

## INFLUENCE OF THE ELECTRON ENERGY DISTRIBUTION FUNCTION ON THE CALCULATION OF IONIZATION RATE IN HOT PLASMA

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*For a radiative collisional model, population densities of atomic levels are determined by a system of equations containing the various atomic process rates. The electron impact ionization is an important atomic process in the collisional radiative model as well as for the study of ionization balance. In many types of plasmas it has been observed that some electrons (hot) are governed by a non-Maxwellian energy distribution. The illustration of the effect of a non-Maxwellian distribution is provided for neutral helium emission lines and effective ionization rate coefficients. The ionization rates are generated from cross sections obtained by the Flexible Atomic Code (FAC), weighted by this distribution. We present, in this work, the effects of hot electrons on the ionization rates of Beryllium by using a non-Maxwellian distribution of hot electrons for different fractions. We study the influence of electron energy distribution functions on the calculation of ionization rate for neutral helium using a non-Maxwellian energy distribution in the case of weak values of hot electron fractions. The use of non-Maxwellian energy distribution for different fractions of hot electrons showed the sensitivity of these rates to the fractions of hot electrons and the forms of the electron energy distribution. The results are in good agreement compared to those found in the literature.*

**Keywords:** collisional radiative model, electron impact ionization, FAC, distribution function, non-Maxwellian distribution of electrons.

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### 1. Introduction

The electron impact ionization is an important atomic process in the description of line radiative emissions and also for the study of ion balance. Many problems related to the study of laboratory plasmas, astrophysics and controlled thermonuclear fusion require the knowledge of the atomic structure such as the energies of different levels and cross sections. Understanding the role of hot electrons in plasmas is particularly important because of their influence on the plasma dynamics, radiation production and energy balances[1]. Such electrons can lead to significant energy losses and have negative effects on the plasma stability and control. Non-Maxwellian and suprathermal (or 'hot') electrons turn out to be an important new topic to consider in plasma physics and fusion because these electrons can play an important role in the formation, evolution, and radiative properties of a wide variety of plasma sources. Distribution of non-Maxwellian electrons energy was predicted and detected in various laboratory sources including tokamak and laser plasmas [1], pulsed

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force plasmas [2], as well as astrophysical sources of solar flares [3] and active galactic nuclei, where they are produced by strong electric fields due to resonant laser-plasma interactions [4]. In addition, the collisional X-ray sources (RX) that measure the basic atomic processes, such as traps of electron beam ions are typically conducted by electron beams, which are mainly non-Maxwellian [5]. Atomic calculations of non-Maxwellian plasmas are not a recent topic: the work by Smith (2003) [6] attempts to explain anomalous helium resonance line intensities in the solar transition region by considering the effect of non-Maxwellian distributions. The distributions are approximated as locally Maxwellian below a certain velocity, and with a power-law decline above this velocity. Excitation and ionization rates are calculated based on these distributions, leading to estimates of the line intensities of interest.

Also, the calculation of rate coefficients is based on analytic expressions for the cross-sections which are drawn from dated sources, primarily Mihalas and Stone (1968) [7].

Further examples of non-Maxwellian electron distribution calculations include the work of MacNeice et al. on the solar atmosphere (1991) [8]. These authors calculated the distribution function through a solution of the Fokker-Planck equation applied to loops in the corona. Perhaps surprisingly, the results show no significant differences to the ionization balance of O, Ne or Si atoms in comparison with those calculated in the Maxwellian regime. This differs from the preponderant results of the literature; such as the substantial amount of work published by Dzifcakova (1992, 2002) [9] and Dzifcakova et al. (2003) [10] on the effects of non-Maxwellian distributions on coronal elements. Dzifcakova (1992) [11] calculated the ionization balance of Fe under the influence of the  $k$  distribution and found considerable differences in the fractions of  $\text{Fe}^{+15} - \text{Fe}^{+17}$  in the temperature range ( $10^5 \dots 10^8$ ) K with  $k = 2$ . Updated values for these calculations can be found in Dzifcakova (2002) [9]. A similar analysis has been carried out for C and O atoms (Dzifcakova et al. 2003) [10], the ionization peaks of the latter being found to be wider and the level populations lower for the  $k$  distribution compared to the Maxwellian one. Other authors, namely Owocki et al. (1983) [12] and Doyle et al. (2003) [13], showed that the  $\text{Fe}^{+8}$  171 Å line is shifted to  $6 \times 10^5 \text{K}$  for a Maxwellian distribution and to less than  $5 \times 10^5 \text{K}$  with a non-Maxwellian distribution. Owocki et al (1983) [12], using the  $k$  distribution, found that the high-energy tail decreases slightly the degree of ionization of  $\text{Fe}^{+11}$  to  $\text{Fe}^{+12}$ , but can significantly increase the ionization of  $\text{O}^{+6}$  to  $\text{O}^{+7}$ . Doyle et al. (2003) [13] also used the  $k$  distribution and found that the temperature at which  $\text{Fe}^{+8}$  lines are produced in detectable quantities is lowered from  $\approx 8 \times 10^5 \text{K}$  to  $\approx 3 \times 10^5 \text{K}$  with  $k$  in the range 2-10. Doyle et al. (2003) [13] showed that the  $\text{Fe}^{+8}$  171 Å line is shifted to  $6 \times 10^5 \text{K}$  for a Maxwellian distribution and to less than  $5 \times 10^5 \text{K}$  with a non-Maxwellian distribution.

Several authors, for many types of plasmas [14, 15, 16, 17, 18, 19, 20, 21], have used non-Maxwellian energy distributions of hot electrons to simulate the line spectra and to study the influence of hot electrons on radiative properties of a helium plasma [22].

Hansen et al. (2004) [23] present the results of a broad investigation into the effects of the electron energy distribution function on the predictions of non-LTE collisional-radiative atomic kinetics models. They studied the effects of the non-Maxwellian and suprathermal (“hot”) electrons distribution on collisional rates (including three-body recombination). It is shown that most collisional rates are fairly insensitive to the functional form and characteristic energy of the electron distribution function as long as the characteristic energy is larger than the threshold energy for the collisional process. Collisional excitation and

ionization rates however are highly sensitive to the fraction of hot electrons. This permits the development of robust spectroscopic diagnostics that can be used to characterize the electron density, bulk electron temperature, and hot electron fraction of plasmas with non-equilibrium electron distribution functions (EDFs). The effects of hot electrons on modeled K-shell lines have been extensively studied using two temperature electron distribution functions [24, 25].

The effects of the hot electron fractions on the ionization rate of neutral helium plasmas was studied (2013) [26]: the fraction of the hot electrons is represented by a non-maxwellian energy distribution. The ionization rates are generated from cross sections obtained by the flexible atomic code, weighted by this distribution. The use of a non-maxwellian energy distribution of hot electrons for different fractions allowed us to show the sensitivity of these rates with respect of the hot electron fractions.

These studies of hot electrons were adapted to particular experiments, and the obtained results were limited to fixed forms of energy distribution used to describe the hot electrons. Gaussian electronic energy distributions have been used to describe the hot electrons produced by intense laser pulses on gas target groups [27, 28, 29, 30]. Hot electrons in the plasma created by laser irradiation of solid targets have been described with Gaussian [31] and Maxwellian [24, 25] distribution functions. In pulsed power plasmas, they have been studied using Gaussian [16, 21] and power-law [18] distributions.

The objective of the work is to present the effects of hot electrons on the ionization rates of Beryllium by using a non-Maxwellian distribution of hot electrons for different fractions. .

Our main concern is focused on studying the influence of electron energy distribution functions on the calculation of ionization rate for neutral helium using a non-Maxwellian energy distribution in the case of weak values of hot electron fractions. We have done this, because the use of the non-maxwellian distribution gives unacceptable results for weak hot electron fractions.

This paper is organized as follows: we begin with an introduction, and then we calculate the ionization cross sections of Beryllium from the FAC in Section 2. Indeed, we present the effects of hot electrons on the calculation of ionization rate for Be using a non-Maxwellian distribution in Section 3. We discuss the results and we present comparisons with literature in Section 4. Section 5 is devoted to present the influence of electron energy distribution functions on the calculation of ionization rate for neutral helium and particularly establish different expressions of electron energy distribution functions. Some numerical results are reported in Section 6. Indeed, we present our contribution to regarding the effects of hot electrons fraction and the influence of electron energy distribution function on the calculation of ionization rate for neutral helium. Finally, we discuss the results and we close this work with a conclusion in Section 7.

## 2. Ionization Cross sections

Two models for the calculation of ionization cross sections by electron impact on atoms, the Binary-Encouter-Bethe and the Deutsch-Mark models, have been implemented [32]. Concerning the electron impact ionization of neutral particles, a large amount of experimental and theoretical work has been devoted in this century to determinate an accurate electron impact ionization cross-section functions (cross-sections versus electron energy) [33]. Because of the numerous potential neutral targets (atoms, molecules, radicals, clusters) and

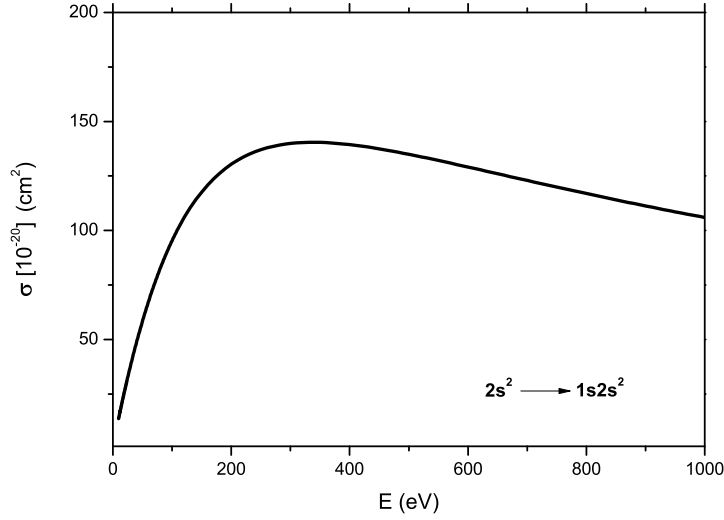


FIGURE 1. Electron impact ionization cross-section of Be obtained by FAC code for the transition:  $2s^2 \rightarrow 1s2s^2$ .

the formidable theoretical and experimental difficulties, the situation concerning quantitative knowledge of absolute electron impact ionization cross-sections is still unsatisfactory [33, 34]. In particular, the measurement and/or calculation of integrated (over all subshells) partial ionization cross-sections for the production of specific ions are not yet as accurate and numerous as necessary for the many areas of application [35].

Although significant progress has been made in recent years, no complete theoretical results are obtained so far. Ionization cross-section by electron impact can be calculated by the FAC code using the relativistic approximation "Distorted Wave method, DW" both with a method of interpolation-factorization [36, 37]. In our work, the ionization cross sections of Be were obtained by using FAC code. The obtained results are shown in Figure. 1 in the energy range (0-1000) eV.

### 3. The effects of hot electrons on the calculation of ionization rate

In plasma, free electrons are characterized by a certain distribution of energy. The interesting quantity is the ionization rate coefficient by electron impact which is obtained by averaging the product of the velocity of the electron by the ionization cross section. In the case of direct ionization, the coefficient of the ionization rate is given by [22, 23]:

$$\tau = \int \nu \sigma(E) F(E) dE, \quad (\text{cm}^3 \text{s}^{-1}). \quad (1)$$

where  $v$  and  $E$  are the velocity and energy, respectively, of the incident electron,  $\sigma(E)$  the impact ionization cross sections calculated by FAC code,  $F(E)$  is the electron energy distribution function,  $E$  is the energy of impact electron. We use a non-Maxwellian distribution function of energy  $F(E)$  to calculate the rate of ionization from cross sections. Low pressure produced plasmas often exhibit functions of non-Maxwellian distributions for electrons that

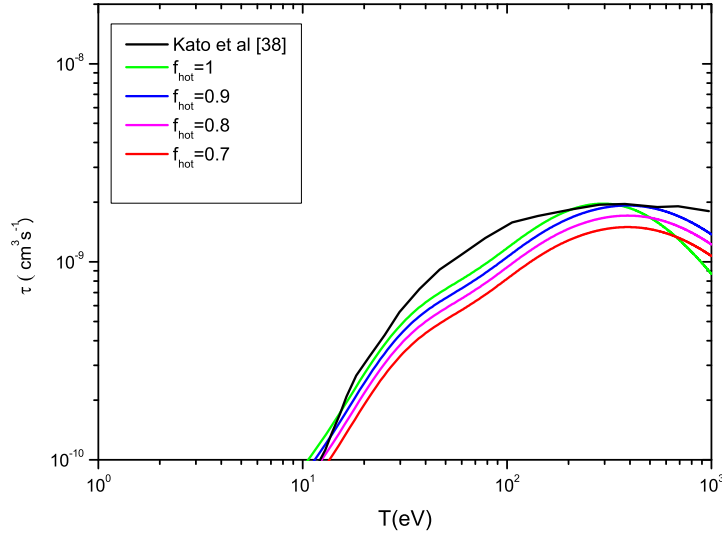


FIGURE 2. Coefficient of the ionization rate to Be obtained by a non-Maxwellian distribution for different values of hot electrons fraction:  $f_{hot} = 0.7, 0.8, 0.9$  and  $1.0$ .

can be represented by a distribution at two temperatures corresponding to a hot population and to a cold one. To study the effects of hot electrons on ionization rate of Beryllium; we have choose the following non-Maxwellian distribution [22]:

$$F_{NM}(E) = (1 - f_{hot}) F_M(T_{bulk}) + f_{hot} F_M(T_{hot}), \quad (2)$$

where  $f_{hot}$  is the normalized hot electron fraction,  $F_M$  is the Maxwell energy distribution function and  $T_{bulk}$  and  $T_{hot}$  are the bulk and hot electron temperatures, respectively. Substituting Equation (2) in Equation (1), with the effective ionization cross sections calculated by the FAC code of the Be enabled us to obtain the ionization rate for different values of hot electrons fraction  $f_{hot}$ .

#### 4. Discussion

The rate coefficients at very low temperatures are very sensitive to the cross section behavior near the threshold. There exist significant discrepancies between various theoretical calculations and/ or empirical scalings. The plane wave Born approximation is not valid at low energy and gives typically lower cross sections than DW computation near threshold by a factor 2 [38]. We plotted in Figure. 2 the curves representing the variations of the coefficients ionization rates of Be for the non-Maxwellian distribution for different values of hot electrons fraction  $f_{hot}$  as a function of the electron temperature and in this electronic temperature area  $T$  between  $1.0$  and  $10^3$  eV. We also included the results obtained by applying a Maxwell distribution for  $f_{hot} = 1$ . The temperature  $T_{bulk}$  was taken equal to an average value of  $k_B T_{bulk} = 0.85$  eV [26]. Indeed fractions of cold electrons are less than hot electrons ones. However, regarding Figure. 2 we note that the curves (of this work)

TABLE 1. The relative differences of the ionization rate in the case of non-Maxwellian distribution:

(a)  $f_{hot}$  is the normalized hot electron fraction

(b)  $\tau_{NM}$ : the coefficient of the ionization rate obtained by non-Maxwellian distribution function

(c)  $\frac{\Delta\tau_{NM}}{\tau_{Kato}} = \frac{\tau_{NM} - \tau_{Kato}}{\tau_{Kato}}$ : the relative differences of coefficient of the ionization rate obtained by non-Maxwellian distribution

$T$ (eV)	$\tau_{Kato}(\text{cm}^3\text{s}^{-1})$	$f_{hot}^{(a)}$	$\tau_{NM}^{(b)}(\text{cm}^3\text{s}^{-1})$	$\frac{\Delta\tau_{NM}}{\tau_{Kato}}^{(c)}$
15	$1.7 \times 10^{-10}$	0.7	$1.18 \times 10^{-10}$	0.30
		0.8	$1.35 \times 10^{-10}$	0.20
		0.9	$1.52 \times 10^{-10}$	0.10
		1.0	$1.68 \times 10^{-10}$	0.01
100	$1.58 \times 10^{-9}$	0.7	$8.20 \times 10^{-10}$	0.48
		0.8	$9.38 \times 10^{-10}$	0.41
		0.9	$1.05 \times 10^{-10}$	0.93
		1.0	$1.17 \times 10^{-9}$	0.25
500	$1.87 \times 10^{-9}$	0.7	$1.46 \times 10^{-9}$	0.21
		0.8	$1.67 \times 10^{-9}$	0.10
		0.9	$1.88 \times 10^{-9}$	0.005
		1.0	$1.67 \times 10^{-9}$	0.10
1000	$1.80 \times 10^{-9}$	0.7	$1.09 \times 10^{-9}$	0.39
		0.8	$1.24 \times 10^{-9}$	0.31
		0.9	$1.40 \times 10^{-9}$	0.22
		1.0	$8.99 \times 10^{-10}$	0.50

for the various fractions (70%, 80%, 90%) are generally quite close to that plotted for the fraction  $f_{hot} = 1$  and represent ionization rates for a Maxwellian distribution. As a matter of fact, in the case of low temperatures, the ionization rates are very sensitive to the behavior of the cross sections [38]. There are considerable differences between various theoretical and experimental methods. The curves of ionization rates in Figure. 2 move progressively away from that obtained by the Maxwellian distribution for  $f_{hot} = 1$  progressively as the hot electron fraction decreases. This shows a remarkable sensitivity of the ionization rates based on hot electrons fractions. We are now able to compare the ionization rate with the results published by Kato et al. [38]. Generally, a good agreement has been noted on the curve of ionization rate for a Maxwellian distribution for and that of Kato et al. [38] as shown in Figure. 2. Table. 1 shows the relative differences of coefficient of the ionization rate obtained by non-Maxwellian distribution. There are relative differences in the range [100 -1000] (eV); these differences are of the order of 30% except in the case where  $f_{hot} = 0.9$  and the temperature equal to 100 eV. The relative differences between the two Maxwellian and non-Maxwellian distributions were calculated for different values of hot electrons fraction. Significant differences are observed for low temperatures in the energy range [20-100] (eV) where  $f_{hot} = 0.7 - 0.8$ , then they are too weak around 500 eV where  $f_{hot} = 0.9$ . They are of the order of 5% to 10%.

### 5. Influence of the electrons energy distributions functions on the calculation of ionization rates

Collisional-radiative atomic models that include the effects of non-Maxwellian and hot electron energy distributions are therefore of significant interest in atomic physics data as well as in spectroscopic tools that can determine the presence and characteristics of the electrons distribution function (EDF) in plasmas from non-invasive spectroscopic measurements [23]. For single-temperature plasmas with Maxwellian electron energy distributions, deexcitation and recombination rates can be obtained directly from collisional excitation and ionization rate coefficients through detailed balance. For plasmas that have electrons in non-Maxwellian distributions, the cross sections of these reverse rates must be integrated over the entire electron energy distribution. Because Helium is one of the most important species for plasma fusion magnetic confinement devices, we selected it for the calculation of ionization rate from the cross sections. Particular experiences and studies on hot electrons have led to fix some forms of energy distribution function. Such forms are given by the following expressions:

$$\text{Maxwellian: } F_M(\epsilon, T_e) = 2\sqrt{\frac{\epsilon}{\pi T_e^3}} e^{-\frac{\epsilon}{T_e}}, \quad (3)$$

$$\text{Gaussian: } F_G(\epsilon, T_e) = \frac{1}{\sqrt{\pi} T_e} \left( \frac{2}{1 + \operatorname{erf}\left(\frac{\epsilon_0}{T_e}\right)} \right) e^{-\left(\frac{\epsilon - \epsilon_0}{T_e}\right)^2}, \quad (4)$$

$$\text{Power-law: } F_p(\epsilon, T_e) = \frac{\gamma - 1}{T_e^{\gamma-1}} \epsilon^{-\gamma}, \epsilon \geq T_e, \quad (5)$$

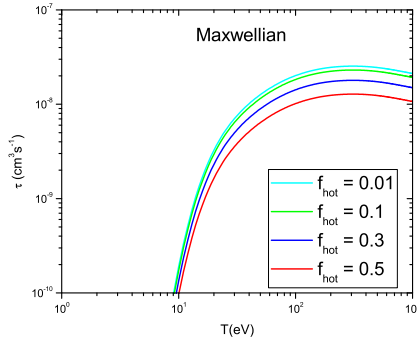
where  $T_e$ ,  $\epsilon$ ,  $\epsilon_0$  are the energies of electrons corresponding to each distribution and  $\gamma$  is a decay constant. For the calculation of ionization rate from the cross sections, we use an energy distribution. This allows us to study the influence of electrons energy distributions functions on the calculation of ionization rate and we take the following form:

$$F(\epsilon) = (1 - f_{hot}) F_M(\epsilon, T_e) + f_{hot} F_X(\epsilon, T_e), \quad (6)$$

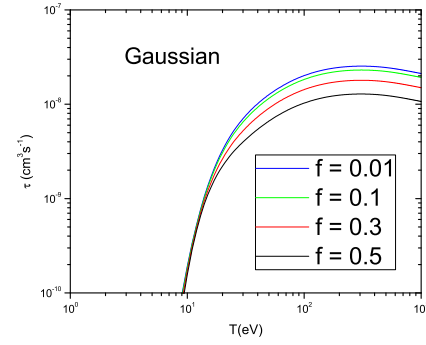
where  $f_{hot}$  is the normalized hot electron fraction,  $F_M(\epsilon, T_e)$  the Maxwell energy distribution function and  $F_X(\epsilon, T_e)$  is the electron energy distribution function. Substituting Equation (6) into Equation (1), and replacing the electron energy distribution functions by Maxwellian, Gaussian and power-law, respectively, and the effective ionization cross sections calculated by the FAC code [36, 37] for neutral helium, allowed us to obtain the ionization rates for different values of hot electrons fraction  $f_{hot}$ .

### 6. Results and Discussions

Figures. 3 and 4 show the results of calculating the ionization rates of neutral helium for different energy distribution functions for different values of hot electrons fraction. However, in Figure. 3(a), if we are interested in high temperatures, it is noted that the curves of ionization rates are very sensitive to the hot electrons fraction, and we can observe that the curves get away from each other progressively as the hot electrons fraction increases. In Figure. 3(b), for a Gaussian distribution of energy and low temperatures, there is a good improvement curves regardless of the value of electrons fractions. With regard to high temperatures and for low hot electrons fractions (0.01-0.1), the curves approach those obtained by the Maxwellian distribution. Figure. 4 shows the ionization rate for an electron energy distribution function of the power-law for different values of the decay constant  $\gamma$ .



(A) Maxwellian distribution



(B) Gaussian distribution

FIGURE 3. Coefficients of the ionization rates to He: The coefficients rates are obtained using the electrons energy distribution functions in (a) Maxwellian and (b) Gaussian and the effects of various hot electrons fraction  $f_{hot} = 0.01, 0.1, 0.3$  and  $0.5$

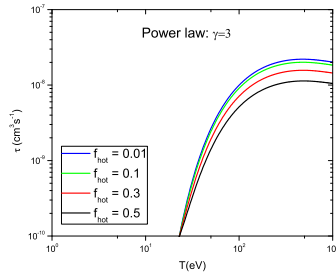
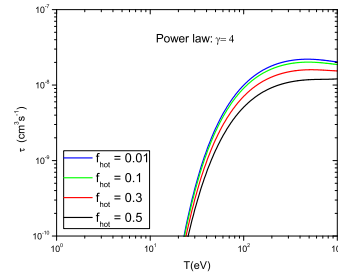
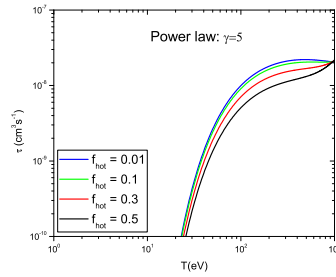
(A) Power-law:  $\gamma = 3$ (B) Power-law:  $\gamma = 4$ (C) Power-law:  $\gamma = 5$ 

FIGURE 4. Coefficients of the ionization rates to He: The coefficients rates are obtained using the electrons energy distribution functions in power-law for various decay constants:  $\gamma = 3$  (a),  $\gamma = 4$  (b) and  $\gamma = 5$  (c) and the effects of various hot electrons fraction  $f_{hot} = 0.01, 0.1, 0.3$  and  $0.5$ .



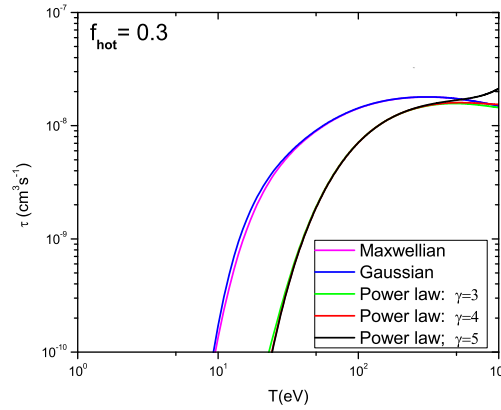


FIGURE 5. Coefficients of the ionization rates to He: The coefficients rates are obtained using the electrons energy distributions functions: Maxwellian, Gaussian and the power-law for various decay constants:  $\gamma = 3, 4, 5$ , and for hot electrons fraction  $f_{hot} = 0.3$ .

The power-law distribution, which is commonly used in astrophysical models, becomes nonzero at its characteristic electron energy and decays more or less rapidly with energy according to the value of  $\gamma$ . It is plain that collisional ionization rates are strongly dependent on the functional form and characteristic energy of the electron energy distribution when the characteristic distribution energy  $T_e$  smaller than the threshold energy. This is understandable because of the wide variations in the number of electrons with sufficient energy to induce the transition among the various distributions. When the characteristic distribution energy  $T_e$  is very small than the threshold energy, the narrowest distribution (the power-law function with  $\gamma = 5$ ) include very small numbers of electrons with energies larger than the threshold energy for excitation and give much smaller rate coefficients than the broader distributions. As the characteristic energies increase, all distributions accumulate larger numbers of energetic electrons and the rate coefficients for ionization processes increase accordingly. It is important to note that when the characteristic energies of the electron distributions are larger than the threshold energy, much of the strong dependence of the rate coefficients on the functional forms and characteristic energies of the distributions vanishes. In particular, coefficients of the ionization rates shown in Figure. 4 are only weakly dependent on the characteristic energy and functional form of the electron distribution as long as the characteristic distribution energy  $T_e$  is very large than the threshold energy. Only when the cross section decays very rapidly do the functional forms and characteristic energies of the distributions have significant impact on the rate coefficients. However for Figure. 4 (a), (b) and (c) and at low temperatures, we observe acceptable differences in the range [20-100] (eV) while starting from 500 eV. At high temperatures, the curves show sensitivity with respect to hot electrons fractions as well as increasing the value of the decay constant  $\gamma$ . It is important to note that in using the electrons energy distributions functions in the calculation of ionization rates for He, there is a good improvement in curves especially for Gaussian and power-law distribution functions to the value of  $\gamma = 2$  and that in low temperatures for any value of  $f_{hot}$  and low hot electrons fractions in high temperatures. In

Figure. 5, we can notice a very good agreement between the two curves of the ionization rate when using the electrons energy distributions functions, Maxwellian and Gaussian, respectively, and the entire energy range and for the hot electrons fraction of 30%. Regarding the ionization rates obtained by using the electron energy distribution function of power-law, we note that the value of  $\gamma$  does not influence the calculation and this for a fixed value of the hot electrons fraction. This shows a remarkable sensitivity of the ionization rates based on the hot electrons fractions and the electrons energy distributions functions.

## 7. Conclusion

The coefficients of the ionization rates of neutral helium and Beryllium were calculated from the effective cross sections. These latter were obtained by the FAC code. To achieve the calculation, we have used two non-Maxwellian distributions: one of them serves to study the effects of hot electrons fraction on the ionization rate of Beryllium. The second distribution stands on basic functions: Maxwellian, Gaussian and the power-law, permit to show their influence on the ionization rate of neutral helium. In the case of Beryllium, we have also shown that the curves of ionization rate are responsive to the hot electrons fractions (70% and 80%). The curve of the ionization rate approaches that of Kato et al. [38] for the fraction of 100% of hot electrons. For large values of  $f_{hot}$  and  $\gamma > 5$ , we have shown the remarkable sensitivity of the electrons energy distributions functions as well as fractions of the hot electrons on the calculation of ionization rate of neutral helium.

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