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On the Determination of Electron Temperature in Diffusion-Dominated Non-L.T.E. Plasmas

H. W. Drawin and F. Emard

Association EURATOM-CEA sur la Fusion
Département de Physique du Plasma et de la Fusion Contrôlée
Centre d'Etudes Nucléaires
92260 Fontenay-aux-Roses (France)

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Population densities of atomic hydrogen levels have been calculated for homogeneous stationary and diffusion-dominated stationary plasmas. The results show strong overpopulation of the lower lying excited states when the actual number density of ground state atoms is larger than the density obtained for the homogeneous stationary state. At low electron and high ground state densities the so-called Boltzmann slope is not further a characteristic quantity for the determination of electron temperatures, since the slope constant changes with quantum number. — The partial L.T.E. condition for diffusion-dominated plasmas is reexamined.

Introduction

Spectroscopic measurements of line emission coefficients made by different authors on wall-stabilized arcs operated at relatively high pressures ¹⁻⁵ and on high-temperature magnetically confined vacuum arcs ⁶⁻⁸ have shown over- and underpopulations for a limited or a large number of quantum states $|i\rangle$ when compared with the Saha density n_i^{Saha} given by the relation

$$n_i^{\text{Saha}} = n_+ n_e \frac{g_i}{2 g_+} \frac{h^3}{(2 \pi m_e k T_e)^{3/2}} \exp \frac{E_i - \nabla E}{k T_e} \quad (1)$$

and when compared with the Boltzmann population density $n_i^{\text{Boltzm.}}$ based on the complete L.T.E. assumption. Population densities n_i satisfying Eq. (1) are said to be in partial L.T.E. The electron temperature T_e of a non-L.T.E. plasma can be determined

from a Boltzmann plot when only levels i are considered which are in partial L.T.E. with respect to n_e and T_e (which implicitly means that only electronic collisions are responsible in populating and depopulating these levels). We show in the following that strong diffusion may destroy any possibility of determining electron temperatures from a "Boltzmann plot", since the diffusion effect pushes the usual partial L.T.E. condition to so high quantum levels that it becomes impossible to determine the slope of the Boltzmann plot with sufficient precision.

General Form of Rate Equations and their Solutions

We consider the level system of atomic hydrogen. The number density n_i of the i -th level (in the following i denotes the principal quantum number) is given by the relation

$$\partial n_i / \partial t + \nabla \cdot (n_i \bar{\mathbf{v}}_i) = (\partial n_i / \partial t)_{\text{coll, rad}}, \quad i = 1, 2, 3, \dots, p \quad (2)$$

Reprint requests to Dr. H.-W. Drawin, Association Euratom-CEA sur la Fusion, Département de Physique du Plasma, Centre d'Etudes Nucléaires, Boîte Postale n° 6, F-92260 Fontenay-aux-Roses, France.



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where $\bar{\mathbf{v}}_i$ is the mean diffusion velocity of particles in level i . The expression on the r.h.s. contains all collisional-radiative interaction terms. We make the assumption of a stationary state, i.e. all time derivatives $\partial n_i / \partial t$ become equal to zero.

We distinguish now between two different idealized physical situations:

a) *Homogeneous stationary state:* We assume the plasma to be homogeneous and stationary. In this case all l.h.s. of system (2) are equal to zero, since

$$\partial n_i / \partial t = 0, \quad \nabla \cdot (n_i \bar{\mathbf{v}}_i) = 0, \quad i \geq 1 \quad (3)$$

holds. System (2) thus reduces to p coupled equations of the following kind

$$0 = (\partial n_i / \partial t)_{\text{coll, rad}} = a_{i1} n_1 + a_{i2} n_2 + \dots + a_{ij} n_j + \dots + a_{ip} n_p + \delta_i, \quad i \geq 1. \quad (4)$$

The coefficients a_{ij} are reaction frequencies and the δ_i are the recombination rates into level i . We make the assumption that $n_e = n_+$ and assume further that only electron collisions and radiative processes are responsible in populating and de-populating the p coupled levels. In our case, radiative absorption is accounted for by optical reduction (escape) factors A_{ij} for bound-bound and A_i for free-bound transitions (see e.g. ⁹⁻¹⁰). For given values of A_{ij} and A_i the coefficients a_{ij} and δ_i thus become a function of n_e and T_e only. When the values of A_{ij} , A_i , n_e and T_e are given the p coupled equations of system (4) yield the population densities n_i of the p bound levels for the *homogeneous stationary (HS) state*. These solutions may be characterized by the symbol n_i^{HS} . Especially the number density of the ground state is then equal to n_1^{HS} .

b) *Inhomogeneous stationary state:* We assume the plasma to be strongly inhomogeneous. Diffusion fluxes will then influence the local population densities. The contribution of excited particles to the total diffusion flux of neutrals is generally very small compared to the diffusion fluxes of ground state particles or electron-ion pairs, since the number density $n_{i>1}$ of excited particles is by several orders of magnitude smaller than n_1 for the ground level and since the length $\lambda_{i>1}$ which the excited particles have to diffuse in order to attain a quasi-steady state with respect to the ground state particles and to the electrons is much shorter than the length λ_1 which the ground state particles must diffuse in order to

come into a quasi-steady state with respect to the electrons alone. Indeed, λ_i is given by the relation $\lambda_i \approx (\tau_i D_i)^{1/2}$ with $i = 1, 2, \dots, p$. D_i is the diffusion coefficient, τ_1 the relaxation time for the ground state particles to come into a quasi-steady state with respect to the electrons, $\tau_{i>1}$ the relaxation time for the excited particles to attain a quasi-steady state population with respect to the electrons and to the actual number of ground state particles. Since $D_{i>1} \approx D_1$ and $\tau_{i>1} \ll \tau_1$ holds ¹¹ it follows that $\lambda_{i>1} \ll \lambda_1$. Under the condition that the smallest lateral dimension of the plasma in direction of the gradient is larger than $\lambda_{i>1}$ and that the conditions

$$\left| \frac{T_e(l + \lambda_{i>1}) - T_e(l)}{T_e(l)} \right| < 1, \\ \left| \frac{n_e(l + \lambda_{i>1}) - n_e(l)}{n_e(l)} \right| < 1$$

are fulfilled, the excited particles can be assumed to be already in a quasi-steady state with respect to n_e and n_1 within dimensions of the order of $\lambda_{i>1}$, whereas the ground state particles can still deviate from the quasi-steady state population, since their "relaxation length" λ_1 is much larger than $\lambda_{i>1}$. For regions which are not smaller than $\lambda_{i>1}$ the rate equations for the excited states can therefore individually be put equal to zero. One obtains for the $p-1$ excited states the following coupled system of rate equations

$$0 = (\partial n_i / \partial t)_{\text{coll, rad}} = a_{i1} n_1 + a_{i2} n_2 + \dots + a_{ij} n_j + \dots + a_{ip} n_p + \delta_i, \quad i \geq 2. \quad (5)$$

When the values A_{ij} , A_i , n_e , T_e , and n_1 are given the $p-1$ population densities $n_{i>1}$ can be calculated from system (5). The solutions $n_{i>1}$ may be termed *solutions for the inhomogeneous stationary state*. From the theory of linear coupled equations follows that the $n_{i>1}$ can be put into the following mathematical form

$$n_{i>1} = n_{i>1}^{(0)}(A_{ij}, A_i, n_e, T_e) + g_{i>1}^{(1)}(A_{ij}, A_i, n_e, T_e) n_1 \quad (6)$$

where the $n_{i>1}^{(0)}$ are the solutions of system (5) when all $a_{i1} n_1$ are put equal to zero, whereas the $g_{i>1}^{(1)}$ are the solutions of system (5) when all $\delta_{i>1}$ are put equal to zero and n_1 is put equal to unity.

The solution for the ground state density, n_1 , follows from the relation

$$\nabla \cdot (n_1 \bar{\mathbf{v}}_1) = (\partial n_1 / \partial t)_{\text{coll, rad}} = a_{11} n_1 + a_{12} n_2 + \dots + a_{1j} n_j + \dots + a_{1p} n_p + \delta_1 \quad (7)$$

which can also be put into the following form (with $n_e = n_+$)

$$\nabla \cdot (n_1 \bar{\mathbf{v}}_1) = - \nabla \cdot (n_e \bar{\mathbf{v}}_A) = n_e^2 \alpha - n_e n_1 S \quad (8)$$

where α and S denote the collisional-radiative recombination and ionization coefficients respectively. α and S depend only on A_{ij} , A_i , n_e and T_e . $\bar{\mathbf{v}}_A$ is the mean ambipolar diffusion velocity. When the divergence of the diffusion flux of ground state atoms or of electron-ion pairs is known Eq. (8) yields the local value n_1 for the inhomogeneous state. It is evident that the local values of n_1 will strongly depend on the local values of $\nabla \cdot (n_1 \bar{\mathbf{v}}_1)$ or $\nabla \cdot (n_e \bar{\mathbf{v}}_A)$ respectively.

Numerical Results for Atomic Hydrogen

The rate equations have been solved with the rate coefficients as published in ¹² (with atom-atom collisions neglected). A maximum number of one hundred levels of principal quantum number i has been taken into account. We have assumed that the resonance lines are all optically thick ($A_{ij}=0$), whereas all other bound-bound and free-bound transitions have assumed to be optically thin (i.e. $A_{ij}=1$ for $i>1$, $A_i=1$ for all i). Typical numerical results obtained are shown in Figs. 1 to 4 in semi-logarithmic presentation for different values of n_e and T_e . The values on the abscissa, $1/i^2$, are proportional to the ionization energies E_1^H/i^2 with E_1^H equal to 13.58 eV.

a) *Homogeneous stationary state:* System (4) yields the ground state density n_1^{HS} as well as the particle densities of all excited levels. The numerical value of n_1^{HS} is indicated on each figure together with the Saha decrement b_1^{HS} for the ground state. b_1^{HS} is equal to n_1^{HS} divided by the corresponding Saha density n_1^{Saha} calculated from Eq. (1) for $i=1$. The population densities of the excited particles, divided by the statistical weight $g_i=2i^2$, are characterized on each figure by the curve parameter n_1^{HS} . One sees that above some critical quantum number c all n_i/g_i lie on a straight line. This is a well-known result: For $i \geq c$ all quantum states are in partial L.T.E. The slope of the straight line characterized by $\tan \alpha$ (Boltzmann slope) is proportional to $1/T_e$. The value of the critical quantum number c depends on n_e and T_e and is nearly independent of the degree of reabsorption

except at low electron densities and high temperatures. The numerical values for c are in agreement with the usually applied partial L.T.E. conditions (see e.g. ¹³).

b) *Inhomogeneous stationary state:* We assume now different values for the diffusion term $\nabla \cdot (n_1 \bar{\mathbf{v}}_1)$. The values of A_{ij} , A_i , n_e , and T_e shall be the same as used under a. According to the different values of $\nabla \cdot (n_1 \bar{\mathbf{v}}_1)$ one obtains from Eqs. (7) or (8) different values for n_1 . We assume that the diffusion term has values such that the local ground state density n_1 becomes equal to $10^{-1} n_1^{\text{HS}}$, $10 n_1^{\text{HS}}$, $10^2 n_1^{\text{HS}}$ These values appear as a curve parameter in Figs. 1 to 4. The curve parameters in parentheses are the values of $\nabla \cdot (n_1 \bar{\mathbf{v}}_1)$ (in units $\text{cm}^{-3} \text{sec}^{-1}$) which have been inserted into Eqs. (7) or (8) respectively for the calculation of n_1 . They are compatible with values met under many experimental conditions.

The values obtained for n_1 can now be used to calculate the corresponding local particle densities $n_{i>1}$ of the excited states according to Equation (6). Dividing by g_i yields the values n_i/g_i as shown in Figs. 1 to 4. In Figs. 1, 3, and 4 one sees additionally the values of n_i/g_i when n_1 is equal to the ground state density n_1 (1 Atm) at a total plasma pressure of $P=1$ Atm. n_1 (1 Atm) has been calculated using the L.T.E. assumption

$$P = (n_1 + \sum_{i>1}^p n_i + 2 n_e) k T, \quad T = T_e. \quad (9)$$

For the cases treated here n_1 (1 Atm) is always larger than n_1^{HS} for the homogeneous stationary state. This means that the plasma is submitted to a diffusion flux which has divergences different from zero.

Discussion and Conclusion

The numerical values presented in Figs. 1 to 4 exhibit the following general behavior of the curves $\ln(n_i/g_i)$ as a function of $1/i^2$: At low electron densities most of the $n_{i>1}$ lie far above the homogeneous stationary state solutions n_i^{HS} when $n_1 > n_1^{\text{HS}}$. For $n_1 < n_1^{\text{HS}}$ the lower lying excited states have population densities $n_{i>1} < n_i^{\text{HS}}$, but the effect is less pronounced than for $n_1 > n_1^{\text{HS}}$. With increasing electron density all excited state populations approach the solutions for the homogeneous stationary state.

When the actual ground state density n_1 is equal or close to the homogeneous stationary state solu-

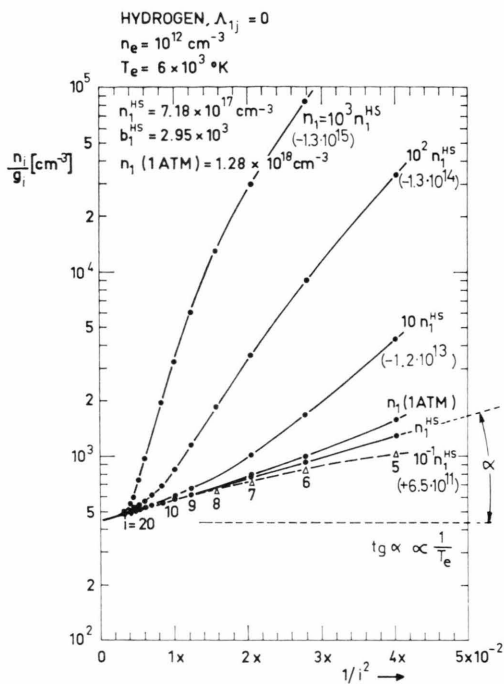


Fig. 1. Population densities n_i/g_i of atomic hydrogen as a function of ionization energy in units E_1^{H} . All resonance lines are assumed to be optically thick (i.e. $\Lambda_{1j}=0$). The ground state density n_1 is indicated on each curve, the values in parentheses are the corresponding divergences of the diffusion fluxes necessary to ensure the values of n_1 for the given values of n_e and T_e . $\text{tg } \alpha$ is proportional to $1/T_e$ with T_e equal to $6 \cdot 10^3 \text{ }^\circ\text{K}$.

tion n_1^{HS} the Boltzmann slope is well defined even at relatively low electron densities, since most of the excited levels are in partial L.T.E. and the energy differences are sufficiently large (which is a necessary condition for a precise determination of the slope constant). It follows from this that the electron temperature can be obtained from a relatively small number of excited state populations.

When the ground state is strongly over- or underpopulated relative to the (already overpopulated) stationary state solution the slope of the curve $\ln(n_i/g_i)$ vs. $1/i^2$ changes continuously with quantum number i until a new critical quantum number c' which is larger than c . Applied to an experimental situation this means: When in a diffusion-dominated plasma of low electron density only a few number of population densities of the lower lying excited states is measured one will not be sure to obtain the correct value of the electron temperature from the slope of the curve $\ln(n_i/g_i)$ vs. $1/i^2$ connecting the measured values. In order to obtain a straight line

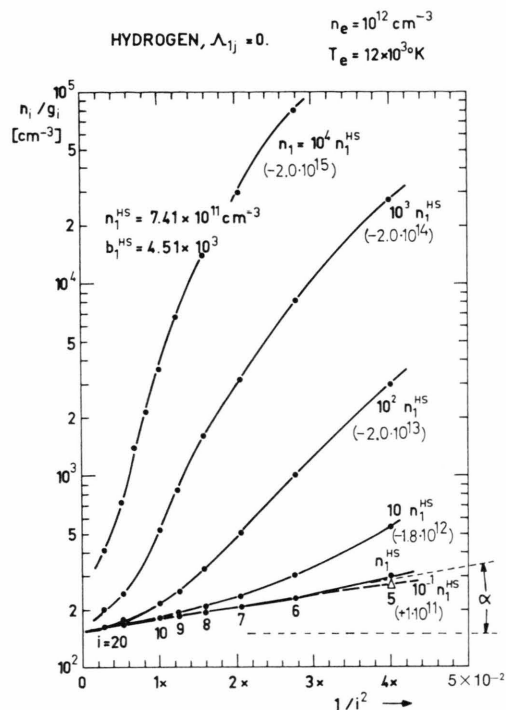


Fig. 2. Population densities n_i/g_i of atomic hydrogen as a function of ionization energy in units E_1^{H} . n_e and T_e are equal to 10^{12} cm^{-3} and $1.2 \cdot 10^4 \text{ }^\circ\text{K}$ respectively.

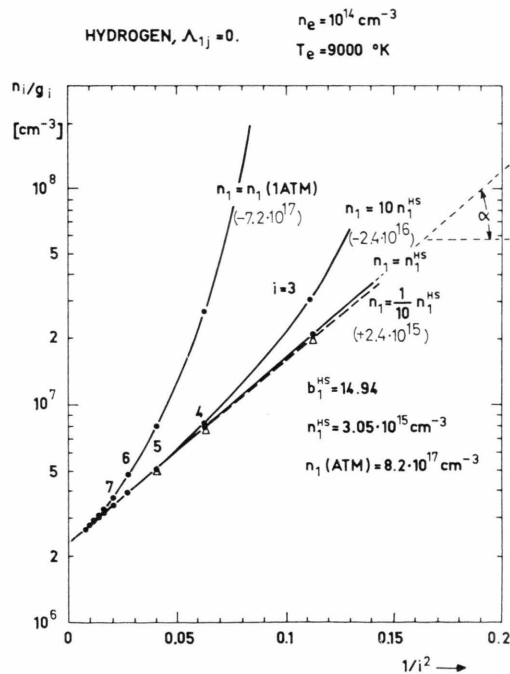


Fig. 3. Population densities n_i/g_i of atomic hydrogen as a function of ionization energy in units E_1^{H} . n_e and T_e are equal to 10^{14} cm^{-3} and $9000 \text{ }^\circ\text{K}$ respectively.

