Atomic level population for nonideal plasmas in strong electric fields

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Starting from the rate equations that are derived from quantum kinetic equations, the level population of the different atomic states is calculated for a nonideal hydrogen plasma in strong electric fields. A change in the balance between excitation and deexcitation processes is produced by the non-Maxwellian form of the electron distribution function that accounts for field and density effects. The result is a considerably higher population of the excited atomic states for densities where both field and density effects are of importance.

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The developments in the field of laser-produced plasmas and capillary discharge x-ray lasers lead to a growing interest in the population kinetics of dense plasmas [1–5]. It is well known that the degree of ionization as well as the population of the different atomic levels in dense plasmas in thermodynamic equilibrium is determined by a nonideal Saha equation [6,7], which accounts for correlation effects such as screening, self-energy, and lowering of the ionization energy. This equation represents a mass action law, which results from the detailed balance relation of the reaction processes in the plasma.

But for nonequilibrium plasmas, found in static electric and magnetic fields or produced by a high-energy laser pulse, this theory is not always justified because of deviations of the momentum distribution function from its Maxwellian form. Physical observables such as, for instance, the opacity would be certainly affected by non-Maxwellian occupation numbers. In this paper we will consider a dense plasma in an electric field where the distribution function deviates from the Maxwellian form as the field strength increases. There follows a field-induced change of the balance between the excitation and deexcitation processes. The ionization equilibrium between the free and the bound particles will be modified. Such plasma conditions could be relevant for short times in dense Z pinches formed from frozen hydrogen fibers through which currents are driven [8]. These high-density Z pinches are of interest as a possible alternative approach to fusion.

In recent papers [9,10], the plasma composition in strong electric fields was considered for a hydrogen plasma. Introducing a Maxwell-like distribution function with a field-dependent electron temperature, the plasma composition was determined by a Saha-type but field-dependent mass action law.

Of course, such a treatment represents a first approximation only because the applied strong electric field produces a nonequilibrium plasma state. This requires that the plasma composition has to be determined in a consequent way from the system of rate equations instead of a modified Saha equation. Especially, there is no relation between excitation (ionization) and deexcitation (recombination) coefficients as it exists if a Maxwellian form of the electron distribution function is assumed. That means, all the rate coefficients have to be calculated in a direct way from their quantum statistical expressions.

The aim of this paper is to solve the problem in such a strict manner starting from the set of rate equations. Field and nonideality effects will be taken into account by the field and density dependence of the rate coefficients for the different excitation and reaction processes. These rate coefficients will be calculated quantum statistically from generalized kinetic equations considered here for a hydrogen plasma that consists of free electrons, protons, and hydrogen atoms. It will be shown to what extent the combination of nonideality and a strong electric field will change the ionization equilibrium. Especially, an interesting new behavior for the population of the excited atomic states will be found following from the competition of field and density effects.

As mentioned above, the composition and level population of a dense partially ionized plasma follows in general from the set of rate equations that reads for a hydrogen plasma [12]

$$\frac{d}{dt}n_H^j = \sum_{j'} \left(n_e n_H^{j'} K_{j'j} - n_e n_H^j K_{jj'} \right) + n_e^3 \beta_j - n_e n_H^j \alpha_j . \tag{1}$$

Here n_e and n_H^j are the number densities of electrons and atoms where j denotes the set of quantum number of the atomic states. The total electron density is

$$n_e^{\mathrm{tot}} = n_e + \sum_j n_H^j .$$

The K_{ij}, α_j, and β_j are the coefficients of excitation (deexcitation), impact ionization, and three-body recombination, respectively. They have to be considered as in-medium reaction rates because dense plasma effects influence essentially the scattering processes. Therefore, to model the population kinetics, a foundation of rate equations is required starting from quantum kinetic equations valid for dense many-particle systems with bound states. This problem was considered in a series of papers [11–15]. The final result is that the rate coefficients are given in terms of bound-bound and bound-free transition T matrices averaged by the corresponding set of distribution functions of free and bound particles. For a nondegenerate plasma in a constant electric field, the coefficients of ionization can be written as

$$\alpha_j = \frac{8\pi m_e}{(2\pi\hbar)^3}\int_{I_j^{\rm eff}}^{\infty} d\varepsilon\varepsilon \int_0^{\bar{p}_{\rm max}} d\bar{p}\, d\sigma_j^{\rm ion}(\varepsilon,\bar{p}) f_e^0(\varepsilon,E), \quad (2)$$

and the three-body recombination coefficient is

$$\beta_j = \frac{8\pi m_e}{(2\pi\hbar)^3}\int_0^{\infty} d\varepsilon\varepsilon \int_0^{\bar{p}_{\rm max}} d\bar{p}\, d\sigma_j^{\rm ion}(\varepsilon,\bar{p}) \times f_e^0(\varepsilon,E) f_e^0\left(\frac{\bar{p}^2}{2m_e},E\right). \quad (3)$$

Here, the adiabatic approximation ($m_e/m_p \ll 1$) was applied. Thus only the field-dependent electron distribution function occurs in the formulas. The $d\sigma_j^{\rm ion}$ is the in-medium differential cross section of ionization, which depends on the impact energy of the incident electron and the energy of the ejected electron. $I_j^{\rm eff}$ is the effective ionization energy and E denotes the electric field stength. Similar expressions follow for the coefficients of excitation and deexcitation.

In order to determine the rate coefficients, one has to solve two problems: (i) The cross sections must be calculated from the transition T matrices. (ii) The field-dependent electron distribution function has to be determined from the kinetic equation.

Let us consider first the calculation of the cross sections. In a generalized Born approximation, the total ionization cross section is given by ($\varepsilon = \frac{p_e^2}{2m_e}$)

$$\sigma_j^{\rm ion}(\varepsilon) = \int_0^{\bar{p}_{\rm max}} d\bar{p}\, d\sigma_j^{\rm ion}(\varepsilon,\bar{p}) = \frac{8\pi\hbar^2}{p_e^2 a_B^2}\int_0^{\bar{p}_{\rm max}} d\bar{p}\bar{p}^2 d\Omega_{\bar{p}} \int_{q_{\rm min}}^{q_{\rm max}} q dq \times \left|V_{ee}^{\rm eff}(q) P_{j\bar{p}}(q)\right|^2, \quad (4)$$

where the limits of integration are determined by energy conservation in the in-medium ionization process. In (4) $P_{j\bar{\mathbf{p}}}$ denotes the atomic form factor

$$P_{j\mathbf{p}}(\mathbf{q}) = \int d^3\bar{r}\Psi_j^*(\mathbf{r})\Psi_{\mathbf{p}}^+(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}}. \quad (5)$$

At this point, it is worth noting that in a nonideal plasma the two-particle properties, i.e., the wave functions and the energies, are essentially influenced by the surrounding plasma. Therefore, these quantities have to be determined from an effective wave equation that is given by [16]

$$\left(\frac{p_e^2}{2m_e} + \frac{p_p^2}{2m_p} + \Delta_{ep}^{\rm eff}(\mathbf{p}_e\mathbf{p}_p z) - z\right)\Psi_{ep}(\mathbf{p}_e\mathbf{p}_p z) + \left[1 - f_e(p_e) - f_p(p_p)\right]\int d^3q\, V_{ep}^{\rm eff}(\mathbf{p}_e\mathbf{p}_p\mathbf{q}z)\Psi_{ep}(\mathbf{p}_e+\mathbf{q},\mathbf{p}_p-\mathbf{q},z) = 0. \quad (6)$$

In comparison to a Schrödinger equation of an isolated pair of particles, there are self-energy corrections $\Delta_{ep}^{\rm eff}$ to the kinetic energy and an effective potential $V_{ab}^{\rm eff}$. Both include many-body effects and therefore they are complicated functions of dynamical screening.

In this paper, the static approximation for the screening will be used and momentum-independent quasiparticle shifts are assumed (rigid shift approximation [17]). Therefore effective potential and quasiparticle shifts are given by

$$V_{ep}^{\rm eff}(q) = \frac{4\pi e^2}{q^2+\kappa^2}; \quad \kappa^2 = \sum_a \frac{4\pi e^2 n_a}{k_B T}, \quad (7)$$

and

$$\Delta_{ep}^{\rm eff} = \Delta_e + \Delta_p; \quad \Delta_a = \frac{\int d^3p {\rm Re}\Sigma_a^R \frac{\partial}{\partial\mu^{id}} f_a}{\int d^3p \frac{\partial}{\partial\mu^{id}} f_a}, \quad (8)$$

with ${\rm Re}\Sigma_a^R$ denoting the real part of the retarded self-energy [16]. In lowest order, the quasiparticle shift is $\Delta_a = -\frac{1}{2}\kappa e_a^2$. Then the effective ionization energy is

$$I_j^{\rm eff} = |E_j| - \Delta_j + \Delta_e + \Delta_p, \quad (9)$$

where E_j is the binding energy in the atomic state $|j\rangle$ and Δ_j is the corresponding self-energy shift following from the effective wave equation (6). According to (4) and (5), the determination of the cross section requires the knowledge of the wave functions. After partial wave expansion, the atomic form factor can be calculated numerically from the radial Schrödinger equation with the effective potential and the self-energy corrections given by (7) and (8). In Fig. 1, results are shown for the ionization cross section of the $2p$ atomic state as a function of the electron impact energy for different screening parameters. Due to the influence of the dense plasma medium, the behavior of the cross section is determined by the

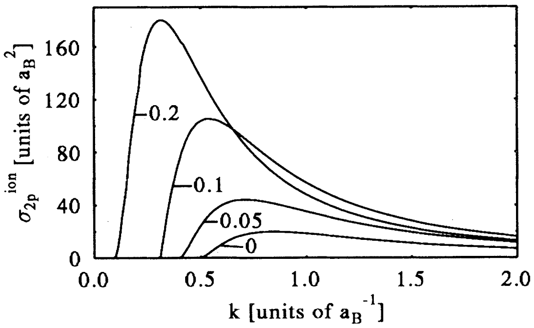

FIG. 1. Total cross section of impact ionization from the $2p$ atomic level as a function of the electron wave number for different screening parameters κa_B.

effective scattering potential, the screened atomic form factor, and the effective density and temperature dependent threshold energy. All these effects modify the cross section in comparison to the low-density case ($\kappa = 0$) where many-body effects are negligible. Especially, the ionization threshold (9) moves down to zero energy with growing plasma density. A similar behavior can be found for the ionization cross sections of other atomic states and for the different excitation cross sections [14,15].

The second problem in order to calculate rate coefficients is the determination of the electron distribution function in the nonideal partially ionized plasma under the influence of a strong electric field. The anisotropy shall be accounted for in a first approximation, i.e.,

$$f_e(\mathbf{p}) = f_e^0(p) + f_e^1(p)\cos\vartheta, \qquad (10)$$

where f_e^0 is the isotropic part, which already includes an explicit field dependence. In the anisotropy correction term, ϑ is the angle between field direction and electron momentum. Adopting this so-called diffusion approximation, the following well-known system of equations for f_e^0 and f_e^1 can be derived from the basic kinetic equation given in [9,10]. It reads in the stationary case

$$\frac{1}{p^2}\frac{\partial}{\partial p}\left\{p^2\left(\frac{eE}{3}f_e^1 - \frac{m_e}{m_H}\frac{1}{\tau_e}\left[pf_e^0 + mkT\frac{\partial}{\partial p}f_e^0\right]\right)\right\} = 0,$$
$$eE\frac{\partial}{\partial p}f_0^0 = -\frac{1}{\tau_p}f_e^1. \qquad (11)$$

The influence of collisions is accounted for in the energy and momentum relaxation times τ_e and τ_p, respectively. They are determined by the collision integrals and can be written in terms of the collision frequencies of the different elastic and inelastic scattering processes

$$\tau_e^{-1} = \left(\nu_a + \nu_p + \nu_{a0} + \frac{m_H}{m_a}\nu_e\right),$$
$$\tau_p^{-1} = (\nu_a + \nu_p + \nu_{a1}). \qquad (12)$$

Here, ν_e describes the electron-electron scattering, ν_p the electron-proton scattering, ν_a the elastic scattering on the atom, and ν_{a0}, ν_{a1} the excitation processes [18]. In the case of electron-electron and electron-proton scattering, the collision frequencies were calculated by numerical solution of the radial Schrödinger equation with the effective potential given by (7). The elastic scattering of electrons on hydrogen atoms was treated by applying the method of close coupling equations in the adiabatic exchange model [19,20]. Here, the effective electron-atom interaction includes a static part and a screened polarization potential. In order to account for the excitation processes in the electron distribution function, a fit formula for the total cross section was used [21].

Because the collision frequencies are dependent on the densities, the distribution function is strongly influenced by the plasma composition. With Eqs. (1) and (11), a self-consistent system of equations for the determination of the plasma composition and the electron distribution function is to be solved. Results for the isotropic part of the distribution function are shown in Fig. 2. The curves in Fig. 2(a) demonstrate the behavior in dependence of the plasma density for a fixed field strength. One observes a very different behavior at low and high densities. In the low-density case, the electrons are strongly accelerated by the electric field, and a high-energy tail of the distribution function is formed (non-Maxwellian tail). The situation is different at high densities where the collision frequencies are higher. The electrons lose the energy

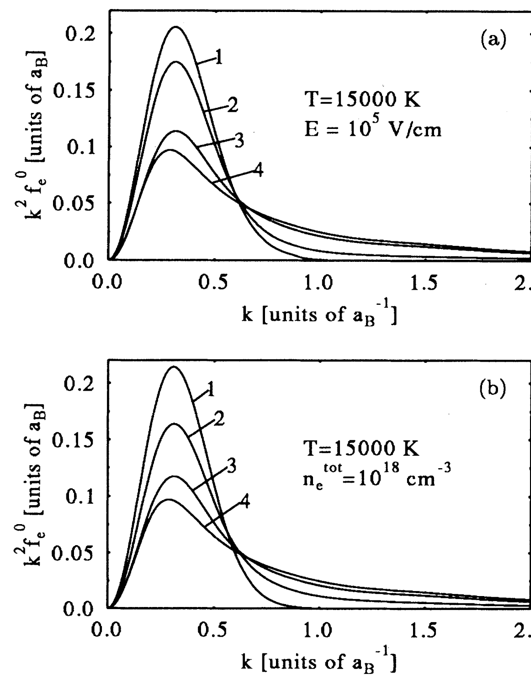

FIG. 2. Field-dependent electron distribution function f_e^0 vs momentum. (a) For a given field strength $E = 10^5$ V/cm and different electron densities $n_e^{\rm tot}$ (1: 10^{18} cm^{-3}, 2: $10^{18.5}$ cm^{-3}, 3: 10^{19} cm^{-3}, 4 : 10^{20} cm^{-3}). (b) For a given electron density $n_e^{\rm tot} = 10^{18}$ cm^{-3} and different field strengths E (1: 0 V/cm, 2: $E = 2\times10^4$ V/cm, 3: 4×10^4 V/cm, 4: 10^5 V/cm).

they gained from the electric field more efficiently and the distribution function tends to the Maxwellian form. The dependence of the distribution function on the electric field strength for a fixed density is shown in Fig. 2(b). As expected, the deformations of the Maxwellian form increase with increasing field strength.

Now the influence of field and density effects on the rate coefficients shall be considered. In Fig. 3, coefficients of impact ionization and three-body recombination of the $2p$ atomic state and the $1s - 2p$ excitation coefficient are shown as a function of the free electron density for different fields. Two density regions can be observed with a different behavior of the rate coefficients. At lower densities, there are strong field effects. The non-Maxwellian tail of the electron distribution function gives rise to considerably higher ionization rates. On the other hand, the recombination rates are lowered more than two orders of magnitude in comparison to the zero-field case. At high densities, the influence of the field becomes smaller. But now, the rate coefficients' behavior is dominated by many-body effects, especially by the lowering of the ionization energy and the Mott effect, i.e., the pressure ionization of atomic states in the dense nonideal plasma. The main result is the strong increase of the impact ionization coefficients with growing density. The density dependence of the excitation, deexcitation, and recombination rates at high densities is smaller because it is determined not directly by the lowering of the ionization threshold but only by the effective potential and the screened atomic form factor in the in-medium cross section.

With the knowledge of the rate coefficients, it is possible to determine the field-dependent level population of the atomic states in a nonideal hydrogen plasma. This was done solving the stationary system of rate equations in a self-consistent manner with the determination of the electron distribution function given by (11). The numerical results for the degree of ionization $c_e = n_e/n_e^{\rm tot}$ for different electric fields are shown in Fig. 4(a). Both the field and medium effects produce changes in the degree of ionization. An enhancement of c_e at low densities can be observed, which follows from the higher ionization

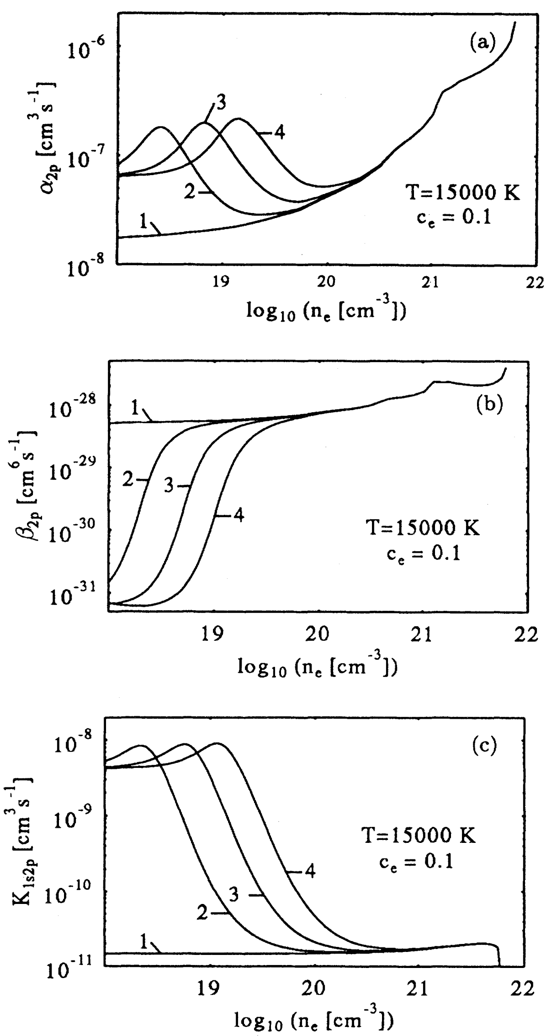

FIG. 3. Different rate coefficients as a function of the free electron density for different field strengths E (1: 0 V/cm , 2: 2×10^4 V/cm, 3: 4×10^4 V/cm, 4: 10^5 V/cm). The degree of ionization is $c_e = n_e/n_e^{\rm tot} = 0.1$. (a) Impact ionization coefficient for the $2p$ atomic state. (b) Three-body recombination coefficient for the $2p$ atomic state. (c) Excitation coefficient for the $1s$-$2p$ transition of hydrogen.

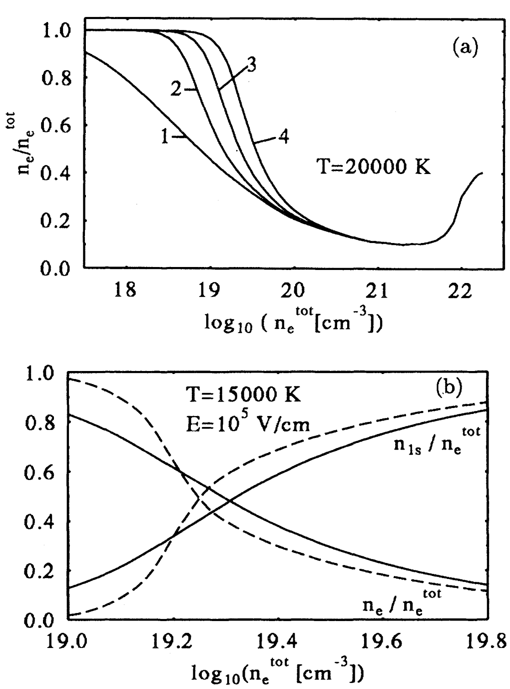

FIG. 4. Degree of ionization for a nonideal hydrogen plasma as a function of the total electron density. (a) For different field strengths (same as in Fig. 3). (b) Comparison of the present calculations with the effective temperature model of [9] (dashed lines).

rates due to the electric field. The effect of the field can be neglected at higher densities. But now the influence of many-body effects on the ionization threshold begins to dominate the plasma composition. Again, there is an increase of the degree of ionization. Here, the Mott transition is indicated by a strong increase of the ionization degree. In Fig. 4(b), a comparison of the degree of ionization is given with results obtained in an earlier paper [9] where a Maxwellian distribution function with an effective field-dependent electron temperature was assumed. In the present calculations, considerably lower values of c_e follow at lower densities compared with the effective temperature approach. That means, the effective Maxwellian-like momentum distribution overestimates the ionization rates. With increasing density, the situation changes, and the degree of ionization obtained here is higher up to densities where field effects can be neglected.

Finally, the results obtained for the field-dependent population of atomic states in the nonideal hydrogen plasma shall be discussed. In Fig. 5(a), the level population is shown for the states with the principal quantum numbers n=1, n=2, and n=3. The full lines are the results for a field strength $E = 10^5$ V cm^{-1} and, for comparison, the dashed lines give the zero-field case. An interesting feature is the enhanced population of the excited atomic levels when the electric field is applied.

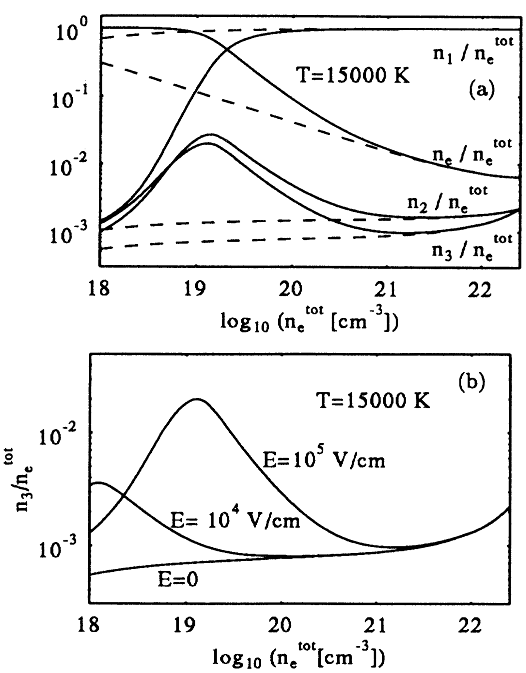

FIG. 5. Population of the different atomic levels for a nonideal hydrogen plasma vs the total electron density. (a) For a field strength $E = 10^5$ V/cm (full lines). A comparison is given with the zero-field case (dashed lines). (b) Total population of the atomic hydrogen levels with the principal quantum number n=3 (3s+3p+3d) for different field strengths.

Especially, well developed maxima of the number fractions are formed in a density region around $n_e = 10^{19}$ cm^{-3}, which tend to be ten times higher than that in the field free case. This behavior is determined by the non-Maxwellian electron distribution function and results from a competition between field and density effects in the plasma. In order to demonstrate the effect of the field, the total population of states with n=3 is shown in Fig. 5(b) for different field strengths. With increasing field, the maximum increases and moves to higher electron densities. At very high densities, the field effects disappear and the nonideality of the plasma governs the population dynamics leading to the Mott effect discussed above.

In order to study the field and density effects on the population dynamics in more detail, the effective population flows between the different levels are shown in Fig. 6. Effective population flow means the net flow of the populating and depopulating processes (deexcitation, excitation and recombination, ionization, respectively) for a certain transition. The nonvanishing effective population flows, presented in Fig. 6, correspond to a field-induced deviation from the detailed balance valid in thermodynamic equilibrium. Negative values describe a change to higher deexcitation rates, positive values to higher excitation rates for the considered transition process. The stationary level population is realized by a vanishing sum of the different flows that determine the population and depopulation rates of the level. At low densities, where the occupation numbers of the atomic states are small, the effective population flows are, of course, also small. At higher densities (around 10^{19} cm^{-3}), a maximum behavior can be observed that describes a strong deviation from the detailed balance caused by the non-Maxwellian electron distribution function. The comparison with the results given in Fig. 5 shows that this behavior is related

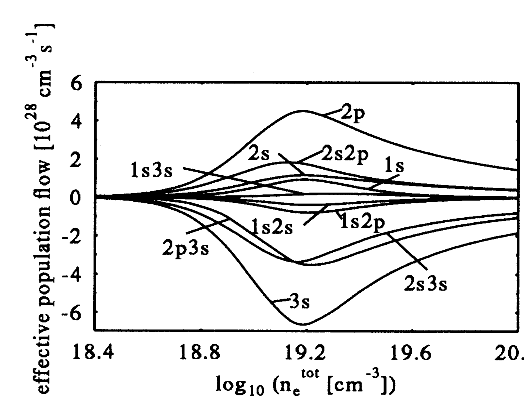

FIG. 6. Effective population flows between the different atomic levels (denoted by the two quantum numbers) and between atomic levels and the continuum (one quantum number), respectively, vs total electron density for a field strength $E = 10^5$ V/cm. Negative values describe a higher deexcitation rate, positive values higher excitation rates for the considered transition process.

to the increased level population of the excited atomic states in that density region. At higher densities, the effective population flows tend to zero because the influence of the electric field becomes negligibly small, and the electron distribution function becomes Maxwellian. The population dynamics is determined then by the detailed balance of the different in- and out-scattering rates and the composition of the dense plasma is given now by the nonideal Saha equation.

As a possible experimental situation with parameters we used, we could think, as already mentioned in the introductory remarks, of a high-density Z pinch in its initial phase. In order to see spectroscopically the influence of the field and nonideality effects on the population in different atomic levels, the occupation of the ground state should be measured absolutely by absorption of Lyman-α, whereas the occupation of the excited levels should be determined from emission measurements.

We can conclude that for certain ratios of field strength and density the population of atomic states in the dense plasma deviates significantly from that of thermodynamic equilibrium. The reason is that even the isotropic part of the electron distribution function becomes non-Maxwellian and, therefore, there is no detailed balance for the different processes. In the stationary case, the composition of the dense plasma has to be determined from the rate equations now instead of the Saha equation. It is important to take into account both nonideality and field effects. An interesting feature is the enhanced population of the excited atomic levels.

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