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Out of Maxwell-Boltzmann equilibrium Collisional Radiative Model

F. Catoire[1,2,*], H. Capes[1], Y. Marandet[1], A. Mekkaoui[1], M. Koubiti[1], J. Rosato[1] and R. Stamm[1]

[1] *PIIM, UMR 6633 Université de Provence / CNRS, Centre de St.-Jérôme, Case 232, 13397 Marseille Cedex 20, France*
[2] *CELIA, UMR 5107 Université de Bordeaux I / CNRS / CEA, 351 cours de la Libération, 33405 Talence, France*

Abstract. In this work we address the effect of plasma turbulence on atomic levels population. The plasma turbulence is considered in Collisional Radiative Modeling through fluctuations of macroscopic quantities such as the electron temperature and/or density. This study focuses on the effect of the Probability Density Function of the electron temperature on the average level populations, in the case where the turbulence frequency is either larger or smaller than any atomic time scales. Then we study the effect of the introduction of a non-Maxwellian Velocity Distribution Function using a κ-function.

1. INTRODUCTION

Collisional Radiative Models (CRM) are extensively used in plasma physics in order to determine the population of atomic (or molecular) energy levels. The purpose of this work is to investigate the effects of a turbulent plasma on the levels population. This topic is of prime importance for spectroscopy since the intensity of a line is proportional to the upper levels population. We have developed a model describing plasma fluctuations (characterized by the frequency ν_{turb}) by including stochastic macroscopic quantities (*e.g.* electron temperature or density) in CRM. Here, the only fluctuating quantity is the electron temperature. The latter is described by a kangaroo process [1], *i.e.* the electron temperature is constant on time intervals. The value of the temperature is assumed to be independent on each time interval and distributed according to a given Probability Density Function (PDF). The probability of having a jump at each interval is linked to the Waiting Time Distribution (WTD). In the case where the moments of the WTD are finite, one can define two regimes, namely the case where the turbulence frequency (ν_{turb}) is either larger or smaller than atomic characteristic time scales. These two regimes respectively correspond to what we call the Diabatic and Static regime which are independent of the WTD, but not of the PDF. The Diabatic and Static regimes are supposed to occur for turbulence frequencies smaller that the ion-electron collision (ν_{i-e}) frequency, allowing to describe the Velocity Distribution Function (VDF) by a Maxwell distribution. In the case where $\nu_{turb} \gg \nu_{i-e}$ the VDF cannot be described by a Maxwell distribution anymore and reaches a different equilibrium. The purpose of this work is also to investigate the effect on levels population of a regime that is out of the Maxwell-Boltzmann equilibrium.

*e-mail: catoire@piim.up.univ-mrs.fr

This paper is organized as follows : first we describe the model we have developed to account for plasma turbulence in the collisional radiative model. Then we discuss the effect of various PDF and finally that of a non-Maxwellian VDF.

2. DESCRIPTION OF THE MODEL

CRM give a description of the evolution of the populations as a function of the plasma parameters. The time evolution of the vector containing the levels population, noted X, is governed by a differential equation given by : $dX(t)/dt = M(t)X(t)$ where the matrix M contains the rates of collisional and radiative processes. The matrix M is a function of the fluctuating plasma parameters through the rates. Usually, in CRM only the Quasy-Steady State (M time-independent) is considered [2]. In this work, the case where the matrix M depends on the fluctuations of electron temperature (*i.e.* a time-dependent case) is investigated.

In this model, the electron temperature is described by a kangaroo process. The time interval $[0,t]$ is split in N subintervals $[t_i, t_{i+1}]$ on which the temperatures are assumed to be constant and equal to T_i. The value of the temperature at each subinterval, is chosen independently from the previous ones. The set of T_i is statistically characterized by its PDF (noted $p(T)$) from which we can fit the two first moments, $\langle T\rangle = \int dT\,T\,p(T)$ and $\langle T^2\rangle = \int dT\,T^2\,p(T)$, to experimental values. From the latter averages, the fluctuation rate r is defined by $r^2 = \frac{\langle T^2\rangle - \langle T\rangle^2}{\langle T\rangle^2}$. The probability of having a jump in the range of time t_i and $t_i + dt$ is given by $\varphi(t_i)dt$, where $\varphi(t)$ is the WTD. As a consequence the probability of having no jump in the interval of time $[0,t]$ is given by: $\Phi(t) = 1 - \int_0^t dx\,\varphi(x)$. The solution we are seeking for is written:

$$\lim_{t\to\infty}\langle X(t)\rangle = \lim_{p\to 0} p\langle\tilde{X}(p)\rangle \quad \text{where} \quad \langle X(t)\rangle = \int dT\,p(T)X_{[T]}(t) \quad \text{and} \quad \langle\tilde{X}(p)\rangle$$

is the Laplace transform of the previous quantity. Some further analysis [3] allows us to calculate $\langle\tilde{X}(p)\rangle$ explicitly:

$$\langle\tilde{X}(p)\rangle = \widetilde{\Phi G}_{ST}(p)(I - \widetilde{\varphi G}_{ST}(p))^{-1}X_0 \tag{1}$$

where $X_0 = X(t=0)$ is set by the initial conditions and

$$\widetilde{\Phi G}_{ST}(p) = \int_0^\infty dt\,\exp(-pt)G_{ST}(t)\Phi(t), \quad \widetilde{\varphi G}_{ST}(p) = \int_0^\infty dt\,\exp(-pt)G_{ST}(t)\varphi(t)$$

$G_{ST}(t)$ being the Green function of the differential equation governing the evolution of levels population vector, for a time-independent M. The turbulence frequency is defined by $\nu_{turb}^{-1} = \int_0^\infty dt\,\varphi(t)\times t$. Two regimes can be distinguished : $\nu_{turb} \ll \nu_{at}$ and $\nu_{turb} \gg \nu_{at}$ where ν_{at} is the characteristic atomic frequency. In the first case, called the Static case, the turbulence dynamics is much slower than atomic processes, and the solution is given by the average of the stationary solution, over the PDF of the electron temperature. On the other hand, the Diabatic regime corresponds to the case where the turbulence dynamics is much faster than atomic processes, and the solution is then given by the stationary solution for which the matrix M has been averaged over the PDF of the electron temperature [3]. These two solutions do not depend on the WTD, hence the WTD only affects the intermediate turbulence frequencies.

We now apply the model to the case of a reduced atomic hydrogen system. We consider only the levels $n = 2$ and $n = 1$. The main mechanisms involved are the electron impact excitation from the ground state to the two excited states (2s and 2p), the ion impact leading to the transition from 2s to 2p, and the spontaneous emission from the 2p state to the ground state. The matrix M is filled up with rates corresponding to the previously quoted reactions. Rates are linear in N_e but not in T_e. The de-excitation from excited states to the ground state by electron impact is calculated by using the detailed balance law [4]. In the case investigated here, the coronal regime is reached meaning that de-excitation by collisions are negligible. The rate coefficients as used in the matrix M are given by $k_{g\to e} = \int d^3v \sigma_{g\to e} v f_{Max}(v)$ where $\sigma_{g\to e}$ is the cross section leading to the transition from g to e states and $f_{Max}(v)$ is the VDF assumed to be a Maxwell distribution since in this section the turbulence frequency is smaller than the electron-electron or ion collisions. The cross-sections used in this work are found in [5]. In the next paragraphs we investigate the effect of the PDF in the Diabatic and the Static limits.

In Fig. 1a the average population of the 2s state of atomic Hydrogen as a function of the turbulence frequency is presented. The turbulence free case is indicated by the blue dot-dashed curve. On this graph a clear transition form the Diabatic limit (large values of ν_{turb}) to the Static limit (small values of ν_{turb}) is noticed. The value of the average population in the Diabatic limit is larger than the Static limit value (by a factor of two for this illustration). This can be explained by the Jensen inequality and the fact that the turbulence free population of the 2s state as a function of the temperature is convex.

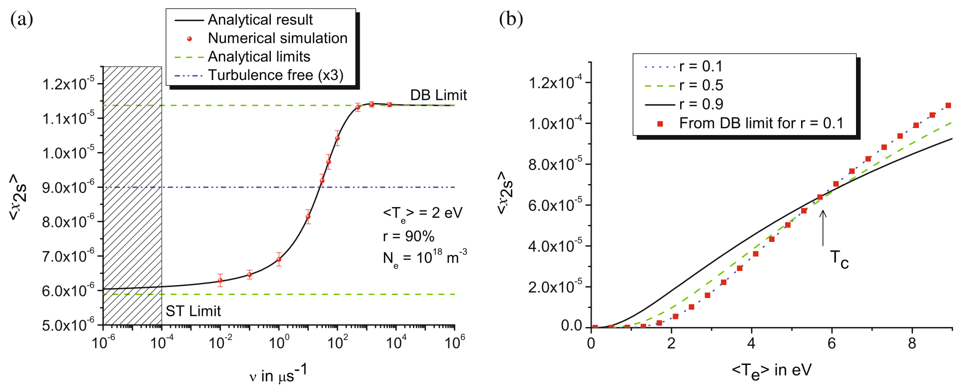

Figure 1. a) Plot of the population as a function of the turbulence frequency. The full curve is the analytical results while the points corresponds to the numerical calculations. The dashed curves are the two limits indicated in the text. b) Plot of the fraction population as a function of fluctuation rate of the electron temperature for different average electron temperature. $N_e = 10^{19}\,\mathrm{cm}^{-3}$, $\nu = 1000\,\mu\mathrm{s}^{-1}$.

In Fig. 1b a plot of the average population of the 2s level as a function of the average electron temperature is presented for different values of the fluctuation rate.

The curves intersect at $\langle T_e\rangle \approx 5.8\,\mathrm{eV} \equiv T_c$ characterizing a regime independent of the fluctuation rate. For $\langle T_e\rangle < T_c$ the average population increases r with r, while the behavior of the average population is opposite for $\langle T_e\rangle > T_c$. Whereas the calculation of Figure 1b has been performed in the Diabatic regime, the behavior is similar in the Static regime and can be explained in a more simple way. The average population at a given average electron temperature, up to the second order in $\langle T\rangle$, is given by:

$$\langle X\rangle(\langle T\rangle) = X(\langle T\rangle) + \frac{d^2X}{dT^2}(\langle T\rangle)r^2\langle T\rangle^2. \tag{2}$$

From this formula the temperature T_c corresponds to the inflexion point of $X(T)$, explaining the behavior of Fig. 1b.

We now compare, in Fig. 2, the average population as a function of the fluctuation rate for different PDF and average temperatures. Figure 2a, has been obtained for an average electron temperate of 2 eV,

Figure 2b for 5 eV, Fig. 2c for 8 eV. The electron density is set to 10^{18} m^{-3}. First, for $\langle T_e \rangle \leq T_c$, the average population decreases with r either in the Diabatic and the Static regime. Clearly a change of the PDF affects the behavior of the average population as a function of the fluctuation rate. Nonetheless, the trend is the same whatever the PDF or the regime is. It can be noticed that only the average population for Log-Normal PDF is independent of the fluctuation rate in the Static regime, which is expected since T_c is PDF-dependent and has been defined for the latter PDF.

3. NON-MAXWELLIAN REGIME

3.1. General description

In the above description of the dynamics, the turbulence frequency is assumed to be small compared to ν_{i-e} and ν_{e-e} in order to describe the VDF by a Maxwell distribution. Here we investigate the case where the VDF is described by a more general distribution going beyond the Maxwell-Boltzmann equilibrium. This function is called the κ-function (or generalized Lorentzian) [6,7] and could describe the case where the turbulence frequency is higher than electron-electron or ion frequencies. The use of this distribution is consistent with astrophysical observations [8,9]. In the following, this regime is called the Non-Maxwellian regime. The expression of the κ-function is given by:

$$f_\kappa(v) = N(1 + \beta v^2)^{-(\kappa+1)}, \tag{3}$$

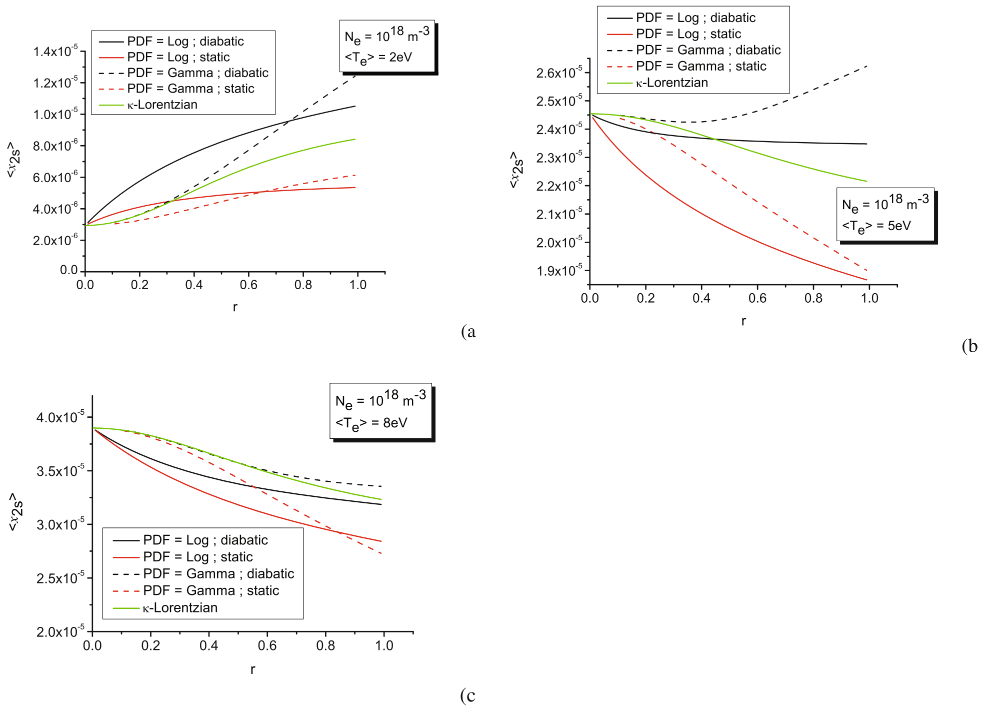

Figure 2. Plot of the population as a function of fluctuation rate of the electron temperature for different PDF in the Diabatic and Static regime. The solid red curve corresponds to a Log-Normal PDF in the Static regime, the full black curve to a Log-Normal PDF in the Diabatic regime, the dashed red curve to a Gamma PDF in the Static regime and the dashed black curve to a Gamma PDF in the Diabatic regime. The green curve corresponds to the Very High Frequency regime.

The scale-parameter β is given by $\beta = (k_B T(\kappa - 3/2))^{-1}$ with T the kinetic temperature such that $\langle E \rangle = \frac{3}{2} k_B T$. N is the normalization constant and is equal $(\frac{\beta}{\pi})^{3/2} \frac{\Gamma(\kappa+1)}{\Gamma(\kappa-1/2)}$. It can be noticed that there are two parameters characterizing this VDF, one describing the kinetic temperature (as defined by $\langle E \rangle$) and the other one, denoted by κ, describing the shape of the distribution. The limit $\kappa \to \infty$ corresponds to the Maxwell-Boltzmann equilibrium. In the Non-Maxwellian regime, the rates introduced in the matrix M are written $k_{g\to e} = \int d^3 v \sigma_{g\to e} v f_\kappa(v)$. The solution of Eq. (1) is simply given by the stationary solution for which the rates of M are modified as previously mentioned. As a consequence, the turbulence free case (Maxwell VDF) is retrieved for $\kappa \to \infty$.

3.2. LINK BETWEEN THE NON-MAXWELLIAN AND THE DIABATIC REGIME

We now focus on the study of the solution in the Diabatic limit. In that case, the average population vector (X) satisfies the relation $\langle M \rangle X = 0$ and neither M nor $\langle M \rangle$ are invertible. The elements of the matrix $\langle M \rangle$ are given by : $\langle M \rangle_{ij} = \iint dT d^3 v \sigma_{ij} v f^T_{Max}(v) p(T)$. Here, it has to be noted that the VDF is a function of the temperature T. If one permutes the two integrals the following results is obtained:

$$\langle M \rangle_{ij} = \int d^3 v \sigma_{ij} v \int dT f^T_{max}(v) p(T) = \int d^3 v \sigma_{ij} v f_{eff}(v)$$

where $f_{eff}(v) = \int dT p(T) f^T_{Max}(v)$. So, generally speaking, the diabatic and the Non-Maxwellian regime cannot be distinguished. More particularly, elements of the matrix $\langle M \rangle_{ij}$ expressed as $\langle M \rangle_{ij} = \int d^3 v \sigma_{ij} v f_{eff}(v)$ are similar to that of Non-Maxwellian regime if one replaces $f_{eff}(v)$ by the κ-function. The question addressed for this work is to know if a PDF is able to fulfill this condition. Clearly such a PDF exists and corresponds to the inverse gamma distribution. It can be shown that the temperature defined by the κ-function and the average temperature defined by $f_{eff}(v)$ are the same and the dimensionless κ term is related to the fluctuation rate (r) of the PDF by the relation $\kappa = \frac{5}{2} + 1/r^2$.

3.3. DISCUSSION OF THE RESULTS IN THE NON-MAXWELLIAN REGIME

A thermodynamical analysis of the κ-function [6] allows us to define the β term as in usual thermodynamics and kinetic theory. This term is written : $\beta = (k_B T(\kappa - 3/2))^{-1}$, which is meaningful only if $\kappa > \frac{3}{2}$. Moreover, by considering the Diabatic regime, we have shown that the κ term, related to the fluctuation rate, belongs to the interval [0,1] (since we deal with inverse Gamma PDF). Then, in Diabatic regime, κ has to be larger than $\frac{7}{2}$, meaning that the Diabatic and the Non-Maxwellian regimes cannot be distinguished to each other if $\kappa \geq \frac{7}{2}$. On the other hand, only the Non-Maxwellian regime can be described by a value of κ in the range $\frac{3}{2} \leq \kappa < \frac{7}{2}$.

Provided the use of a κ-function are given in Fig. 2 by the full green curve. The behavior of the average population as a function of r is similar to that of the others PDF. This can be explained by the fact that on this figure the NM regime is restricted to the Diabatic behavior. To see a drastic change associated the NM regime, one needs to plot the average population as a function of the average temperature for a value of κ in the range $\frac{3}{2} \leq \kappa < \frac{7}{2}$ only attributed to the NM regime. What we have observed in that case is a drastically different trend of the average population as a function of $\langle T \rangle$.

4. CONCLUSION

In this work we have investigated the effect of plasma turbulence on atomic hydrogen level populations. We have shown that the average population exhibits the same trend at a given average temperature independently of the choice of the PDF or regime. We have also demonstrated that the Non-Maxwellian equilibrium corresponding to deviation from the Maxwell-Boltzmann equilibrium cannot always be distinguished from the Diabatic regime.

References

[1] U. Frisch and A. Brissaud, J. Quant. Spectrosc. Radiat. Transfer **11**, 1753 (1971)
[2] T. Fujimoto, *Plasma Spectroscopy* (Oxford University Press, 2004)
[3] Catoire *et al.*, To be published in PRA
[4] B. Diu, C. Guthmann, D. Lederer and B. Roulet, *Statistical Physics* (Hermann, 1989)
[5] R.K. Janev, W.D. Langer, K. Evans Jr. and D.E. Post Jr., *Cross Sections and reaction Rate Coefficients* (Springer Series on Atoms and Plasmas, 1987)
[6] R.A. Treumann, Phys. Scr. **59**, 19 (1999)
[7] P.H. Yoon, PRL **95**, 215003 (2005)
[8] Bryant D.A., J. Plasma Physics **56**, 87 (1996)
[9] Bryant D.A., Ph. D. thesis (1995)