Population of Excited Levels of Atoms and Ions: Electron Temperature and Density from Relative Line Intensities of the Ions C IV, N V, and O VI

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The theory of the population of excited levels for atoms and ions is given for stationary, nonthermal plasmas. Simplified expressions were obtained, with the aid of which populations of the levels $2P$, $3P$, and $3D$ were determined for the ions C IV, N V, and O VI. It is shown that the populations obtained by this method are in very good agreement with the populations determined directly from the balance of excitation and de-excitation processes. Plots are given which enable the determination of electron density and temperature from relative intensities of three chosen lines from a given ion.

1. INTRODUCTION

THE spectroscopic methods of measurements of plasma parameters are not sufficiently well developed for the range of electron densities lying between the solar-corona type of equilibrium and the thermodynamic equilibrium. It is true that, using the continuum spectrum of hydrogen plasma, one can determine the electron temperature kT_e and density for a wide range of changes of electron density N_e. However, because of very intense impurity lines, such measurements are possible only for extremely pure plasmas.[1–3] In previous works[4–6] the measurements of electron temperature from the relative intensities of lines from the same ion have been presented. Unfortunately, the relations determined in these references between intensities of lines and electron temperature are valid only for plasmas of relatively low densities, when one can still apply the solar-corona equilibrium relations. For the range of N_e between that defined by the solar-corona equilibrium relations and the thermodynamic equilibrium, a method for electron-density determination has been given,[7] using the absolute intensities of lines. However, the determination of plasma electron densities from absolute line intensities is much more troublesome than their determination from relative line intensities. Elsewhere,[8] the method of determination of N_e from relative line intensities of the same ion was expressly mentioned. It is shown in the present work that from relative intensities of three chosen lines of a given ion, one can determine electron temperature and density for nonthermal plasmas and for a broad range of changes of N_e.

In all these cases a knowledge of the population of the excited levels considered is required for the known electron velocity distribution. Unfortunately, the lack of experimental data for excitations of ions makes it difficult to choose the proper function for the cross section. In the present work the expression given in Ref. 9 is used; for not too high values of kT_e, it is close to the expression of Seaton.[10] In the method of calculation of electron density and temperature given below, other functions for the excitations can obviously be used. The use of other cross sections can cause some changes of relative line intensities, but it does not influence the validity of the method itself.

2. ANALYSIS OF THE POPULATION OF EXCITED LEVELS OF ATOMS AND IONS

We consider the populations of levels of excited atoms and ions for an optically thin, stationary plasma which does not interact with the chamber walls. For such plasmas we can neglect the radiative excitations as well as the radiative induced transitions. As the electron temperatures of the considered plasmas are not higher than 20–30 eV, the collisions of atoms with ions and of ions with ions can also be neglected in comparison with the collisions of electrons with atoms or ions.

Taking all these assumptions into account, we can write an expression for the population of an excited level n for the range of densities N_e, for which the collisional excitations play an essential role in the population of this level and are balanced by the radiative de-excitations from the level n. This expression has the form[7]

$$N_n/N_m = B_n^*(g_n/g_m)\exp[-(E_n-E_m)/kT_e], \quad (1)$$

where

$$B_n^* = \sum_i \prod_{k<n} \tau_{k+1,\,k}^{(i)}.$$

In the expression for B_n^* the multiplication takes into

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account the excitation of the level n from the ground level m, by stepwise excitations of the intermediate levels lying between n and m for a given mode of population i, whereas the summation over i takes into consideration all the paths leading to the population of the level n. The quantities N_n and N_m are the densities of atoms and ions in the excited state n and in the ground state m, respectively; g_n and g_m are the statistical weights of levels n and m; E_n and E_m are the energies of excitation of levels n and m; and the coefficients $\tau_{k+1,\,k}$ are defined by the following expression:

$$\tau_{k+1,\,k}=\frac{N_e\langle\sigma_{k,\,k+1}V_e\rangle}{\sum_{t\leqslant k}A_{k+1,\,t}}\frac{g_k}{g_{k+1}}\exp\left(\frac{E_{k+1}-E_k}{kT_e}\right). \quad (2)$$

In this expression $A_{k+1,\,t}$ is the coefficient of spontaneous radiation from level $k+1$ to level t, and $\langle\sigma_{k,\,k+1}V_e\rangle$ is the rate coefficient for excitation of an atom or ion from level k into level $k+1$ by an electron impact.

Consider the case where electron densities in a plasma are so small that one must also take into consideration in Eq. (1) the cascade transitions from higher levels which contribute to the population of the level n, as well as the optically forbidden transitions. Then instead of Eq. (1) one gets

$$\frac{N_n}{N_m}=B_n{}^*\frac{g_n}{g_m}\exp\left(-\frac{E_n-E_m}{kT_e}\right)+\sum_{t>n}B_t{}^*\frac{A_{tn}}{\sum A_{nk}}\frac{g_t}{g_m}\times\exp\left(-\frac{E_t-E_m}{kT_e}\right)+\tau_{nm}{}^{\text{band}}\frac{g_n}{g_m}\exp\left(-\frac{E_n-E_m}{kT_e}\right). \quad (3)$$

In this expression the second term gives the population of the level n by the cascade transitions, and the third term gives the population by the optically forbidden transitions. $\tau_{nm}{}^{\text{band}}$ is defined here by Eq. (2), in which $\sigma_{k,\,k+1}$ is replaced by $\sigma_{mn}{}^{\text{band}}$. For the levels which are populated directly from ground state by the optically allowed transitions (e.g., *s*-*p* transitions), one can neglect the influence of the optically forbidden transitions. When electron densities in a plasma are sufficiently high, in the expression for the population of an excited level, the collisional de-excitations must be also taken into account.

Further, the plasma will be considered to be one for which we can assume a Maxwellian velocity distribution of electrons. Such an assumption is valid for most experiments.

Using the Klein-Rosseland relation for the cross sections for excitation and de-excitation of atoms and ions by an electron impact and taking $\langle\sigma V_e\rangle$ from Eq. (2), one can write the expression for the population of levels in the form

$$N_n/N_m=B_n(g_n/g_m)\exp[-(E_n-E_m)/kT_e], \quad (4)$$

where

$$B_n=\sum_i\prod_{k<n}\frac{\tau_{k+1,\,k}{}^{(i)}}{1+\sum_{r\leqslant k}\tau_{k+1,\,r}{}^{(i)}}.$$

For large N_e ($\sum_{r\leqslant k}\tau_{k+1,\,r}\gg 1$ for each k), we have $B_n\approx 1$, and Eq. (4) tends towards the Boltzmann statistical expression.

Using (3) and (4), we can obtain a single, more general expression:

$$\frac{N_n}{N_m}=\left(B_n+\frac{\tau_{nm}{}^{\text{band}}}{1+\sum_{r<n}\tau_{nr}}\right)\frac{g_n}{g_m}\exp\left(-\frac{E_n-E_m}{kT_e}\right)+\sum_{t>n}B_t\frac{A_{tn}g_t}{\sum_{k<n}A_{nk}g_m}\exp\left(-\frac{E_t-E_m}{kT_e}\right). \quad (5)$$

3. DEPENDENCE OF THE RELATIVE POPULATIONS OF EXCITED LEVELS ON N_e AND kT_e

To determine the ratios of the population of excited levels as a function of electron density, it is convenient to express the above-mentioned formulas as explicit functions of N_e. For this purpose we write $\tau_{k+1,\,k}{}^{(i)}=N_e\beta_{k+1,\,k}{}^{(i)}$, where the expression for $\beta_{k+1,\,k}$ is obtained from Eq. (2).

If the population of a level n is going from the ground level m, for every way of population, through the same number of intermediate levels, then Eq. (1) with the aid of $\beta_{k+1,\,k}$ can be presented in the form

$$\frac{N_n}{N_m}=N_e{}^{n-m+1}D_n{}^*\frac{g_n}{g_m}\exp\left(-\frac{E_n-E_m}{kT_e}\right), \quad (6)$$

where

$$D_n{}^*=\sum_i\prod_{k<n}\beta_{k+1,\,k}{}^{(i)}.$$

In this expression the value of the exponent $n-m$ of N_e is equal to the number of intermediate levels between the ground level m and the excited level n. It follows immediately from Eq. (6) that if two levels, n and n', have $|(E_n-E_{n'})/kT_e|\ll 1$, and there are different numbers of intermediate levels between the ground level m and the levels n and n' ($n-m\neq n'-m$), then their population ratio will be strongly dependent on N_e, whereas the dependence on kT_e will be slight. This enables the determination of the electron density from the ratio of intensities of two lines belonging to the same ion. Taking into consideration that the line intensity is given by

$$I_{nk}=N_nA_{nk}h\nu_{nk},$$

we get the following expression for the determination of the electron density:

$$N_e{}^{n'-n}=\frac{I_{n'k'}A_{nk}\nu_{nk}}{I_{nk}A_{n'k'}\nu_{n'k'}}\frac{D_n{}^*}{D_{n'}{}^*}\frac{g_n}{g_{n'}}\exp\left(\frac{E_{n'}-E_n}{kT_e}\right). \quad (7)$$

When the number of intermediate levels is different for each mode of populating, then one cannot find such simple relations between N_e and the ratio of $I_{nk}/I_{n'k'}$. Nevertheless, knowing the relations $I_{nk}/I_{n'k'}=f(N_e)$, one can also determine N_e easily.

Equation (6) is valid for the same range of electron densities for which Eq. (1) is valid. For lower densities, the population of excited levels by the cascade transitions and by the optically forbidden transitions has also to be taken into consideration, using Eq. (3).

On the other hand, for sufficiently high plasma densities, the expression for the electron density is obtained from Eq. (4) in the form

$$N_e{}^{n'-n}=N_{e(7)}{}^{n'-n}\frac{D_{n'}{}^*D_n}{D_n{}^*D_{n'}}, \quad (8)$$

where

$$D_n=\sum_i\prod_{t\leqslant n}\frac{\beta_{k+1,\,k}{}^{(i)}}{1+\sum_{r\leqslant k}\tau_{k+1,\,k}{}^{(i)}}.$$

Here $N_{e(7)}$ means the electron density determined by Eq. (7). Similarly, one can consider the range of low and high electron densities when determining the electron temperature kT_e. But for low electron densities it is not possible, usually, to get kT_e as a simple function of the ratio $I_{nk}/I_{n'k'}$. However, frequently it is convenient, for the determination of kT_e, to use the lines radiated by excited P levels (with S as the ground state). In this case the influence of the cascade and optically forbidden transitions is practically negligible, and the formula for kT_e is the same as in the case of solar-corona equilibrium. Using Eq. (4) for high electron densities, we obtain a general expression for kT_e in the form

$$kT_e=(E_{n'}-E_n)\Big/\left(\ln\frac{I_{nk}A_{n'k'}g_{n'}\nu_{n'k'}}{I_{n'k'}A_{nk}g_n\nu_{nk}}+\ln\frac{B_{n'}}{B_n}\right). \quad (9)$$

For very high electron densities, Eq. (9) evidently tends towards the formula valid for the plasma in thermodynamical equilibrium.

4. DETERMINATION OF N_e AND kT_e FROM THE POPULATION OF IONS C IV, N V, AND O VI

To determine the populations of some excited levels of lithiumlike ions, we shall use the excitation cross section of ions by electron impact given by Griem[9]:

$$\sigma_{mn}\approx4\pi a_0{}^2\xi_m f_{mn}\frac{\chi_H{}^2}{\epsilon(E_n-E_m)}, \quad (10)$$

where a_0, ξ_m, and f_{mn} are the Bohr radius for the hydrogen atom, the number of equivalent electrons in state m,

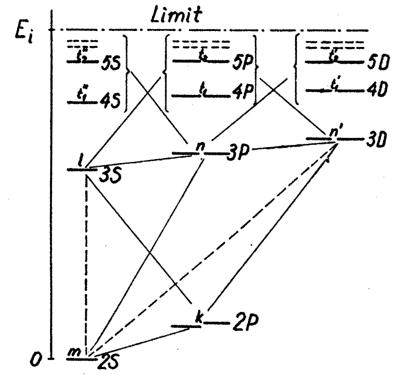

FIG. 1. Simplified scheme of levels for ion C IV, N V, and O VI.

and the absorption oscillator strength for the m-n transitions, respectively; χ_H is the ionization energy of the hydrogen atom, and ϵ is the energy of the colliding electrons (all energies are in eV).

The average Gaunt factor $\bar{g}$ changes only slightly for changes of the ratio $\epsilon/(E_n-E_m)$ over a range from 1 to 5; thus, for not too large values of this ratio, there is relatively good agreement between Eq. (10) and the more precise expression of Seaton.[10] Hence the quantity $\langle\sigma_{mn}V_e\rangle$, calculated for a Maxwellian velocity distribution of electrons, changes only slightly for not too high temperatures kT_e ($kT_e\leqslant2|E_n-E_m|$), if σ_{mn} given by Eq. (10) is used instead of Seaton's cross section. That also means that for this range of kT_e one can use Eq. (10) when determining τ_{nm} from Eq. (2):

$$\tau_{nm}\approx1.6\times10^{-17}\xi_m N_e\frac{A_{nm}}{\sum_{k<n}A_{nk}}\left(\frac{\chi_H}{kT_e}\right)^{1/2}\left(\frac{\chi_H}{E_n-E_m}\right)^3. \quad (11)$$

Further considerations pertain to some chosen excited levels of the ions C IV, N V, and O VI. To determine the electron densities from relative intensities of lines of these ions, it is convenient to compare the populations of the levels $3D$ and $3P$. However, for the determination of the electron temperature, we consider the ratios of populations of levels $3P$ and $2P$. The levels $2P$, $3P$, and $3D$ are relatively well separated from other levels, which fact considerably simplifies the analysis of their populations (Fig. 1). The populations of these levels were calculated with the aid of Eq. (5), yielding the following forms for the above mentioned levels:

$$2^2P_{3/2}\ (k):\quad \frac{N_k}{N_m}=\frac{\tau_{km}}{1+\tau_{km}}\frac{g_k}{g_m}\exp\left(-\frac{E_k-E_m}{kT_e}\right); \quad (12)$$

$3^2P_{1/2,3/2}(n)$:

$$\frac{N_n}{N_m}=\left[\frac{\tau_{nm}}{1+\tau_{nm}+\tau_{nl}}+\frac{\tau_{nl}\tau_{lk}\tau_{km}}{(1+\tau_{nl}+\tau_{nm})(1+\tau_{lk})(1+\tau_{km})}\right]\times\frac{g_{n\frac{1}{2}}+g_{n\frac{3}{2}}}{g_m}\exp\left(-\frac{E_n-E_m}{kT_e}\right), \quad (13)$$

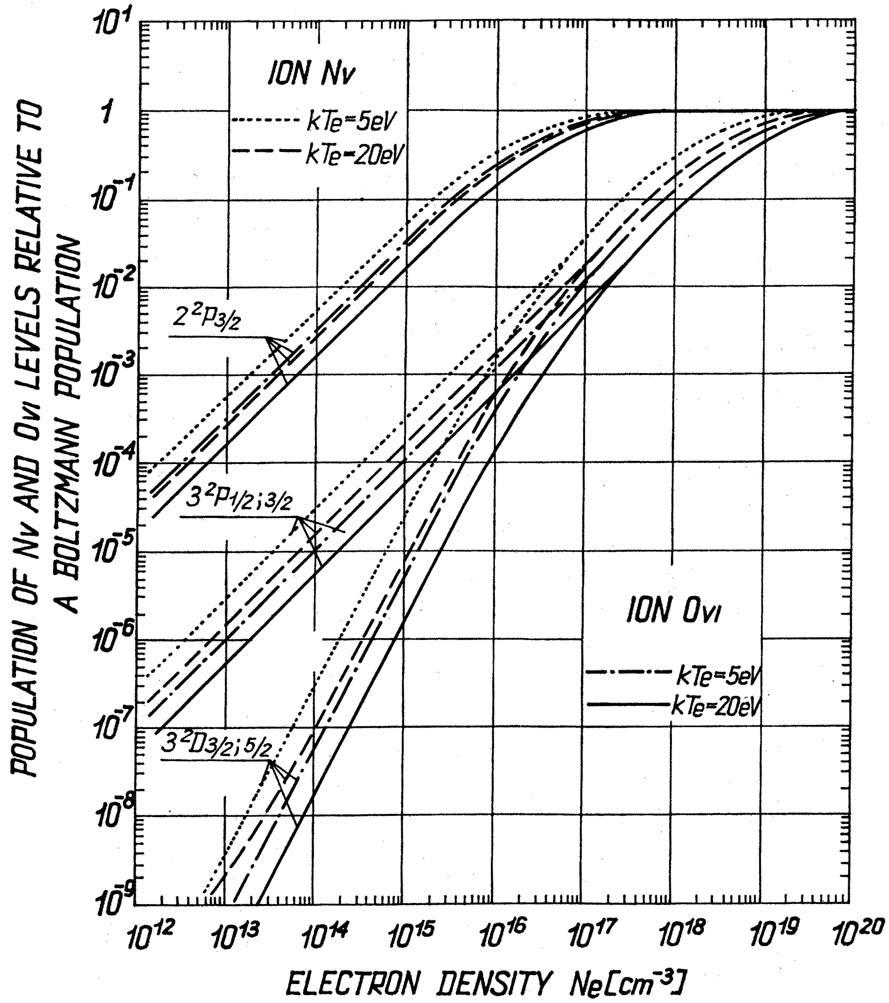

FIG. 2. Ratio of actual and thermal equilibrium populations of the levels $2P$, $3P$, and $3D$ of the ions N v and O vi.

where $\tau_{nm}=\tau_{n\frac{1}{2}m}=\tau_{n\frac{3}{2}m}$, $\tau_{lk}=\tau_{lk\frac{1}{2}}+\tau_{lk\frac{3}{2}}$, and the numbers $\frac{1}{2}$ and $\frac{3}{2}$ connected with the subscripts n and k denote the quantum number J of a given sublevel.

$$3^2D_{3/2,5/2}\ (n'):\quad \frac{N_{n'}}{N_m}=\Bigg[\frac{\tau_{n'k}\tau_{km}}{(1+\tau_{n'k}+\tau_{n'n})(1+\tau_{km})}$$

$$+\frac{N_n}{N_m}\frac{\tau_{n'n}}{(1+\tau_{n'k}+\tau_{n'n}}\Bigg]\frac{g_{n'\frac{3}{2}}+g_{n'\frac{5}{2}}}{g_m}\exp\left(-\frac{E_{n'}-E_m}{kT_e}\right)$$

$$+\sum_{t>n}\tau_{tm}\frac{A_{tn'}}{\sum_{k<n'}A_{n'k}}\frac{g_t}{g_m}\exp\left(-\frac{E_t-E_m}{kT_e}\right).\quad (14)$$

In Fig. 2 the ratios of populations of the levels $2P$, $3P$, and $3D$ of the ions N v and O vi, calculated according to the Eqs. (12)–(14), to populations determined by the statistical Boltzmann formula are presented as a function of N_e for the two temperatures $kT_e=5$ and $kT_e=20$ eV.

From the ratio of intensities of lines of the levels $3D$ and $3P$ as a function of N_e, one gets the curves enabling the determination of electron densities. It can be seen from Fig. 3 that this ratio depends only slightly on kT_e for a wide range of changes of N_e. For high electron densities the ratio of intensities of lines is close to that obtained from the Boltzmann formula.

For the rectilinear part of the curves, the electron density is given by a simple relation following from Eq. (7).

Comparing now the intensities of lines from the levels $3P$ and $2P$, one gets the dependence of their ratio on temperature. This is presented in Fig. 4. At densities $N_e\leqslant 10^{15}$ the ratios of intensities of these lines do not depend on N_e, in agreement with the results of other authors.[4–6]

One should still consider to what extent the populations of excited levels, calculated with the aid of the method given above, coincide with the solutions of the set of equations which were obtained as the result of a

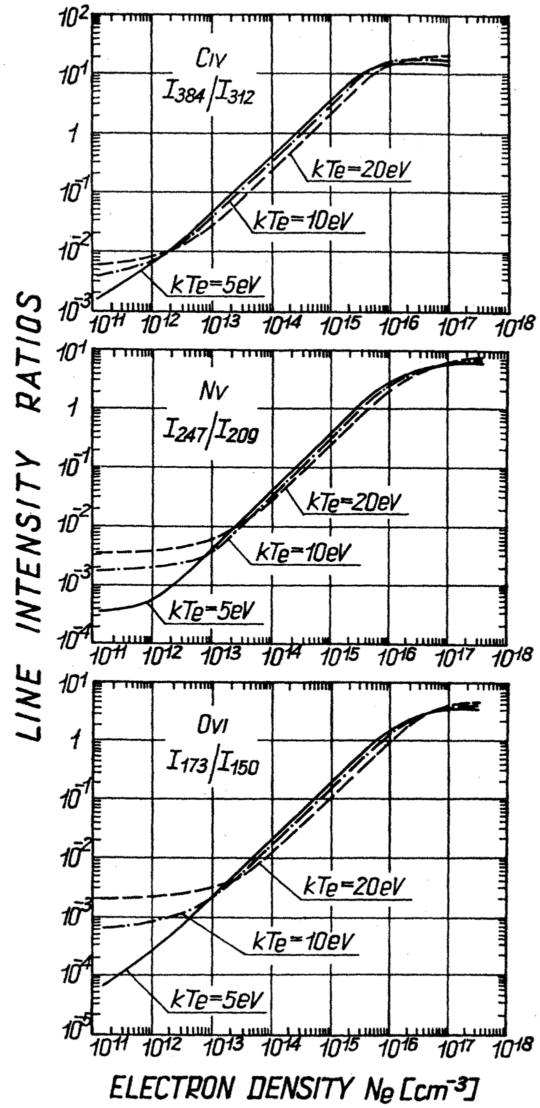

FIG. 3. Relative line intensities of the ions C IV, N V, and O VI as a function of electron density N_e for different electron temperatures.

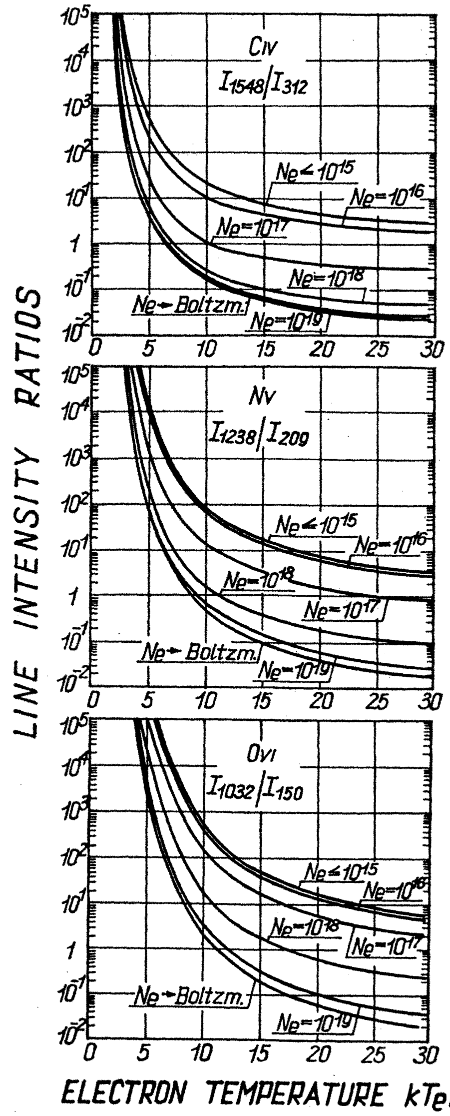

FIG. 4. Relative line intensities of the ion C IV, N V, and O VI as a function of electron temperature.

balance of the processes leading to the excitation and de-excitation of the levels considered.

In the equation obtained from the balance of excitation and de-excitation processes and determining the population of the level $2P$, and also of the corresponding expressions for the $3P$ and $3D$ levels, the excitation cross sections can be taken from the expression (10). Also, $\langle \sigma V_e \rangle$ can be expressed by τ, which is given by Eq. (11) [as in Eqs. (12)–(14) above].

Then the equation for the population of the level $2P_{3/2}$ has the form

$$\frac{N_k}{N_m}=\left\{\frac{\tau_{km}}{1+\tau_{km}}\frac{g_k}{g_m}\exp\left(-\frac{E_k-E_m}{kT_e}\right)+\left[\sum_{n_S=3}^{5}\frac{N_{n_S}}{N_m}A_{n_Sk}\left(1+\tau_{n_Sk}\sum_{n_P<n_S}A_{n_Sn_P}/A_{n_Sk}\right)\right.\right.$$
$$\left.\left.+\sum_{n_D=3}^{5}\frac{N_{n_D}}{N_m}A_{n_Dk}\left(1+\tau_{n_Dk}\sum_{n_P<n_D}A_{n_Dn_P}/A_{n_Dk}\right)\right][A_{km}(1+\tau_{km})]^{-1}\right\}\left\{1+[g_kA_{km}(1+\tau_{km})]^{-1}\right.$$
$$\left.\times\left[\sum_{n_S=3}^{5}\tau_{n_Sk}\sum_{n_P<n_S}A_{n_Sn_P}g_{n_S}\exp\left(-\frac{E_{n_S}-E_k}{kT_e}\right)+\sum_{n_D=3}^{5}\tau_{n_Dk}\sum_{n_P<n_D}A_{n_Dn_P}g_{n_D}\exp\left(-\frac{E_{n_D}-E_k}{kT_e}\right)\right]\right\}^{-1}. \quad (15)$$

TABLE I. Populations of levels for ion N V calculated from Eqs. (12)–(14) and compared with those obtained from Eqs. (15), (15′), and (15″). N with subscript "Boltz" denotes a population obtained from the Boltzmann statistical formula.

N_e	Level $2^2P_{3/2}(k)$ $N_k/N_{k\,\mathrm{Boltz}}$ Eq. (12)	Level $2^2P_{3/2}(k)$ $N_k/N_{k\,\mathrm{Boltz}}$ Eq. (15)	Level $3^2P_{3/2}(n)$ $N_n/N_{n\,\mathrm{Boltz}}$ Eq. (13)	Level $3^2P_{3/2}(n)$ $N_n/N_{n\,\mathrm{Boltz}}$ Eq. (15′)	Level $3^2D_{5/2}(n')$ $N_{n'}/N_{n'\,\mathrm{Boltz}}$ Eq. (14)	Level $3^2D_{5/2}(n')$ $N_{n'}/N_{n'\,\mathrm{Boltz}}$ Eq. (15″)
			$kT_e=5$ eV			
10^{11}	6.64×10^{-6}	6.64×10^{-6}	3.19×10^{-8}	3.19×10^{-8}	2.25×10^{-12}	2.25×10^{-12}
10^{12}	6.64×10^{-5}	6.64×10^{-5}	3.19×10^{-7}	3.19×10^{-7}	5.50×10^{-11}	5.50×10^{-11}
10^{13}	6.63×10^{-4}	6.63×10^{-4}	3.18×10^{-6}	3.19×10^{-6}	3.80×10^{-9}	3.80×10^{-9}
10^{14}	6.59×10^{-3}	6.50×10^{-3}	3.18×10^{-5}	3.18×10^{-5}	3.61×10^{-7}	3.61×10^{-7}
10^{15}	6.22×10^{-2}	6.22×10^{-2}	3.15×10^{-4}	3.12×10^{-4}	3.38×10^{-5}	3.38×10^{-5}
10^{16}	3.99×10^{-1}	3.99×10^{-1}	3.12×10^{-3}	3.03×10^{-3}	2.13×10^{-3}	2.13×10^{-3}
10^{17}	8.69×10^{-1}	8.69×10^{-1}	4.31×10^{-2}	4.33×10^{-2}	4.37×10^{-2}	4.37×10^{-2}
10^{18}	9.85×10^{-1}	9.85×10^{-1}	3.77×10^{-1}	3.70×10^{-1}	3.64×10^{-1}	3.64×10^{-1}
10^{19}	9.98×10^{-1}	9.99×10^{-1}	8.64×10^{-1}	8.61×10^{-1}	8.59×10^{-1}	8.59×10^{-1}
10^{20}	1.00	1.00	9.85×10^{-1}	9.84×10^{-1}	9.84×10^{-1}	9.84×10^{-1}
			$kT_e=20$ eV			
10^{11}	3.32×10^{-6}	3.32×10^{-6}	1.59×10^{-8}	1.59×10^{-8}	1.12×10^{-11}	1.19×10^{-11}
10^{12}	3.32×10^{-5}	3.32×10^{-5}	1.59×10^{-7}	1.59×10^{-7}	1.22×10^{-10}	1.27×10^{-10}
10^{13}	3.32×10^{-4}	3.32×10^{-4}	1.59×10^{-6}	1.59×10^{-6}	2.05×10^{-9}	2.09×10^{-9}
10^{14}	3.31×10^{-3}	3.31×10^{-3}	1.59×10^{-5}	1.59×10^{-5}	1.01×10^{-7}	1.02×10^{-7}
10^{15}	3.21×10^{-2}	3.22×10^{-2}	1.59×10^{-4}	1.59×10^{-4}	8.73×10^{-6}	8.85×10^{-6}
10^{16}	2.49×10^{-1}	2.54×10^{-1}	1.55×10^{-3}	1.56×10^{-3}	6.72×10^{-4}	6.73×10^{-4}
10^{17}	7.68×10^{-1}	8.09×10^{-1}	1.89×10^{-2}	1.96×10^{-2}	1.98×10^{-2}	1.98×10^{-2}
10^{18}	9.71×10^{-1}	1.05	2.24×10^{-1}	2.16×10^{-1}	2.14×10^{-1}	2.14×10^{-1}
10^{19}	9.97×10^{-1}	1.07	7.59×10^{-1}	7.53×10^{-1}	7.51×10^{-1}	7.51×10^{-1}
10^{20}	1.00	1.07	9.69×10^{-1}	9.69×10^{-1}	9.68×10^{-1}	9.68×10^{-1}

Here n_S, n_P, and n_D are the principal quantum numbers for the terms S, P, and D, respectively. The summation here is only up to the levels with principal quantum number equal to $n=5$, as the influence of higher levels on the population of the level $2P$ is slight, and the calculations for higher levels become much more difficult.

The expressions for the population of the levels $3P$ and $3D$ are like Eq. (15), and we denote them by (15′) and (15″), respectively.

To solve (15) for N_k, one should write similar equations for N_{nS} and N_{nD}, thus getting a set of equations, the solution of which is very laborious. In this connection, the method of successive approximations was applied, assuming from the outset that the densities N_{nS}, N_{nD} (and for the level $3D$ also N_{nP}) are determined by Eq. (5). It appeared that with this assumption the populations calculated from Eq. (15), and from the similar equations (15′) and (15″) for the levels $3P$ and $3D$, are in a very good agreement with those calculated from Eqs. (12)–(14). This is illustrated in Table I, which was obtained with the aid of the GIER computer.

It follows from these considerations that, as far as the population of excited levels is concerned, the more complicated equations of the type of Eq. (15) can be replaced by the simpler Eqs. (12)–(14), resulting from Eq. (5). Note that the form of these equations is similar to that of the Boltzmann equation.

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