_1\psi_1(x,\xi) + u_2\psi_2(x,\xi) \tag{66}$$

where functions $u_1(x)$ and $u_2(x)$ are determined after the imposition of the initial conditions expressed by equations (46a) and (46b) and of the imposition of the nullity of the expression:

$$u'_1(x)\psi_1(x,\xi) + u'_2(x)\psi_2(x,\xi) = 0, \tag{67}$$

That, along with the condition,

$$u'_1(x)\psi'_1(x,\xi) + u'_2(x)\psi'_2(x,\xi) = \frac{\xi^4}{4}, \tag{68}$$

Which results from the very equation (45), form a linear system whose solution is given by the equations:

$$u'_1(x) = -\frac{\xi^2}{2}\exp\left(\frac{\xi^2 x^2}{4}\right)\sin\left(\frac{\xi^2 x}{2}\right) \Rightarrow u_1(x) = -\frac{\xi^2}{2}\int_0^x dx' \exp\left(\frac{\xi^2 x'^2}{4}\right)\sin\left(\frac{\xi^2 x'}{2}\right) \tag{69}$$

$$u'_2(x) = \frac{\xi^2}{2}\exp\left(\frac{\xi^2 x^2}{4}\right)\cos\left(\frac{\xi^2 x}{2}\right) \Rightarrow u_2(x) = \frac{\xi^2}{2}\int_0^x dx' \exp\left(\frac{\xi^2 x'^2}{4}\right)\cos\left(\frac{\xi^2 x'}{2}\right). \tag{70}$$

Integrating equations (69) and (70),

$$u_1(x) = \frac{\xi\sqrt{\pi}}{4}\exp\left(\frac{\xi^2}{4}\right)\left[erf\left(\frac{i\xi x - \xi}{2}\right) - erf\left(\frac{i\xi x + \xi}{2}\right) + 2erf\left(\frac{\xi}{2}\right)\right] \tag{71}$$

$$u_2(x) = -i\frac{\xi\sqrt{\pi}}{4}\exp\left(\frac{\xi^2}{4}\right)\left[erf\left(\frac{i\xi x-\xi}{2}\right)+erf\left(\frac{i\xi x+\xi}{2}\right)\right], \tag{72}$$

it is possible to write the solution particular of equation (45) as follows:

$$\begin{aligned}\psi_p(x,\xi) = &-i\frac{\xi\sqrt{\pi}}{4}\sin\left(\frac{\xi^2 x}{2}\right)\exp\left[-\frac{\xi^2}{4}\left(x^2-1\right)\right]\left[erf\left(\frac{i\xi x-\xi}{2}\right)+erf\left(\frac{i\xi x+\xi}{2}\right)\right]+\\ &\frac{\xi\sqrt{\pi}}{4}\cos\left(\frac{\xi^2 x}{2}\right)\exp\left[-\frac{\xi^2}{4}\left(x^2-1\right)\right]\left[erf\left(\frac{i\xi x-\xi}{2}\right)-erf\left(\frac{i\xi x+\xi}{2}\right)+2erf\left(\frac{\xi}{2}\right)\right].\end{aligned} \tag{73}$$

As the general solution of differential equation (45) is the sum of the solution of the homogeneous and particular equations, the initial conditions are imposed, as expressed by equations (46a) and (46b), to determine the constants:

$$k_1 = \frac{\xi\sqrt{\pi}}{2}\exp\left(\frac{\xi^2}{4}\right)\left[1-erf\left(\frac{\xi}{2}\right)\right] \tag{74}$$

$$k_2 = 0. \tag{75}$$

Finally, according to the Frobenius Method, the Doppler Broadening function can be written thus:

$$\begin{aligned}\psi(x,\xi) = &\frac{\xi\sqrt{\pi}}{2}\exp\left[-\frac{1}{4}\xi^2\left(x^2-1\right)\right]\cos\left(\frac{\xi^2 x}{2}\right)\times\\ &\left\{1+\operatorname{Re}\phi(x,\xi)+\tan\left(\frac{\xi^2 x}{2}\right)\operatorname{Im}\phi(x,\xi)\right\},\end{aligned} \tag{76}$$

where $\phi(x,\ \xi)=erf\left(\frac{i\xi x-\xi}{2}\right)$.

5.6. Fourier transform method

In doing the transformation of variables $u=\frac{\xi}{2}(x-y)$ in the full representation of the Doppler broadening function, equation (30), one obtains the expression

$$\psi(\xi,x) = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{+\infty}\frac{e^{-u^2}du}{1+\left(x-2\frac{u}{\xi}\right)^2}\ , \tag{77}$$

that can be mathematically interpreted as the convolution of the Lorentzian function with a gaussian function, as exemplified by the equation below:

$$\psi(\xi,\ x) = f * g \equiv \int_{-\infty}^{+\infty} g(u)\ f(x - u)\ du\ , \tag{78}$$

where $f(x - u) = \dfrac{1}{1 + \left(x - 2\dfrac{u}{\xi}\right)^2}$ is the lorentzian function and $g(u) = \dfrac{1}{\sqrt{\pi}} e^{-u^2}$ the gaussian function. Function $f(x - u)$ admits a full representation through the Fourier cosine transform (Polyanin and Manzhirov, 1998), as being

$$f(x - u) = \int_0^{\infty} e^{-w} \cos\left[\left(x - 2\frac{u}{\xi}\right) w\right] dw. \tag{79}$$

In replacing-se equation (79) in the integer of convolution, as given by equation (78), applying the properties of the integrals of convolution one gets to the following expression:

$$\psi(\xi,\ x) = f * g \equiv \int_0^{\infty} e^{-w} \int_{-\infty}^{+\infty} g(u)\ \cos\left[\left(x - 2\frac{u}{\xi}\right) w\right] du\ dw = \int_0^{\infty} e^{-w}\ I(w)\ dw\ , \tag{80}$$

where,

$$\begin{aligned} I(w) \ &\equiv\ \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-u^2} \ \cos\left[\left(x - 2\frac{u}{\xi}\right)\ w\right] du \\ &= \frac{1}{\sqrt{\pi}} \cos(xw) \int_{-\infty}^{+\infty} e^{-u^2} \cos\left[\left(2\frac{u}{\xi}\right)\ w\right] du = e^{-\frac{w^2}{\xi^2}}\ \cos(xw). \end{aligned} \tag{81}$$

In replacing equation (81) in the equation (80), one obtains a new full representation of the Doppler broadening function, interpreted as a Fourier cosine transform (Gonçalves et. al., 2008):

$$\psi(\xi,x) = \int_0^{\infty} e^{-\frac{w^2}{\xi^2} - w} \cos(wx)\ dw = \frac{1}{2}\left[\int_0^{\infty} e^{-\frac{w^2}{\xi^2} - 2wa} dw + \int_0^{\infty} e^{-\frac{w^2}{\xi^2} - 2wb} dw\right], \tag{82}$$

where $a \equiv \dfrac{(1 - ix)}{2}$ and $b \equiv \dfrac{(1 + ix)}{2}$.

The integrals on the right side of equations (3.25) and (3.26) are known as complementary error functions, in which case one can conclude that:

$$\int_0^\infty e^{-\frac{w^2}{\xi^2}-2\,wa}\,dw = \frac{\xi\sqrt{\pi}}{2}e^{\frac{(\mathrm{xi}-1)^2}{4}\xi^2}\,\mathrm{erfc}\left(\frac{\xi - i\xi x}{2}\right) \tag{83}$$

$$\int_0^\infty e^{-\frac{w^2}{\xi^2}-2\,wb}\,dw = \frac{\xi\sqrt{\pi}}{2}e^{\frac{(\mathrm{xi}+1)^2}{4}\xi^2}\,\mathrm{erfc}\left(\frac{\xi + i\xi x}{2}\right). \tag{84}$$

In replacing equations (83) and (84) in equation (82) it is possible to write the following expression for the Doppler broadening function:

$$\psi(x,\xi) = \frac{\xi\sqrt{\pi}}{4}e^{\frac{(xi-1)^2\xi^2}{4}}\left[1 + erf\left(\frac{i\xi x - \xi}{2}\right)\right] + \frac{\xi\sqrt{\pi}}{4}e^{\frac{(xi+1)^2\xi^2}{4}}\left[1 - erf\left(\frac{i\xi x + \xi}{2}\right)\right]. \tag{85}$$

With some algebraic manipulation it is easy to prove that the Fourier transform method and the Frobenius method, equations (85) and (76) respectively, provide identical results.

5.7. Fourier series method

From the representation of the Doppler broadening function in a Fourier cosine transform, equation (82), it is possible to write

$$\psi(\xi,x) = \int_0^\infty e^{-\frac{w^2}{\xi^2}-w}\cos(wx)\,dw = \int_0^\infty G(w)e^{-w}\cos(wx)\,dw, \tag{86}$$

where function $G(w)=e^{-\frac{w^2}{\xi^2}}$ is even and can be expanded into a Fourier series in cosines:

$$G(w) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi w}{L}\right), \tag{87}$$

where

$$a_0 = \frac{\xi\sqrt{\pi}}{L}erf\left(\frac{L}{\xi}\right) \tag{88}$$

$$a_n = \frac{\xi\sqrt{\pi}}{2L}e^{-\left(\frac{n\pi\xi}{2L}\right)^2}\left[erf\left(\frac{2L + n\pi\xi^2 i}{2\xi L}\right) + erf\left(\frac{2L - n\pi\xi^2 i}{2\xi L}\right)\right]. \tag{89}$$

In replacing equation (87) in equation (86) and integrand, it is possible to write the following expression for the Doppler broadening function in the form of Fourier series:

$$\psi(x,\xi) = \frac{\xi\sqrt{\pi}}{2L\left(1+x^2\right)} erf\left(\frac{L}{\xi}\right) + \frac{\xi\sqrt{\pi}}{L}\sum_{n=1}^{\infty} F_n(x,\xi,L)\,\mathrm{Re}\left[Z(\xi,L)\right], \tag{90}$$

where

$$F_n(x,\xi,L) \equiv \frac{\left[(n\pi)^2 + L^2\left(1+x^2\right)\right] e^{-\left(\frac{n\pi\xi}{2L}\right)^2}}{L^2\left(1+x^2\right)^2 + (n\pi)^2\left(2-2x^2+(n\pi/L)^2\right)}, \tag{91}$$

$$Z(n,\xi,L) = erf\left(\frac{n\pi\xi^2 i + 2L^2}{2\xi L}\right). \tag{92}$$

5.8. Representation of function $\psi(x,\ \xi)$ using Salzer expansions

Although the formulations obtained for function $\psi(x,\ \xi)$ from the Frobenius method, Fourier transform and Fourier series methods only contain functions that are well-known in literature, it can be inconvenient to work with error functions that contain an imaginary argument. One of the ways to overcome this situation is to calculate the real and imaginary parts of function $\phi(x,\ \xi)$ using the expansions proposed by Salzer (Palma and Martinez, 2009)

$$\phi(x,\xi) = erf\left(\frac{i\xi x - \xi}{2}\right) = \mathrm{Re}\,\phi(x,\xi) + \mathrm{Im}\,\phi(x,\xi)\,i, \tag{93}$$

where:

$$\mathrm{Re}\,\phi(x,\xi) \cong -erf\left(\frac{\xi}{2}\right) + \exp\left(-\frac{\xi^2}{4}\right) \times \left\{\frac{1}{\pi\xi}\left[\cos\left(\frac{\xi^2 x}{2}\right) - 1\right] + \frac{2}{\pi}\sum_{n=1}^{n\max}\frac{\exp\left(-n^2/4\right)}{n^2+\xi^2} f_n(x,\xi)\right\} \tag{94}$$

$$\mathrm{Im}\,\phi(x,\xi) \cong \exp\left(-\frac{\xi^2}{4}\right)\left\{\frac{1}{\pi\xi}\sin\left(\frac{\xi^2 x}{2}\right) + \frac{2}{\pi}\sum_{n=1}^{n\max}\frac{\exp\left(-n^2/4\right)}{n^2+\xi^2} g_n(x,\xi)\right\}, \tag{95}$$

where auxiliary functions $f_n(x,\ \xi)$ and $g_n(x,\ \xi)$ are written by:

$$f_n(x,\xi) = -\xi + \xi\cosh\left(\frac{n\xi x}{2}\right)\cos\left(\frac{\xi^2 x}{2}\right) - n\sinh\left(\frac{n\xi x}{2}\right)\sin\left(\frac{\xi^2 x}{2}\right), \tag{96}$$

$$g_n(x,\xi) = \xi \cosh\left(\frac{n\xi x}{2}\right)\sin\left(\frac{\xi^2 x}{2}\right) + n\sinh\left(\frac{n\xi x}{2}\right)\cos\left(\frac{\xi^2 x}{2}\right). \tag{97}$$

5.9. The Mamedov method

Mamedov (Mamedov, 2009) put forward an analytical formulation to calculate function $\psi(x,\ \xi)$, based on its representation in the form of a Fourier transform, equation (82). Using the expansions in series of the exponential and cosine functions,

$$e^{-x} = \lim_{N\to\infty}\sum_{i=1}^{N}\frac{(-1)^i x^i}{i!}, \tag{98}$$

$$\cos x = \lim_{N\to\infty}\sum_{i=0}^{N}\frac{(-1)^i x^{2i}}{(2i)!}, \tag{99}$$

and the well-known binomial expansion

$$(x \pm y)^n = \lim_{N\to\infty}\sum_{m=0}^{N}(\pm 1)^m F_m(n) x^{n-m} y^m, \tag{100}$$

Mamedov proposed the following expressions for the Doppler broadening function:

for $\xi > 1$ and $x > 1$

$$\begin{aligned}\psi(x,\xi) = {} & \frac{\xi}{2\sqrt{\pi}}\lim_{L\to\infty}\sum_{i=0}^{L}F_i(-1)\Bigg\{\frac{1}{(x^2+1)^{i+1}}\sum_{j=0}^{i}F_j(i)\left[1+(-1)^j\right] \\ & \times\frac{2^{2i}x^j}{\xi^{2i-j+1}}\gamma\left(\frac{2i-j+1}{2},\frac{\xi^2(x^2+1)^2}{4}\right) + (x^2+1)^i\lim_{M\to\infty}\sum_{k=0}^{M}F_k(-1-i) \\ & \times\left[1-(-1)^k\right]\frac{x^k\xi^{2i+k+1}}{2^{2i+2}}\Gamma\left(-\frac{2i+k+1}{2},\frac{\xi^2(x^2+1)^2}{4}\right)\Bigg\},\end{aligned} \tag{101}$$

for $\xi \le 1$ and $x \le 15$

$$\psi(x,\xi) = \frac{\xi}{2\sqrt{\pi}}\lim_{L\to\infty}\sum_{i=0}^{L}\sum_{j=0}^{M}\frac{(-1)^{i+j}x^{2j}\xi^{2j+i+1}}{2i!(2j!)}\Gamma\left(\frac{i+2j+1}{2}\right), \tag{102}$$

for $\xi \le 1$ and $x = 0$

$$\psi(x,\xi)=\frac{\xi}{2\sqrt{\pi}}\lim_{L\to\infty}\sum_{i=0}^{L}\frac{(-1)^{i}\,\xi^{i+1}}{2i!}\Gamma\left(\frac{i+1}{2}\right), \tag{103}$$

where $\Gamma(x,\ \xi)$, $\gamma(x,\ \xi)$ and $\Gamma(x)$ are the well-know incomplete Gamma functions and $F_m(n)$ are binomials coefficients defined by:

$$F_m(n)=\begin{cases}\dfrac{n(n-1)\ldots(n-m+1)}{m!}, & \text{for integer n}\\[2ex] \dfrac{(-1)^{m}\,\Gamma(m-n)}{m!\,\Gamma(-n)}, & \text{for non-integer n}\end{cases} \tag{104}$$

6. Numerical calculation of function $\psi(x,\ \xi)$

The numerical calculation of the Doppler broadening function consists of calculating a defined integral. There are many methods in the literature for this calculation, but in this chapter we will describe a numerical reference method based on the Gauss-Legendre quadrature. In basic terms, the Gauss-Legendre quadrature method consists of approximating a defined integer through the following expression:

$$\int_{-1}^{1} f\left(\frac{b-a}{2}\eta+\frac{b+a}{2}\right)dx\approx\frac{b-a}{2}\sum_{i=1}^{N}w_i f\left(\frac{b-a}{2}\eta_i+\frac{b+a}{2}\right), \tag{105}$$

where N is the order of the quadrature, $\eta_i$is the point of the quadrature and w_i the weight corresponding to the point of quadrature. The points of the Gauss-Legendre quadrature are the roots of the polynomials of Legendre (Arfken, 1985) in the interval $[-1,\ 1]$, as generated from the Rodrigues' formula,

$$P_n(x)=\frac{1}{2^n n!}\frac{d^n}{dx^n}\left\{(x^2-1)^n\right\}. \tag{106}$$

for an isotope at a given temperature, that is, for a fixed value for variable ξ, the function $\psi(x,\ \xi)$ decreases rapidly and a very high value is not necessary for what we will consider our numerical infinite. This fact can be evidenced at Figure 1.

For that an adequate numerical infinite ($x=5000$) was considered, as well as a high-order quadrature ($N=15$), whose points of Legendre and respective weights are found in Table 3. The results obtained with this method, whose handicap is the high computing cost, can be seen in Table 4.

i	x_i	$\omega(x_i)$
1	0.9879925	0.0307532
2	0.9372734	0.0703660
3	0.8482066	0.1071592
4	0.7244177	0.1395707
5	0.5709722	0.1662692
6	0.3941513	0.1861610
7	0.2011941	0.1984315
8	0.0000000	0.2025782
9	-0.2011941	0.1984315
10	-0.3941513	0.1861610
11	-0.5709722	0.1662692
12	-0.7244177	0.1395707
13	-0.8482066	0.1071592
14	-0.9372734	0.0703660
15	-0.9879925	0.0307532

Table 3. Points of Legendre η_i and respective w_i weights.

ξ / x	0	0.5	1	2	4	6	8	10	20	40
0.01	0.00881	0.00881	0.00881	0.00881	0.00881	0.00880	0.00880	0.00879	0.00873	0.00847
0.02	0.01753	0.01753	0.01752	0.01752	0.01750	0.01746	0.01742	0.01735	0.01685	0.01496
0.03	0.02614	0.02614	0.02614	0.02612	0.02605	0.02594	0.02578	0.02557	0.02393	0.01836
0.04	0.03466	0.03466	0.03465	0.03461	0.03445	0.03418	0.03381	0.03333	0.02965	0.01857
0.05	0.04309	0.04308	0.04306	0.04298	0.04267	0.04216	0.04145	0.04055	0.03380	0.01639
0.10	0.08384	0.08379	0.08364	0.08305	0.08073	0.07700	0.07208	0.06623	0.03291	0.00262
0.15	0.12239	0.12223	0.12176	0.11989	0.11268	0.10165	0.08805	0.07328	0.01695	0.00080
0.20	0.15889	0.15854	0.15748	0.15331	0.13777	0.11540	0.09027	0.06614	0.00713	0.00070
0.25	0.19347	0.19281	0.19086	0.18325	0.15584	0.11934	0.08277	0.05253	0.00394	0.00067
0.30	0.22624	0.22516	0.22197	0.20968	0.16729	0.11571	0.07043	0.03881	0.00314	0.00065
0.35	0.25731	0.25569	0.25091	0.23271	0.17288	0.10713	0.05726	0.02816	0.00289	0.00064
0.40	0.28679	0.28450	0.27776	0.25245	0.17360	0.09604	0.04569	0.02110	0.00277	0.00064
0.45	0.31477	0.31168	0.30261	0.26909	0.17052	0.08439	0.03670	0.01687	0.00270	0.00064
0.50	0.34135	0.33733	0.32557	0.28286	0.16469	0.07346	0.03025	0.01446	0.00266	0.00063

Table 4. Reference values for Doppler Broadening Function $\psi(x, \xi)$.

7. Conclusion

A brief retrospective look at the calculation methodologies for the Doppler broadening function considering the approximations of Beth-Plackzec according to the formalism ofBriet-Wigner was presented in this chapter.

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