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Calculation of Deformed Cross Sections Applying Kaniadakis Distribution Using FRENDY Code

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1. Introduction

Over the years, numerical and analytical solutions have been developed for calculating the Doppler broadening function using the Kaniadakis deformed statistics. This distribution presents the factor κ that expresses the level of deformation regarding the standard Maxwell-Boltzmann distribution and is defined by [1]:

$$f_\kappa(V,T) = A(\kappa)\exp_\kappa\left(-\frac{MV^2}{2k_\mathrm{B}T}\right), \tag{1}$$

where M is the nucleus mass, V is the velocity of the target nucleus, T is the temperature of the medium and $A(\kappa)$ is defined as:

$$A(\kappa) = \left(\frac{|\kappa|M}{\pi k_\mathrm{B}T}\right)^{n/2}\left(1+\frac{3|\kappa|}{2}\right)\frac{\Gamma\left(\frac{1}{2|\kappa|}+\frac{3}{4}\right)}{\Gamma\left(\frac{1}{2|\kappa|}-\frac{3}{4}\right)}. \tag{2}$$

Considering that this type of statistics is not yet applied in current reactors, using this methodology in existing nuclear data generation codes is necessary to validate the results. In this context, the current work applied the deformed numerical solution of Doppler broadening using the aforementioned statistic within the FRENDY nuclear code to generate unprecedented values of deformed cross-sections using official databases. The nuclear code used was developed by the Japanese Atomic Energy Agency (JAEA). Its great advantage is using the latest format for nuclear data, Generalized Structure of Nuclear Data (GNDS). This research compared these values with those generated by the standard Maxwell-Boltzmann statistics calculated by the same nuclear code.

2. Methodology

The starting point from the present work is the new nuclear data processing code called FRENDY. It was developed by the Japan Atomic Energy Agency (JAEA), and it has a similar processing method to that of the NJOY. FRENDY is written in the object-oriented language C++ and was developed with the intention to offer good maintainability, modularity, portability and flexibility [2].

To calculate Doppler broadening cross-sections for the unresolved resonance region, FRENDY uses the $\psi - \chi$ method, which approximately calculates the Doppler broadened cross-sections. In order to do that, the code uses the definitions of the cross-sections:

$$\sigma_\gamma = \sigma_0 \left(\frac{\Gamma_\gamma}{\Gamma}\right)\left(\frac{E_0}{E}\right)^{\frac{1}{2}} \psi(\xi, x) \tag{3}$$

$$\sigma_s = \sigma_0 \frac{\Gamma_n}{\Gamma} \psi(\xi, x) + \sigma_0 \frac{R}{\lambda_0} \chi(\xi, x) + 4\pi R^2, \tag{4}$$

where R represents the nuclear radius, λ_0 corresponds to the reduced neutron wavelength ($\lambda_0 = h/\sqrt{2mE}$), E is the energy of the incident neutron, E_0 is the resonant energy, K_B represents the Boltzmann constant, A is the mass number, T is the temperature of the medium, and Γ is the total width of the resonance as measured in the laboratory coordinates. Besides:

$$x = \frac{2}{\Gamma}(E - E_0) \tag{5}$$

$$\xi \equiv \frac{\Gamma}{\left(\frac{4E_0 K_B T}{A}\right)^{1/2}} \tag{6}$$

To calculate the deformed Kaniadakis Cross-sections (KCS), it is necessary to substitute the expressions $\psi(\xi, x)$ and $\chi(\xi, x)$, which considers the standard Maxwell-Boltzmann distribution for the Kaniadakis expressions, $\psi_\kappa(\xi, x)$ and $\chi_\kappa(\xi, x)$ defined by [3,4]:

$$\psi_\kappa(\xi, x) = \frac{\xi}{2\sqrt{\pi}} B(\kappa) \int_{-\infty}^{+\infty} \frac{dy}{1 + y^2} iexp_\kappa \left[\frac{-\xi^2 (x - y)^2}{4}\right] \tag{7}$$

And

$$\chi_\kappa(\xi, x) = \frac{\xi}{\sqrt{\pi}} B(\kappa) \int_{-\infty}^{+\infty} \frac{y\, dy}{1 + y^2} iexp_\kappa \left[\frac{-\xi^2 (x - y)^2}{4}\right] \tag{8}$$

Where

$$iexp_\kappa\left(\frac{-\xi^2(x-y)^2}{4}\right) \equiv \left(\frac{\kappa^2\left(\frac{-\xi^2(x-y)^2}{4}\right)-\sqrt{1+\kappa^2\left(\frac{-\xi^2(x-y)^2}{4}\right)^2}}{\kappa^2-1}\right) exp_\kappa\left(\frac{-\xi^2(x-y)^2}{4}\right) \tag{9}$$

$$exp_\kappa(x) = \left(\sqrt{1+\kappa^2x^2}+\kappa x\right)^{\frac{1}{\kappa}} \tag{10}$$

$$y = \frac{2}{\Gamma}(E_{CM}-E_0) \tag{11}$$

E_{CM} is the centre-of-mass energy,

$$B(\kappa) = (2|\kappa|)^{\frac{3}{2}}\left(1+\frac{1}{2}3|\kappa|\right)\frac{\Gamma\left(\frac{1}{2|\kappa|}+\frac{3}{4}\right)}{\Gamma\left(\frac{1}{2|\kappa|}-\frac{3}{4}\right)}. \tag{12}$$

An Alternative form that can be used to obtain the deformed values for the deformed Kaniadakis Doppler broadening function is to use the Effective medium temperature concept, which is [5]:

$$\psi_\kappa(\xi,x) \cong \psi_\kappa(\tilde{\xi},x) \cong \frac{\tilde{\xi}\sqrt{\pi}}{2}Re\left[\frac{i}{\sqrt{\pi}}\frac{p_0+p_1\tilde{z}+p_2\tilde{z}^2+p_3\tilde{z}^3}{1+q_1\tilde{z}+q_2\tilde{z}^2+q_3\tilde{z}^3+q_4\tilde{z}^4}\right] \tag{13}$$

where:

$$\tilde{z} = \tilde{u} + i\tilde{h} \tag{14}$$

$$\tilde{u} = \tilde{\xi}x/2 \tag{15}$$

$$\tilde{h} = \tilde{\xi}/2 \tag{16}$$

$$\tilde{\xi} = \frac{\Gamma}{\left(\frac{4E_0k_BT_{ef}}{A}\right)^{1/2}} \approx p_\kappa(x,\xi) for \begin{cases} 0.1 \le \kappa \le 0.5 \\ 0 \le x \le 40 \\ 0.05 \le \xi \le 0.5 \end{cases} \tag{17}$$

3. Preliminary results

The preliminary results indicate that the insertion of the deformed Kaniadakis Doppler broadening function in the FRENDY returned successful results, as illustrated in figure 1:

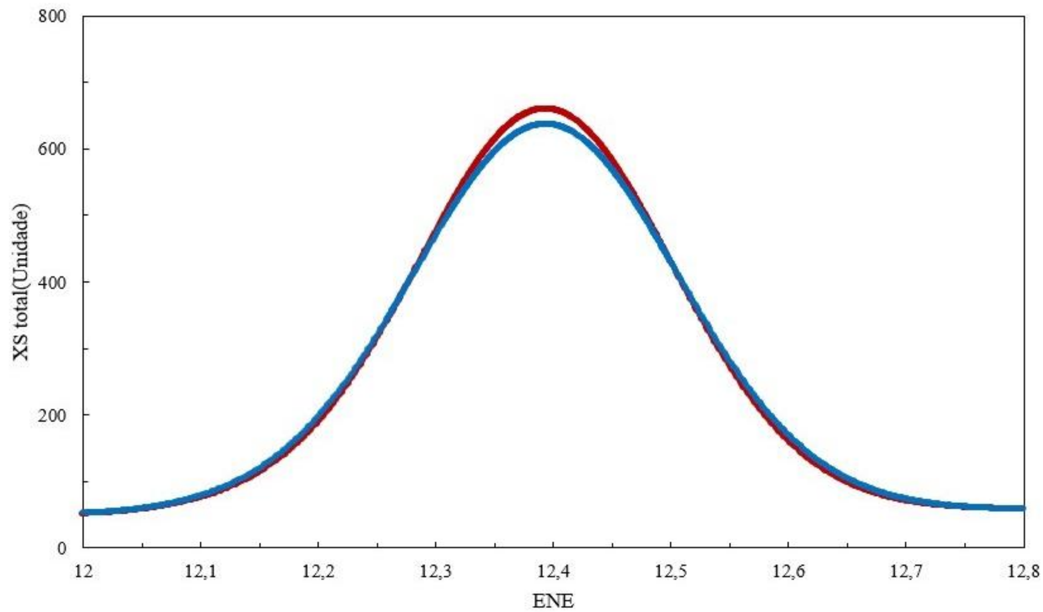

Figure 1: Comparison between XS Total results for Temperature = 1000K and material U-238, using Maxwell-Boltzmann distribution (red line) and Kaniadakis distribution (blue line).

5. Conclusions

The values of the cross-sections generated were compatible with the expected attenuation of the peaks as the value of κ increased. These results indicate that the application of generalized statistics is feasible even in codes developed for standard statistics.

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