Non L.T.E. Populations and Related Quantities for H-H$^+$-e Plasmas as a Function of the Cut-off Level

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The influence of the choice of the cut-off level n^* of the evaluation of the coefficients of quasistationary plasmas has been studied. The numerical results show that the coefficient $r_1(i)$ which represents the contribution of the population density of the ith excited level by direct excitation from the ground level, is strongly affected by the choice of n^*. A minor influence is observed 1) on the coefficient $r_0(i)$ which represents the contribution to the population density of the ith level from the continuum of free electrons 2) on the collisional-radiative recombination (α) and ionization (S) coefficients'.

Introduction

A number of papers [1–4] has appeared in the last few years dealing with the problem of the determination of the ionization coefficients and of population densities of non equilibrium hydrogen plasmas. No explicit attention has received in these papers the problem of the choice of the cut-off level n^*, a problem which has, on the contrary, been considered in detail for equilibrium (see for example Ref. 5) and non equilibrium stationary plasmas [6]. It is the purpose of this paper to discuss the influence of the choice of n^* on typical coefficients of quasistationary plasmas such as $r_0(i)$, $r_1(i)$, α and S [see Eqs. (3) – (5)].

A plasma of atomic hydrogen in different non equilibrium conditions will be considered; the type of results obtained is however of general interest.

Quasistationary Plasmas

It is well known that for a quasistationary plasma one can write

$$\partial n_1/\partial t = -\partial n_e/\partial t = \gamma\, n_+\, n_e = (\alpha - S\, n_1/n_+)\, n_+ n_e\,, \tag{1 a}$$

$$\partial n_i/\partial t = 0 \quad \text{for} \quad i \geqq 2 \tag{1 b}$$

where α and S denote the collisional-radiative recombination and ionization coefficients respectively. The condition $[\partial n_i/\partial t = 0]_{i\,\geqq\,2}$ yields:

$$n_e \sum_{j \neq i} n_j K_{ji} - n_i\, n_e (K_{ic} + \sum_{j \neq i} K_{ij}) + n_e\, n_+ (\beta_i + n_e K_{ci}) - n_i \sum_{j<i} A_{ij} + \sum_{j>i} n_j A_{ji} = 0\,, \tag{2}$$

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Equation (2) refers to a thin plasma when only the electrons are responsible for the collisional processes. The rate coefficients appearing in Eq. (2) are those relative to the collisional ionization (K_{ic}) and recombination (K_{ci}) processes, to the excitation ($K_{ij}\, i<j$) and deexcitation ($K_{ji}\, j>i$) processes, to the spontaneous radiative transitions (A_{ij}) and to the radiative recombination (β_i). They have been calculated according to the recent work of Johnson [7].

The system of linear equations typified by Eq. (2) can be solved by taking the electron number density n_e, the ground state number density n_1 and the electron temperature as parameters. The solutions are usually expressed by means of the coefficients $r_0(i)$ and $r_1(i)$ which are related to the Saha deviation $b(i)$'s through

$$b(i) = n_i/n_{iE} = r_0(i) + r_1(i)\, n_1/n_{1E} \tag{3}$$

(subscript E refers to equilibrium conditions).

The first coefficient, $r_0(i)$, represents the population density of a given quantum state when the ground state number density n_1 is zero, while $r_1(i)$ is the increase in the population density of the same state for an unit increase in the ground state.

α and S can be evaluated by means of the following equations

$$\alpha = [-b + \sum_{j>1} a_j\, r_0(j)]/n_e^2\, n_{1E}\,, \tag{4}$$

$$S = [-c - \sum_{j>1} a_j\, r_1(j)]/n_e\, n \tag{5}$$

where

$$b = -(\beta_1 + n_e K_{c1})\, n_e\, n_+/n_{1E} \tag{6}$$

$$c = -(K_{1c} + \sum_{j \neq i} K_{ij})\, n_e\,, \tag{7}$$

$$a_j = (A_{j1} + n_e K_{j1})\, n_{jE}\, n_{1E}\,. \tag{8}$$

The dimension of the system depends on the number of quantum states considered in the plasma. In principle, one could consider a very high number of quantum states, but the solution of the system might then become quite difficult. Physical reasons do however suggest that a critical level n^* exists above which a quantum state can not be considered bound. This level can be taken as the cut-off level for truncating the system of linear equations [8]; it can be calculated by employing one of the several theories proposed in the literature [9].

Two difficulties arise in this connection i) n^* becomes very large and practically unrealistic at low electron number densities ii) the values of n^* differ according to the theory selected for the calculation. To overcome these difficulties, it was therefore decided to study the influence of the

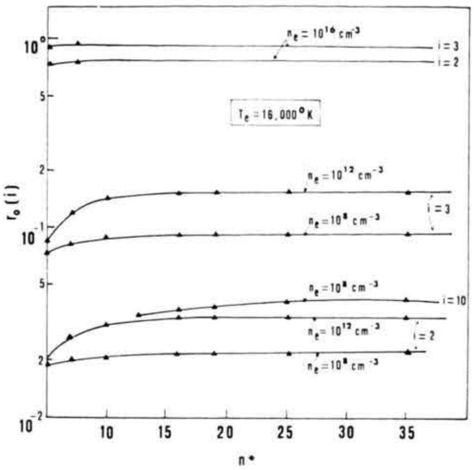

Fig. 1. Values of $r_0(i)$ as a function of n^*.

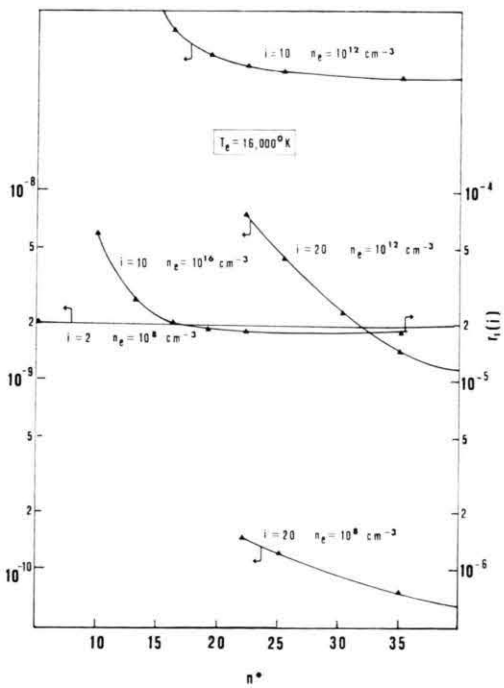

Fig. 2. Values of $r_1(i)$ as a function of n^*.

choice of n^* on the coefficients of non equilibrium plasmas by considering n^* as an arbitrary cut-off level.

Results

Typical results for $r_0(i)$ and $r_1(i)$ as a function of n^*, at different electron number densities, have been reported in Figs. 1 – 3 for selected values of the principal quantum number i.

The following points should be noted: a) the coefficient $r_0(i)$ is affected by the choice of n^* for low lying excited levels, while a slight dependence on n^* is presented by the high lying levels. A reverse behaviour is observed for the coefficient $r_1(i)$. b) The influence of the choice of n^* on $r_0(i)$ and $r_1(i)$ decreases with increasing electron number density n_e and increases with decreasing temperature. c) In all cases the influence of the choice of n^* on $r_0(i)$ is less pronounced than the corresponding influence on $r_1(i)$. As a consequence, c) we can say that the choice of n^* does not significantly affect the accuracy of the population densities of excited states in recombining plasmas [i.e. for plasmas in which $b(i) \cong r_0(i)$], while this will not be true for ionization plasmas (i.e. for plasmas in which $b(i) \cong r_1(i) n_1/n_{1E}$. This behaviour is in agreement with Park's calculations [10].

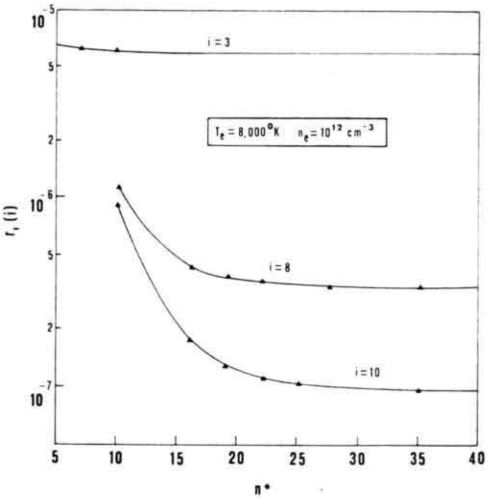

Fig. 3. Values of $r_1(i)$ as a function of n^*.

Table 1 shows the influence of the choice of n^* on the coefficients α and S at different electron number densities and different temperatures. One can see that these coefficients are practically independent of n^* for high and low values of n_e; deviations up to 30% are observed in the intermediate range of n_e. It is worth noting the independence of α and S for $n^* \geqq 10$. This value can be taken as a practical cut-off level for calculating α and S for plasmas containing singly ionized atoms, neutral atoms and electrons. (In this connection see also the results of Norcross and Stone [11] for low temperature Cesium plasmas.)

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Table 1. The influence of n^* on the coefficients $\alpha(\mathrm{cm}^3\,\mathrm{sec}^{-1})$ and $S(\mathrm{cm}^3\,\mathrm{sec}^{-1})$.

				$T_e=16{,}000$ °K				
	$n^*=5$	$n^*=7$	$n^*=10$	$n^*=16$	25	35	42	n_e
α	3.59(−13)	3.81(−13)	3.91(−13)	4.00(−13)	4.08(−13)	4.14(−13)	4.16(−13)	10^8
α	3.72(−13)	4.54(−13)	5.06(−13)	5.32(−13)	5.40(−13)	5.42(−13)	5.43(−13)	10^{12}
α	7.99(−13)	9.81(−13)	1.01(−12)	1.03(−12)	1.03(−12)	1.03(−12)	1.03(−12)	10^{14}
α	4.77(−12)	4.92(−12)	4.95(−12)	4.96(−12)	4.97(−12)	4.97(−12)	4.97(−12)	10^{16}
S	2.01(−13)	2.01(−13)	2.01(−13)	2.01(−13)	2.04(−13)	2.03(−13)	2.09(−13)	10^8
S	2.17(−13)	2.73(−13)	3.17(−13)	3.40(−13)	3.47(−13)	3.50(−13)	3.50(−13)	10^{12}
S	1.50(−12)	1.93(−13)	1.99(−13)	2.02(−13)	2.03(−13)	2.03(−13)	2.03(−13)	10^{14}
S	1.83(−11)	1.88(−11)	1.89(−11)	1.89(−11)	1.89(−11)	1.89(−11)	1.89(−11)	10^{16}
				$T_e=8{,}000$ °K				
α	7.85(−13)	8.27(−13)	8.48(−13)	8.69(−13)	8.90(−13)	9.08(−13)	9.08(−13)	10^8
α	1.81(−12)	1.10(−11)	1.12(−11)	1.36(−11)	1.39(−11)	1.39(−11)	1.39(−11)	10^{12}
S	6.46(−18)	6.46(−18)	6.46(−18)	6.47(−18)	6.55(−18)	6.67−(18)	6.67(−18)	10^8
S	7.74(−18)	1.33(−17)	1.82(−17)	2.05(−17)	2.08(−17)	2.09(−17)	2.10(−17)	10^{12}

1 D. R. Bates, A. E. Kingston, and R. W. P. McWhirter, Proc. Roy. Soc. **A 267**, 297; **A 270**, 150 [1962].

2 H. W. Drawin, Z. Physik **225**, 470, 483 [1970]; H. W. Drawin and F. Emard, report EUR CEA FC-534 [1970].

3 C. Park, J.Q.S.R.T. **12**, 323 [1972].

4 L. C. Johnson and E. Hinnov, J.Q.S.R.T. **13**, 333 [1973].

5 M. Capitelli and E. Molinari, J. Plasma Phys. **4**, 335 [1970].

6 H. W. Drawin, Annalen der Physik **14**, 262 [1964].

7 L. C. Johnson, Astrophys. J. **174**, 227 [1972].

8 An other procedure which has been often used for truncating the linear system is to find a principal quantum number n_0, above which all quantum states are in Saha's equilibrium with the electrons. The difficulty of this method lies in the lack of a rigorous procedure for locating n_0. It can be shown that the values of $r_0(i)$ and $r_1(i)$ calculated by solving the system for a given n^* are practically equal to those obtained by solving a system of dimension n_0 and by considering in the relevant equations the quantum levels from n_0 to n^* in Saha's equilibrium.

9 see for example A. Unsold, ZS. Astrophys. **24**, 355 [1949]; H. R. Griem, Phys. Rev. **128**, 997 [1962]; G. Ecker and W. Weizel, Z. Naturforsch. **12 a**, 859 [1957]; H. Margenau and M. Lewis, Rev. Mod. Phys. **31**, 569 [1959].

10 C. Park, J.Q.S.R.T. **8**, 1633 [1968].

11 D. W. Norcross and P. M. Stone, J.Q.S.R.T. **8**, 655 [1968].