

An analytical excitation for an ionizing plasma

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AN ANALYTICAL EXCITATION MODEL FOR AN IONIZING PLASMA

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From an analytical model for the population of high-lying excited levels in ionizing plasmas it appears that the distribution is a superposition of the equilibrium (Saha) value and an overpopulation. This overpopulation takes the form of a Maxwell distribution for free electrons. Experiments for He II, Na I and Ar I confirm the general validity of the model.

Introduction. The distribution functions of atoms and ions over their excited states are studied in the framework of collisional radiative models (CRM). These models are of great importance for plasma diagnostics, for the description of radiation sources like gas lasers and for impurity radiation loss calculations in fusion plasmas. Most model calculations have been focused on hydrogen and hydrogenic systems [1-3] since for H theoretical and semiempirical expressions for cross sections are available [2,4,5].

In CR models the distribution of the population of excited levels is calculated numerically for a finite number of levels by solving a set of coupled balance equations, one for each level. This approach requires a complete set of collisional rate coefficients and a cut-off of the system at a high-lying level. This cut-off causes the densities of high-lying levels to deviate considerably with respect to measured values.

For many plasma conditions it is possible to treat the problem analytically [6,7], at least for top levels, i.e. levels which are in the so-called excitation saturation phase (ESP) or partial local thermal equilibrium (PLTE). In ESP electronic excitation and deexcitation are assumed to dominate over radiative processes; in PLTE ionization and three-body recombination prevail. In this paper we deal with an analytical model for ionizing plasmas, i.e. plasmas with a ground state overpopulated with respect to the continuum. This overpopulation is distributed over the excited levels, by an excitation flow J from the ground state through

the excitation space to the continuum in a ladder-climbing fashion. Recombination and ionization processes will influence this excitation flow. By treating the excitation space as a continuum, we may equate the divergence of J to the difference of the recombination source R and the ionization sink I in the continuity equation

$$\operatorname{div} J = R - I. \quad (1)$$

The specific meaning of this equation will be discussed later, with either the principal quantum number p or the energy E as independent variable. Eq. (1) can be reformulated as a differential equation for the population density $n(p)$; the solution can be written as a superposition of the PLTE (s: Saha) and the ESP(e) distributions:

$$n(p) = n^s(p) + n^e(p) = n_p^s [1 + \delta b(p)]. \quad (2)$$

Here $1 + \delta b(p)$ is a factor expressing that the density is given by an equilibrium value and an overpopulation. Eq. (2) has a similar form as the solutions of numerical models [2,3]

$$n(p) = n^s(p) [r_p^{(0)} + r_p^{(1)} b(1)], \quad (2a)$$

where $r_p^{(0)}$ and $r_p^{(1)}$ are the so-called collisional radiative coefficients and $b(1)$ is the Saha increment of the overpopulated ground state. In the collision-dominated ESP regime we obtain $r_p^{(0)} = 1$ as in eq. (2). The second term of the r.h.s. of eq. (2a) shows that the overpopulation of the levels p is proportional to the overpopulation

of the ground state and depends on the atomic processes in the lower, corona, part of the atomic system. For hydrogen the ESP distribution can be described by a simple power law in p , as has been shown by Fujimoto [3] and Van der Mullen [8]. Their results suggest that

$$\delta b(p) \equiv b(p) - 1 = b_0 p^{-x}, \quad (3)$$

where $b(p)$ is the Saha increment of level p and b_0 is a constant. The value of b_0 can be obtained from a simple numerical CR model for the small number of lower levels which are not yet in ESP. Expression (3) has been confirmed by many experiments, as shown in fig. 1 for Ar I, He II and Na I [9–11] with a value of about 6 for the exponent. Apparently (3) is also valid for non-hydrogenic systems.

The aim of this letter is to derive the power law, to indicate that it is quite insensitive to atomic structure and that it has a fundamental meaning: it has the same form as the Maxwell distribution for free electrons.

The analytic top model (ATM). We assume as usually that in the plasma to be considered the energy distribution of the free electrons is maxwellian, that heavy-particle collisions can be neglected and that temporal and spatial derivatives for the excited-state densities

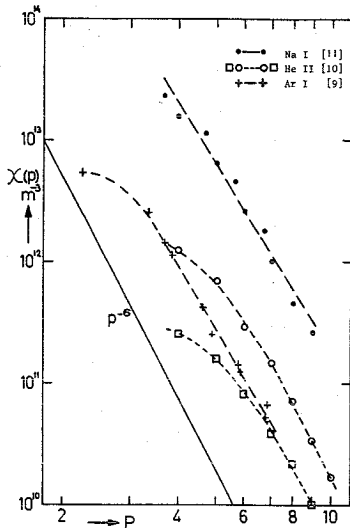


Fig. 1. Normalized population density $\chi(p)$, of excited states as a function of effective quantum number p . The quantity $\chi(p) = \eta(p) \exp(-u_p) = [n(p)/g(p)] \exp(-E_{pi}/kT_e)$ is proportional to $b(p)$, which is nearly equivalent to $\delta b(p)$ if $\delta b(p) \gg 1$. Note, that the predicted p^{-6} slope is observed.

can be ignored. The first two assumptions require the ionization degree to be larger than 10^{-3} . For the ATM we add the two specific assumptions that, first, radiative transitions can be neglected with respect to electronic (de)excitation and, second, the ionization energy E_{pi} of an ATM level is less than the kinetic energy of the free electrons, i.e. $E_{pi}/kT_e < 1$. With the first assumption the balance equation of level p is reduced to

$$n_e \sum [n(q)C(q, p) - n(p)C(p, q)] = n_e n(p)S(p) - n_e^2 n_i Q(p), \quad (4)$$

where $n(p)$, $n(q)$ are the densities of excited states p , q respectively; C is the rate coefficient for electronic (de)excitation, S for ionization and Q for recombination; n_e is the electron density and n_i the ion density. The various theoretical expressions for $C(p, q)$ in the literature [2,6,15] can be written in the general form

$$C(p, q) = 16\pi a_0^2 R^2 (2\pi m_e kT_e)^{-0.5} \times f_{pq} E_{pq}^{-1} \Psi_c(p, q, Z, T) \equiv \epsilon_{pq} f_{pq} E_{pq}^{-1}, \quad (5)$$

with

$$\epsilon_{pq} = 4.35 \times 10^{-12} \hat{T}_e^{-0.5} \Psi_c \quad (6)$$

(in $\text{eV m}^3 \text{s}^{-1}$, \hat{T}_e in eV) and where a_0 is the Bohr radius, R the Rydberg energy and m_e the electron mass; $E_{pq} = RZ^2(p^{-2} - q^{-2})$ is the energy difference between the levels p and q ; f_{pq} is the oscillator strength, which for small values of $\Delta p = q - p$ can be approximated [4] by $f_{pq} = 1.53 p^{-5} q^{-3} (p^{-2} - q^{-2})^{-3}$.

The function $\Psi_c(p, q, Z, T)$ can be adjusted to the various collision theories. For $u_p < 1$, Ψ_c is only a weak function of p, q and the charge number Z . Differences between the various theories have to disappear when $u_p = E_p^1/kT_e$ tends to zero, since in that case the cross sections have to approach the Born–Bethe expression. For hydrogenic ions eq. (6) can be written as

$$C_{pq} = c_{pq} p^4 \Delta p^{-4}, \quad \text{with } c_{pq} \approx 0.1 R^{-1} Z^{-2} \epsilon_{pq}. \quad (7)$$

For the ionization rate coefficient we can use

$$S(p) = \frac{80}{3} \pi a_0^2 R^2 (2\pi m_e kT_e)^{-0.5} E_{pi}^{-0.5} \Psi_s(p, T), \quad (8)$$

in which $\Psi_s(p, T)$ can also be adjusted to the various

collision theories. With $E_{p1} = Rp^{-2}Z^2$ eq. (8) can be written as

$$S(p) = s_p p^2,$$

with

$$s_p = 5.34 \times 10^{-13} \hat{T}_e^{-0.5} Z^{-2} \Psi_s \quad (\text{in } \text{m}^3 \text{s}^{-1}). \quad (9)$$

As can be seen from (7), one-step excitation processes ($\Delta p = 1$) are by far the most probable; the excitation flow which results from $\Delta p = 1$ processes will be called the stepflow. The stepflow at location p is defined as the difference in the number of excitation processes from p to $p + 1$ and the number of deexcitation processes from $p + 1$ to p and can be written

$$J(p, p+1) = n_e n(p) C(p, p+1) - n_e n(p+1) C(p+1, p). \quad (10)$$

By introducing the density per statistical weight $\eta(p) = n(p)/g(p)$ and the Saha increment $b(p) = \eta(p)/\eta^s(p)$ and by applying the principle of detailed balancing (DB) to processes between p and $p + 1$, we get with $g(p) = 2p^2$ and eq. (7) for the stepflow

$$J(p, p+1) = 2n_e \eta^s(p) c_{p,p+1} p^6 [b(p) - b(p+1)]. \quad (11a)$$

In a continuous description we obtain for the excitation flow the approximation

$$J(p) = -2n_e \eta^s(p) c_p p^6 b'(p), \quad (11b)$$

where $b'(p)$ is the first derivative of $b(p)$; c_p contains also $\Delta p \neq 1$ processes, but as a consequence of the $(\Delta p)^{-4}$ dependency in eq. (7) c_p is close to $c_{p,p+1}$.

The ionization sink $I(p)$ can [cf. eq. (9)] be written as

$$I(p) = n_e n(p) = 2n_e \eta^s(p) s_p p^4 b(p) \quad (12)$$

and the recombination source $R(p)$ with detailed balancing as

$$R(p) = n_e n_i Q(p) = 2n_e \eta^s(p) s_p p^4. \quad (13)$$

In the one-dimensional p space $\text{div } J$ can be replaced by $dJ/dp = J'$. By substituting eqs. (11b), (12) and (13) into eq. (1), we can derive a second-order differential equation in $b(p)$. From various collision theories [2,4,15] it appears that the remaining p dependence of $\eta^s(p) c_p$ and of s_p/c_p can be ignored in the $u_p < 1$ limit. Then this equation reads

$$p^2 b''(p) + 6pb'(p) - (s_p/c_p) [b(p) - 1] = 0 \quad (14)$$

and has as a solution

$$b(p) = 1 + b_0 p^{-x} \quad (15a)$$

or

$$\eta(p) = \eta^s(p) (1 + b_0 p^{-x}) = \eta^s(p) + \beta p^{-x} \exp(u_p). \quad (15b)$$

The value of x can be found from

$$x = 2.5 + 2.5 (1 + 0.16 s_p/c_p)^{1/2}. \quad (16)$$

Eq. (15) shows that the population distribution is a superposition of the equilibrium (Saha) value and an overpopulation originating from the overpopulated ground state of the ionizing plasma; b_0 is the *extrapolated* Saha increment and $\beta \exp(u_1)$ is the extrapolated ESP population of the ground state.

As can be seen from eqs. (16), (6) and (9) the value of x depends only weakly on the ratio s_p/c_p and the ratio Ψ_s/Ψ_c . The lowest value, $x = 5$, is obtained if ionization and recombination are neglected. If ionization is included [8], then values of 5.5 to 6.5 are obtained if the results of refs. [2,5] are inserted into eq. (16); so x is always close to 6. Also it is evident that x is nearly Z independent. However, b_0 depends strongly on Z and for high Z large values for p and/or n_e are required to satisfy the theory.

The result of the ATM has been compared with experimental data for different atomic systems, by using for non-hydrogenic systems an effective principal quantum number $p = Z (R/E_{p1})^{1/2}$. As can be seen from fig. 1 there is good agreement between the experimental results and the ATM description for $x = 6$.

The fundamental significance of this power-law dependence can be found if we transform the p metric of the excitation space to the energy metric E and introduce the energy distribution function $f(E)$ according to

$$f(E) dE = \eta(p) g(p) dp, \quad (17)$$

where the energy $E \equiv -E_{p1} = -RZ^2 p^{-2}$ is defined as a negative quantity.

From eq. (15) we can derive that for $x = 6$ the distribution function can be written as

$$f(E) = \eta^s(p) R^{3/2} Z^3 |E|^{-5/2} + \beta R^{-3/2} Z^{-3} |E|^{1/2} \exp(-E/kT). \quad (18)$$

The first term of this expression represents the equilibrium population for bound states, whereas the second term gives the overpopulation. This overpopulation has the same energy dependence as the Maxwell distribution for free electrons. This surprising result can be understood by noting that in the ESP the interaction with free electrons occur more frequently than typical atom events like radiative decay. Apparently, the result of these frequent interactions is that the energy distribution of the free electrons is imposed on the overpopulated bound electrons.

Application of the Fokker-Planck description for the top levels. In order to obtain the energy distribution function directly from the continuity equation in the E -representation, the course of an electron through the excitation space can be considered as a Markov process [13] and the Fokker-Planck description can be used. The excitation flow $J(E)$ can then be written [7,12] as

$$J(E) = f(E) \langle \Delta E \rangle / \Delta t - \frac{1}{2} \partial [f(E) \langle \Delta E^2 \rangle / \Delta t] / \partial E. \quad (19)$$

The first term represents the drift in excitation space. The average change per unit time of the energy of a bound electron with initial energy E can be written as, cf. eq. (6),

$$\langle \Delta E \rangle / \Delta t = n_e \sum C(p, q) E_{pq} = n_e \sum \epsilon_{pq} f_{pq}. \quad (20)$$

The second term represents the diffusion

$$\langle \Delta E^2 \rangle / \Delta t = n_e \sum C(p, q) E_{pq}^2 = n_e \sum \epsilon_{pq} f_{pq} E_{pq}. \quad (21)$$

For the $u_p = 0$ limit $\partial \epsilon_{pq} / \partial p = \partial \epsilon_{pq} / \partial q = 0$ and ϵ_{pq} can be replaced by the constant ϵ . The summations in eqs. (20), (21) are evaluated by employing the atomic summation rules [14]

$$\sum_q f_{pq} = 1 \quad \text{and} \quad \sum_q f_{pq} E_{pq} = -\frac{4}{3} E_p. \quad (22)$$

Herewith eq. (19) can be written as

$$J(E) = \frac{5}{3} n_e \epsilon f(E) + \frac{2}{3} n_e \epsilon \partial f(E) / \partial E. \quad (23)$$

The ionization sink has the form [cf. eq. (12)]

$$I(E) = n_e f(E) s_p R Z^2 |E|^{-1} \quad (24)$$

and the recombination source reads [cf. eq. (13)]

$$R(E) = n_e \eta^s(p) s_p R^{5/2} Z^5 |E|^{-7/2}. \quad (25)$$

By substituting eqs. (23)–(25) in eq. (1), we get a solution which can be shown to be the same solution as

given by eq. (15) for $x = 6$. Only the factor $\exp(u_p)$ has disappeared as a consequence of the $u_p = 0$ limit. The advantages of the Fokker-Planck treatment are that the derivation is not limited to step processes only and that application to more complex atomic systems turns out to be justified if the wave function can be described as a product of a wave function of the outer electron and one of the core.

Conclusions.

The population distribution of a high-lying level in an ionizing plasma is a superposition of a Saha population and an overpopulation.

This overpopulation has the same form as the maxwellian distribution of free electrons.

If overpopulated bound electrons are subjected to frequent interactions with free electrons they will take over the energy distribution of the free electrons. Hence, the atomic structure is only of minor importance. This fact is confirmed by experiments in non-hydrogenic systems.

The problem of CR models for ionizing plasmas is reduced to the determination of the extrapolated ground-state overpopulation.

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