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A new formulation for the Doppler broadening function relaxing the approximations of Beth–Plackzec

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ABSTRACT

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. The thermal agitation movement in the reactor core is adequately represented in the 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 of a nuclear reactor. 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 and used for the approximate calculations of the resonance integrals in heterogeneous fuel cells. In these types of application we can point at the need to develop precise analytical approximations for the Doppler broadening function to be used in the calculation codes that calculate the values of this function. However, the Doppler broadening function is based on a series of approximations proposed by Beth–Plackzec. In this work a relaxation of these approximations is proposed, generating an additional term in the form of an integral. Analytical solutions of this additional term are discussed. The results obtained show that the new term is important for high temperatures.

1. Introduction

The thermal nuclei movement is well represented in the neutron–nuclei interaction through the Doppler broadening function and interference term function (Duderstadt and Hamilton, 1976). Considering an average thermal balance at temperature T where the target nuclei are in movement and their velocities given by the Maxwell–Boltzmann distribution (Lamarsh and Baratta, 2001), the expressions for the cross-section of radioactive capture near any isolated resonance with an energy peak from the Briet–Wigner formalism is written by:

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

where,

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

and A is the mass number, T is the absolute temperature, E is the energy of incident neutron, E_{CM} is the centre-of-mass energy, E_0 is the energy where the resonance occurs, Γ is the total width of the resonance as measured in the lab coordinates, v is the neutron velocity module, $\Gamma_D = (4E_0kT/A)^{1/2}$ is the Doppler width of resonance, $v_r = |v - V|$ is the module of the relative velocity between neutron movement and nucleus movement and $v_{th} = \sqrt{2kT/A}$ is the velocity module for each target nucleus.

Eq. (2) can be found in reference (Duderstadt and Hamilton, 1976) and usually from three proposed approaches for Beth–Placzek, only the first integral remains, generating the conventional Doppler broadening function $\psi(x,\xi)$ well established in the literature:

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

where the following are defined:

$$y = \frac{2}{\Gamma}(E_{CM} - E_0) \tag{4.a}$$

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

$$\xi = \frac{\Gamma}{\Gamma_D} = \frac{\Gamma}{(4E_0 kT/A)^{1/2}}. \tag{4.c}$$

Eq. (3) is obtained by taking into account the following approximations as proposed by Beth–Placzek.

Approximation 1: one neglects the second exponential in Eq. (2), given that $(v + v_r)^2 >> (v - v_r)^2$.

Approximation 2: to extend the lower limit for integration down to $-\infty$ in Eq. (2), given that the ratio between the energy of neutron incidence and the practical width is large.

Approximation 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:

$$E_{CM}^{1/2} = E^{1/2}\left(1 + \frac{E_{CM} - E}{E}\right)^{1/2} \approx E^{1/2}\left(1 + \frac{E_{CM} - E}{2E}\right), \tag{5}$$

This paper will obtain an analytical expression for the second term in Eq. (2), with denoted additional term $\psi_a(x, \xi)$, in the case the first approximation of Beth–Placzek (BP1) be relaxed:

$$\psi_a(x, \xi) = \frac{\xi}{2\sqrt{\pi}} \int_{-2E/\Gamma}^{+\infty} \frac{dy}{1 + y^2}\left[\exp\left(-\frac{(v + v_r)^2}{2v_{th}^2}\right)\right]. \tag{6}$$

In the next section Eq. (5) will be presented.

2. Mathematical formulation

For a heavy nucleus, the following approximation for the reduced mass of the system is valid:

$$M_R = \frac{Am}{A + m} = \frac{m}{1 + m/A} \approx m. \tag{7}$$

From Eqs. (5) and (7), it is possible to write:

$$\left(\frac{M_R v_r^2}{2}\right)^{1/2} = \left(\frac{mv^2}{2}\right)^{1/2}\left(1 + \frac{\frac{M_R v_r^2}{2} - \frac{mv^2}{2}}{mv^2}\right) \Rightarrow v_r = \frac{v_r^2 + v^2}{2v}. \tag{8}$$

From Eq. (8) and bearing in mind that $v_{th} = \sqrt{kT/A}$ one has:

$$\frac{1}{2v_{th}^2}\left(\frac{v^2 + v_r^2}{2v}\right)^2 = \frac{1}{2kTv^2/A}\left(\frac{3v^2 + v_r^2}{2}\right)^2 = \frac{1}{A \cdot 4EkT/A}(3E + E_{CM})^2. \tag{9}$$

In Eq. (9), and bearing in mind that near the resonance $E \approx E_0$, it is possible to recognise the term Γ_D. From Eqs. (4.a) and (4.b) it is possible to write:

$$(3x + y) = \frac{2}{\Gamma}(3E + E_{CM} - 4E_0) \Rightarrow (3E + E_{CM}) = \frac{\Gamma}{2}(3x + y) + 4E_0. \tag{10}$$

Thus, in replacing Eq. (10) into Eq. (9), one has the following expression:

$$\frac{1}{2v_{th}}\left(\frac{v^2 + v_r^2}{2v}\right)^2 = \frac{1}{A \cdot \Gamma_D^2}\left(\frac{(3x + y)\Gamma}{2} + 4E_0\right)^2 = \frac{\xi^2}{A}\left(\frac{(3x + y)}{2} + \frac{4E_0}{\Gamma}\right)^2. \tag{11}$$

Finally, in applying the second approach of Beth–Placzek, the additional term $\psi_a(x, \xi)$ can be written thus:

$$\psi_a(x, \xi) = \frac{\xi}{2\sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{dy}{1 + y^2} \exp\left[-\frac{\xi^2}{A}\left(\frac{(3x + y)}{2} + \frac{4E_0}{\Gamma}\right)^2\right]. \tag{12}$$

In contrast to the Doppler broadening function $\psi(x, \xi)$, where all parameters of the nuclear resonance to be studied are contained in the variable ξ, Eq. (12) explicitly shows in its functional form A, Γ and E_0. In the next section an analytical formulation for Eq. (12) will be proposed.

3. An analytical formulation for $\psi_a(x, \xi)$

In order to obtain an analytical expression for Eq. (12) it is convenient to define the following constants:

$$k_1 = \frac{1}{4A} \tag{13.a}$$

$$k_2 = \frac{8E_0}{\Gamma} + 3x, \tag{13.b}$$

This way, Eq. (12) can be written in a more convenient way:

$$\psi_a(x, \xi) = \frac{\xi}{2\sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{dy}{1 + y^2}\left[\exp(-\xi^2 k_1 (k_2 + y)^2)\right]. \tag{14}$$

Thus, integral Eq. (14) acquires a form similar to Eq. (3), which has a well-established and known solution. There are several approximations in the literature to calculate the function $\psi(x, \xi)$ as the 4-pole Padé approximation (Keshavamurthy and Harish, 1993), Fourier series (Gonçalves et al., 2012) or Binomial expansion (Mamedov, 2009) amongst other methods (Campos and Martinez, 1987; Campos and Martinez, 1989; Gonçalves et al., 2008; Palma et al., 2006; Ferran et al., 2015). In the present paper the Frobenius Method has been selected as it has been shown to be simple, accurate and fast (Campos and Martinez, 1987; Campos and Martinez, 1989; Gonçalves et al., 2008; Palma et al., 2006). From the analytical expression proposed by Palma et al. (2006) for the calculation of the Doppler broadening function $\psi(x, \xi)$,

$$\psi(x, \xi) = \frac{\xi\sqrt{\pi}}{2} \exp\left[-\frac{1}{4}\xi^2(x^2 - 1)\right] \cos\left(\frac{\xi^2 x}{2}\right) \times \left\{1 + \mathrm{Re}\phi(x, \xi) + \tan\left(\frac{\xi^2 x}{2}\right)\mathrm{Im}\phi(x, \xi)\right\}, \tag{15}$$

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

It is possible to use Eq. (15) to obtain an analytical formulation for the additional term $\psi_a(x, \xi)$ as Eqs. (3) and (14) are very similar in their functional forms. For that, it is necessary to make the following mathematical associations between Eqs. (3) and (14):

$$x \to -k_2 \tag{16.a}$$

$$\xi \to 2\sqrt{k_1}\xi. \tag{16.b}$$

Thus, after some algebraic work using Eqs. (16.a) and (16.b) in Eq. (15) it is possible to write the following expression for the additional term $\psi_a(x, \xi)$:

$$\psi_a(x, \xi) = \frac{\xi\sqrt{\pi}}{2} \exp\left[-\xi^2 k_1 (k_2^2 - 1)\right] \cos(2\xi^2 k_1 k_2) \times \left[1 + \mathrm{Re}\,\eta(x, \xi) - \tan(2\xi^2 k_1 k_2)\mathrm{Im}\,\eta(x, \xi)\right]. \tag{17}$$

where

$$\eta(x, \xi) = erf\left[-\xi\sqrt{k_1}(ik_2 + 1)\right] \tag{18}$$

The expression obtained for $\psi_a(x, \xi)$ in this paper, Eq. (17), is valid for any of the variables x and ξ values.