An Improved Kaniadakis Doppler Broadening Function

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INTRODUCTION

The thermal agitation movement in a reactor core is adequately represented by the microscopic cross-section of the neutron-nucleus interaction through the Doppler Broadening Function [1]. The general formalism that describes these reactions is already consolidated and well understood from the physical point of view, with the nuclei velocities in a nuclear reactor usually given by the Maxwell-Boltzmann Distribution [2]:

$$f(V,T) = \left(\frac{M}{2\pi k_B T}\right)^{3/2} e^{-\frac{MV^2}{2k_B T}}, \quad (1)$$

where T is the absolute temperature, M is the target nucleus mass, $\vec{V}$ it's velocity and k_B is the so–called Boltzmann constant.

In this paper, we will consider a nuclei velocity distribution that may be able to describe situations in thermal non-equilibrium, which can operate with thermodynamic configurations other than the current ones, such as temperature, pressure, and volume ranges. The Maxwell-Boltzmann Distribution is obtained from the product of probabilities, independent of the velocity components of the particles (in the case of target nucleus) which may not be valid in certain situations and that would affect reaction rates in the reactor core, deviating from the exponential behaviour in equation (1).

Despite the fact that the Maxwell-Boltzmann distribution describes the velocity distribution on the cores of nuclear reactors so well, new velocity distributions for the target nuclei in nuclear cores and their consequences in the Doppler Broadening Phenomenon have been under investigation, towards a new generation of reactors in which such quasi-Maxwellian velocity distributions are more adequate. Additionally, the effect of relaxing one of the Bethe-Plackzec approximations in the deduction of this new Doppler Broadening Function makes an additional term appears naturally.

Amongst so many velocity distribution functions as described in the literature, the Kaniadakis statistics [3] will be considered to study the effects of Doppler Broadening on a thermal non-equilibrium system. The Kaniadakis statistics is widely used in different areas of knowledge such as the statistics of cosmic rays, defect turbulence, optical lattices, hydrodynamic turbulence, scattering processes in particle physics, gravitationally interacting systems, and Hamiltonian systems with long-range interactions and metastable states.

The Kaniadakis distribution, also known as κ distribution, is based on a Boltzmann's H-theorem generalization, with an explicit functional dependency of a κ parameter that measures the deviation in relation to the Gaussian behaviour of the system. Formally, the κ-distribution is written as:

$$f_{\{\kappa\}}(V,T) = A(\kappa) exp_{\{\kappa\}}\left(-\frac{MV^2}{2k_B T}\right), \quad (2)$$

where

$$A(\kappa) = \left(\frac{|\kappa| M}{\pi k_B T}\right)^{n/2} \left(1 + \frac{1}{2} n|\kappa|\right) \frac{\Gamma(1/2|\kappa| + n/4)}{\Gamma(1/2|\kappa| - n/4)}, \quad (3)$$

n is the system's dimension and the κ-exponential is defined by:

$$exp_{\{\kappa\}}(z) = \left(\sqrt{1+\kappa^2 z^2} + \kappa z\right)^{1/\kappa}, \quad (4)$$

The κ-parameter is such that $|\kappa| < 2/n$, and if the limit $\kappa \to 0$ in equation (2) is taken, it reproduces the standard Maxwell-Boltzmann distribution as well as in the same limit, equation (4) is reduced to the usual exponential function. In the next section a brief review of the Doppler Broadening Function considering a Maxwell-Boltzmann distribution of target nuclei speed will be presented.

THE CONVENTIONAL DOPPLER BROADENING FUNCTION

The expressions for the cross-section of radioactive capture near any isolated resonance with an energy peak from the Breit–Wigner formalism [4] is written by:

$$\overline{\sigma_\gamma}(E,T) = \sigma_o \left(\frac{E_0}{E}\right)^{\frac{1}{2}} \Psi(x,\xi), \quad (5)$$

where,

$$\Psi(x,\xi) = \frac{\xi}{2\sqrt{\pi}} \int_{-\frac{2}{\Gamma}E_{0CM}}^{+\infty} \frac{dy}{1+y^2} \left\{ exp\left[-\frac{v(x)-v_r(y)}{2v_{th}^2}\right] + -exp\left[-\frac{v(x)+v_r(y)}{2v_{th}^2}\right] \right\}, \quad (6)$$

is the so-called Doppler Broadening Function, and the following are defined:

$$y = \frac{2}{\Gamma}(E_{CM} - E_{0CM}), \quad (7)$$
$$x = \frac{2}{\Gamma}(E - E_{0CM}), \quad (8)$$
$$\xi = \frac{\Gamma}{\Gamma_D}, \quad (9)$$

where E is the incident neutron energy, E_{CM} is the two body system's energy, E_{0CM} is the energy where the resonance occurs, both in the centre-of-mass coordinates, Γ is the total width of the resonance as measured in lab coordinates, $\Gamma_D = \sqrt{4Ek_BT/A}$, where A is the target nucleus mass number, is the Doppler width of resonance, $\underset{v}{\rightarrow}$ is the neutron velocity, $\underset{v_r}{\rightarrow} = \underset{v}{\rightarrow} - \underset{V}{\rightarrow}$ is the relative velocity between the neutron and nucleus movement, being v and v_r, respectively, their modules and $v_{th} = \sqrt{k_BT/A}$ is the scale parameter of the distribution. The Doppler Broadening Function as written in equation (6), in addition to having no analytical solution, presents a very complicated form. Thus, the possibility of making some approximations becomes very useful. To manage this problem, Bethe and Plackzec, in dealing with the resonance effects in nuclear processes and in particular the Doppler Broadening function, suggested some approximations for energies near the resonant peak [5]. These approximations are:

1) The second exponential in equation (6) is neglected, that is, it is considered that $[v(x) + v_r(y)]^2 >> [v(x) - v_r(y)]^2$;

2) Based on the fact that the ratio between the energy of neutron incidence and the practical width is large, it is possible to extend the lower integration limit of the remaining integral to $-\infty$;

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:

$$E_{CM}^{1/2} = E^{1/2}\left(1 + \frac{E_{CM-E}}{E}\right)^{1/2} \approx E^{1/2}\left(1 + \frac{E_{CM-E}}{2E}\right), \quad (10)$$

With these approaches taken on equation (6), only the first integral remains, and the conventional Doppler Broadening Function, well established in the literature, is obtained [1]:

$$\Psi(x,\xi) \approx \psi(x,\xi) = \frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{+\infty} \frac{dy}{1+y^2} e^{-\frac{\xi^2}{4}(x-y)^2}, \quad (11)$$

In this paper, it will be considered the Kaniadaks Doppler Broadening Function [6] in the case that the first of the Bethe and Plackzec approximations is not taken into account. That is, the Maxwell-Boltzmann velocity distribution given by equation (1) will be replaced by the Kaniadakis one, given by equation (2), and the first Bethe and Plackzec approximation will not be considered.

THE KANIADAKIS DOPPLER BROADENING FUNCTION

The functional form of the Doppler Broadening Function originates in two distinct formalisms, one of them from the quantum mechanics, through the single level formulation proposed by Briet and Wigner, and another in the statistical mechanics, that considers the agitation movement of the nuclei inside the reactor obeying the Maxwell-Boltzmann statistics, given by equation (1). Thus, in the present paper, the way of understanding the quantum mechanics of the system will be maintained, changing only the statistical distribution of velocities, considering the quasi-Maxwellian distribution known as Kaniadakis distribution. In this context, the Kaniadakis Doppler broadening Function can be written as [6]:

$$\Psi_{\{\kappa\}}(x,\xi) = \frac{\xi}{2\sqrt{\pi}}B(\kappa)\int_{-\frac{2}{\Gamma}E_{0CM}}^{+\infty}\frac{dy}{1+y^2}\left\{iexp_{\{\kappa\}}\left[-\frac{v(x)-v_r(y)}{2v_{th}^2}\right] + -iexp_{\{\kappa\}}\left[-\frac{v(x)+v_r(y)}{2v_{th}^2}\right]\right\}, \quad (12)$$

where $B(\kappa)$ is defined as:

$$B(\kappa) = (2|\kappa|)^{3/2}\left(1 + \frac{3}{2}|\kappa|\right)\frac{\Gamma(1/2|\kappa|+3/4)}{\Gamma(1/2|\kappa|-3/4)}, \quad (13)$$

and the function $iexp_{\{\kappa\}}$ is defined by:

$$iexp_{\{\kappa\}}(x) = \left(\frac{\kappa^2 x - \sqrt{\kappa^2 x^2 + 1}}{\kappa^2 - 1}\right) exp_{\{\kappa\}}(x) \quad (14)$$

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

$$\mu = \frac{Am_n^2}{Am_n + m_n} = \frac{m_n}{1+1/A} \approx m_n, \quad (15)$$

where m_n is the neutron mass. From equations (10) and (15), it is possible to write:

$$v_r(x) = \frac{v_r^2(x) + v^2(y)}{2v(y)}. \quad (16)$$

In order to obtain the enlarged Doppler Broadening function, we will consider only the last two Bethe-Plackzec approximations, in the same way it as in [7] for the usual Doppler Broadening function.

By using equation (16), the arguments of the functions in equation (12) becomes:

$$\frac{v(x)-v_r(y)}{2v_{th}^2} = \frac{\xi^2}{4}(x-y)^2, \quad (17)$$
$$\frac{v(x)+v_r(y)}{2v_{th}^2} = \frac{\xi^2}{A}\left(\frac{3x+y}{2} + \frac{4E_0}{\Gamma}\right)^2. \quad (18)$$

Finally, with equations (17) and (18), equation (12) can be written as:

$$\Psi_{\{\kappa\}}(x,\xi) \approx \psi^E_{\{\kappa\}}(x,\xi) = \psi_{\{\kappa\}}(x,\xi) - \psi^a_{\{\kappa\}}(x,\xi), \quad (19)$$

where,

$$\psi_{\{\kappa\}}(x,\xi) = \frac{\xi}{2\sqrt{\pi}} B(\kappa) \int_{-\infty}^{+\infty} \frac{dy}{1+y^2} iexp_{\{\kappa\}} \left[-\frac{\xi^2}{4}(x-y)^2\right], \quad (20)$$

is the Kaniadakis Doppler Broadening Function, as can be found in [6], and $\psi^a_{\{\kappa\}}(x,\xi)$ is the additional term, given by:

$$\psi^a_{\{\kappa\}}(x,\xi) = \frac{\xi}{2\sqrt{\pi}} B(\kappa) \int_{-\infty}^{+\infty} \frac{dy}{1+y^2} iexp_{\{\kappa\}} \left[-\frac{\xi^2}{A}\left(\frac{3x+y}{2} + \frac{4E_0}{\Gamma}\right)^2\right]. \quad (21)$$

The function denoted by $\psi^E_{\{\kappa\}}(x,\xi)$ is the enlarged Kaniadakis Doppler Broadening Function. It can be noted that, unlike the Kaniadakis Doppler broadening function $\psi_{\{\kappa\}}(x,\xi)$ where all parameters of the nuclear resonance to be studied are contained in the variable ξ, equation (21) explicitly shows in its functional form, A, Γ, and E_0. In the next section, the results obtained will be reported.

RESULTS

In this section the results obtained by considering the additional term $\psi^a_{\{\kappa\}}(x,\xi)$ will be reported. The results were obtained by using the Gauss-Legendre quadrature method [8] for the integrals in equations (20) and (21). This method basically consists of approximating a defined integral according to the expression:

$$\int_a^b f(x)dx = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{b-a}{2}x + \frac{b-a}{2}\right)dx \approx \frac{b-a}{2}\sum_{i=1}^{N} \omega_i f\left(\frac{b-a}{2}x + \frac{b-a}{2}\right), \quad (22)$$

where N is the order of the quadrature, x_i is the point of quadrature, and ω_i is the weight function corresponding to the point of quadrature. The Gauss-Legendre quadrature points are the roots of the Legendre polynomial in the interval $[-1, 1]$. In this paper a 15^0 order method was implemented to generate the data for the construction of the tables present in this section.

Tables 1, 2 and 3 shows, respectively, the results obtained for the functions $\psi^a_{\{\kappa\}}(x,\xi)$ and $\psi^E_{\{\kappa\}}(x,\xi)$ by fixing $\kappa = 0.1, 0.4$ and 0.6 considering the first resonance of the ^{238}U isotope $E_0 = 6.674\ eV$.

The % deviation is calculated by the following expression:

$$\% = 100 \times \left|\frac{\psi^E_{\{\kappa\}}(x,\xi) - \psi_{\{\kappa\}}(x,\xi)}{\psi^E_{\{\kappa\}}(x,\xi)}\right| = 100 \times \left|\frac{\psi^a_{\{\kappa\}}(x,\xi)}{\psi^E_{\{\kappa\}}(x,\xi)}\right|. \quad (23)$$

TABLE 1. Functions $\psi^a_{\{\kappa\}}(x,\xi)$ and $\psi^E_{\{\kappa\}}(x,\xi)$ ranging x and ξ and fixing $\kappa = 0.1$, considering the first resonance of the ^{238}U isotope $E_0 = 6.674\ eV$.

ξ	$x=-30$			$x=-10$			$x=0$			$x=10$			$x=30$		
	$\psi^a_{\{\kappa\}}(x,\xi)$	$\psi^E_{\{\kappa\}}(x,\xi)$	%	$\psi^a_{\{\kappa\}}(x,\xi)$	$\psi^E_{\{\kappa\}}(x,\xi)$	%	$\psi^a_{\{\kappa\}}(x,\xi)$	$\psi^E_{\{\kappa\}}(x,\xi)$	%	$\psi^a_{\{\kappa\}}(x,\xi)$	$\psi^E_{\{\kappa\}}(x,\xi)$	%	$\psi^a_{\{\kappa\}}(x,\xi)$	$\psi^E_{\{\kappa\}}(x,\xi)$	%
0.01	0.00556	0.00295	188.5	0.00542	0.00327	166.0	0.00535	0.00336	159.2	0.00528	0.00341	154.7	0.00513	0.00339	151.6
0.02	0.00293	0.01293	22.6	0.00264	0.01451	18.2	0.00251	0.01481	16.9	0.00238	0.01477	16.1	0.00214	0.01372	15.6
0.03	0.00053	0.02068	2.6	0.00043	0.02484	1.7	0.00039	0.02544	1.5	0.00035	0.02492	1.4	0.00028	0.02094	1.3
0.04	0.00005	0.02415	0.2	0.00004	0.03291	0.1	0.00003	0.03422	0.1	0.00003	0.03292	0.1	0.00002	0.02418	0.1
0.05	0.00000	0.02486	0.0	0.00000	0.04009	0.0	0.00000	0.04258	0.0	0.00000	0.04009	0.0	0.00000	0.02486	0.0

TABLE 2. Functions $\psi^a_{\{\kappa\}}(x,\xi)$ and $\psi^E_{\{\kappa\}}(x,\xi)$ ranging x and ξ and fixing $\kappa = 0.4$, considering the first resonance of the ^{238}U isotope $E_0 = 6.674\ eV$.

ξ	$x=-30$			$x=-10$			$x=0$			$x=10$			$x=30$		
	$\psi^a_{\{\kappa\}}(x,\xi)$	$\psi^E_{\{\kappa\}}(x,\xi)$	%	$\psi^a_{\{\kappa\}}(x,\xi)$	$\psi^E_{\{\kappa\}}(x,\xi)$	%	$\psi^a_{\{\kappa\}}(x,\xi)$	$\psi^E_{\{\kappa\}}(x,\xi)$	%	$\psi^a_{\{\kappa\}}(x,\xi)$	$\psi^E_{\{\kappa\}}(x,\xi)$	%	$\psi^a_{\{\kappa\}}(x,\xi)$	$\psi^E_{\{\kappa\}}(x,\xi)$	%
0.01	0.00471	0.00195	241.3	0.00461	0.00216	213.7	0.00456	0.00222	205.6	0.00451	0.00225	200.4	0.00442	0.00224	197.5
0.02	0.00382	0.00871	43.8	0.00360	0.00978	36.8	0.00350	0.00999	35.0	0.00340	0.00998	34.1	0.00321	0.00932	34.4
0.03	0.00218	0.01491	14.6	0.00202	0.01775	11.4	0.00195	0.01819	10.7	0.00188	0.01790	10.5	0.00174	0.01535	11.4
0.04	0.00130	0.01878	6.9	0.00120	0.02467	4.9	0.00115	0.02557	4.5	0.00111	0.02476	4.5	0.00102	0.01906	5.4
0.05	0.00085	0.02067	4.1	0.00078	0.03082	2.5	0.00075	0.03249	2.3	0.00072	0.03088	2.3	0.00066	0.02085	3.2

TABLE 3. Functions $\psi^a_{\{\kappa\}}(x,\xi)$ and $\psi^E_{\{\kappa\}}(x,\xi)$ ranging x and ξ and fixing $\kappa = 0.6$, considering the first resonance of the ^{238}U isotope $E_0 = 6.674\ eV$.

ξ	$x=-30$			$x=-10$			$x=0$			$x=10$			$x=30$		
	$\psi^a_{\{\kappa\}}(x,\xi)$	$\psi^E_{\{\kappa\}}(x,\xi)$	%	$\psi^a_{\{\kappa\}}(x,\xi)$	$\psi^E_{\{\kappa\}}(x,\xi)$	%	$\psi^a_{\{\kappa\}}(x,\xi)$	$\psi^E_{\{\kappa\}}(x,\xi)$	%	$\psi^a_{\{\kappa\}}(x,\xi)$	$\psi^E_{\{\kappa\}}(x,\xi)$	%	$\psi^a_{\{\kappa\}}(x,\xi)$	$\psi^E_{\{\kappa\}}(x,\xi)$	%
0.01	0.00205	0.00058	350.4	0.00202	0.00065	312.2	0.00201	0.00067	301.3	0.00199	0.00068	294.6	0.00196	0.00067	292.4
0.02	0.00236	0.00267	88.4	0.00229	0.00300	76.3	0.00225	0.00307	73.4	0.00222	0.00307	72.3	0.00215	0.00288	74.7
0.03	0.00218	0.00486	44.9	0.00210	0.00574	36.6	0.00206	0.00588	35.1	0.00203	0.00581	34.9	0.00196	0.00507	38.6
0.04	0.00200	0.00656	30.5	0.00193	0.00837	23.0	0.00189	0.00866	21.9	0.00186	0.00844	22.0	0.00180	0.00677	26.5
0.05	0.00186	0.00776	24.0	0.00180	0.01086	16.5	0.00176	0.01138	15.5	0.00173	0.01092	15.8	0.00167	0.00795	21.0

From the results summarized in the tables 1 to 3 it is possible to conclude that the influence of the additional term $\psi^a_{\{\kappa\}}(x,\xi)$ can not be neglected if $\xi < 0.05$. Also, as the κ-parameter is increased, the influence of the additional term $\psi^a(x,\xi)$ is emphasized. This statement can be justified by the fact that, as κ increases, the limit for which ξ can not be neglected also increases.

CONCLUSIONS

This work evaluated the hypothesis of disregarding the first of the Beth–Plackzec approximations. With it, an additional term to the Kaniadakis Doppler broadening function $\psi^a_{\{\kappa\}}(x,\xi)$ is obtained. Although the effect of considering the additional term $\psi^a_{\{\kappa\}}(x,\xi)$ is small, it can be noted that this term can not be neglected for high temperatures, that is, for small values of ξ. It can also be noted that, if the additional term $\psi^a_{\{\kappa\}}(x,\xi)$is taken into account, then the symmetry of the Kaniadakis Doppler Broadening Function is lost, that is, for a positive value of the x parameter, there is a slightly greater absorption than for its negative symmetric value $-x$. Analyzing the presented results, it is noticed that as κ increases, it becomes increasingly evident the influence of the additional term $\psi^a_{\{\kappa\}}(x,\xi)$ in the Kaniadakis Doppler Broadening Function. Thus, if a system is ruled by the Kaniadakis statistics the inclusion of the additional term is probably not negligible.

ACKNOWLEDGMENT

This research project is supported by the following Brazilian institutions: Brazilian Council for Scientific and Technological Development (CNPq), Brazilian Nuclear Energy Commission (CNEN), and Research Support Foundation of the State of Rio de Janeiro (FAPERJ).

REFERENCES

[1] Duderstadt, J. J. and L. J. Hamilton, *Nuclear Reactor Analisys, 1st Edition*, John Wiley & Sons, New York, NY (1976).

[2] R. K. Pathria and P. D. Beale, *Statistical Mechanics, 3rd Edition*, Elsevier, New York, NY (2011).

[3] G. Kaniadakis, “Non-linear kinetics underlying generalized statistics”, *Physica A: Statistical Mechanics and its Applications*, **296**, 405-425 (2001) doi:10.1016/S0378-4371(01)00184-4.

[4] G. Breit and E. Wigner, “Capture of slow neutrons”, *Physical Review (Series I)*, **49**, 519–531 (1936); doi:10.1103/PhysRev.49.519.

[5] H. A. Bethe and G. Placzek, “Resonance Effects in Nuclear Processes”, *Physical Review (Series I)*, **51**, 450-484 (1937);
doi:10.1103/PhysRev.51.450.

[6] G. Guedes et al., “The Doppler Broadening Function using the Kaniadakis distribution”, *Annals of Nuclear Energy*, **110**, 453-458 (2017); doi: 10.1016/j.anucene.2017.06.057.
doi:10.1016/j.anucene.2017.06.057, in press.

[7] Daniel A. P. Palma et al., “A new formulation for the Doppler Broadening Function relaxing the approximations of Beth–Plackzec”, *Annals of Nuclear Energy*, **88**, 68-72 (2016); doi:10.1016/j.anucene.2015.10.030

[8] R. Burden and J. Faires, *Numerical Analysis, 9th Edition*, Brooks Cole, Boston, MA, (2011).