Impact ionization in nonideal plasmas in a strong electric field

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The influence of an applied electric field on the impact ionization and on the mass-action law of a nonideal hydrogen plasma is discussed. The coupling of field and many-body effects leads to a minimum behavior of the impact-ionization coefficient as a function of the plasma density.

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The effects of an electric field on the atomic processes in plasmas and solids are of current interest for different fields of research [1–4]. Especially, progress in dense-plasma physics requires the study of the influence of strong electric fields on nonideal plasmas [5]. The behavior of a nonideal dense plasma is determined by the degeneracy if we have

$$n\Lambda^3 \geq 1, \qquad \Lambda = \sqrt{2\pi\hbar^2/mk_BT}$$

and by the strong Coulomb correlation if

$$nl^3 > 1, \qquad r_s > 1 \ .$$

Here $l = e^2/(k_BT)$ is the Landau length and $r_s = d/a_0$ is the Brueckner parameter with the mean particle distance d and the Bohr radius a_0. Under these conditions many-particle effects may be expected such as screening, self-energy, and the lowering of the ionization energy. All these effects influence essentially the ionization and recombination processes in a partially ionized plasma. Therefore, a strong modification of the reaction rates at higher plasma densities may be expected [6].

Furthermore, the ionization kinetics in plasmas is connected with the application of a strong electric field in many cases. The latter modifies the ionization rates at lower densities because the mean-free-path length is large and the external electric field accelerates the electrons to energies which are sufficient for impact ionization.

In this paper we will study the impact ionization in plasmas which results from a coupling of nonideality and an applied strong electric field. Thereby we assume that the field strengths are sufficiently high enough for impact ionization but not so strong that field emission takes place. As a test plasma we consider a nonideal hydrogen plasma.

The equations of ionization kinetics may be obtained from generalized Boltzmann equations for reactive systems in external fields in which many particle effects, such as mentioned above, are taken into account [7–10]. Following these papers we obtain for the electron number density n_e

$$\frac{\partial n_e}{\partial t} = \sum_{a=e,p}\sum_j (\alpha_a^j n_a n_j - \beta_a^j n_a n_e n_p) \ . \tag{1}$$

Here n_p and n_j are the number densities of the protons and of the hydrogen atoms in the state $|j\rangle$, respectively. If degeneracy effects are neglected one gets the following statistical expressions for the rate coefficients of ionization and recombination

$$\alpha_a^j = \frac{1}{\hbar V}\int \frac{d^3p_a}{(2\pi\hbar)^3}\frac{d^3p_e}{(2\pi\hbar)^3}\frac{d^3p_p}{(2\pi\hbar)^3}\frac{d^3\bar{P}}{(2\pi\hbar)^3}\frac{d^3\bar{p}_a}{(2\pi\hbar)^3} 2\pi\delta\left(E_a + E_e + E_p - \bar{E}_{Pj} - \bar{E}_a\right) |\langle p_a p_e p_p|T^{02}|j\bar{P}\bar{p}_a\rangle|^2 \frac{f_a}{n_a}\frac{F_j}{n_j}, \tag{2}$$

$$\beta_a^j = \frac{1}{\hbar V}\int \frac{d^3p_a}{(2\pi\hbar)^3}\frac{d^3p_e}{(2\pi\hbar)^3}\frac{d^3p_p}{(2\pi\hbar)^3}\frac{d^3\bar{P}}{(2\pi\hbar)^3}\frac{d^3\bar{p}_a}{(2\pi\hbar)^3} 2\pi\delta\left(E_a + E_e + E_p - \bar{E}_{Pj} - \bar{E}_a\right) |\langle p_a p_e p_p|T^{02}|j\bar{P}\bar{p}_a\rangle|^2 \frac{\bar{f}_a}{n_a}\frac{\bar{f}_e}{n_e}\frac{\bar{f}_p}{n_p} \ . \tag{3}$$

Here T^{02} is the three-particle scattering operator for impact ionization and three-body recombination processes. The energies of the free electrons and protons are quasiparticle energies given by the well-known dispersion relation

$$E_a(p,t) = \frac{p^2}{2m_a} + \mathrm{Re}\Sigma_a^R(p,\omega,t)|_{\hbar\omega=E_a(p,t)} \ . \tag{4}$$

$\Sigma_a^R(p,\omega,t)$ is the quantum-statistical retarded self-energy function. In order to simplify the problem we use the approximation of thermal-averaged shifts [11]

$$E_a(p,t) = \frac{p^2}{2m_a} + \Delta_a(t) \ ,$$

where Δ_a has to be determined from

$$\Delta_a(r,t) = \frac{\int d^3p \, \mathrm{Re}\Sigma_a^R(p,r,t) \frac{\partial}{\partial \mu_a^{\mathrm{id}}} f_a(p,r,t)}{\int d^3p \frac{\partial}{\partial \mu_a^{\mathrm{id}}} f_a(p,r,t)} . \quad (5)$$

It can be shown that the thermal-averaged shift is related to the chemical potential by

$$\mu_a = \mu_a^{\mathrm{id}} + \Delta_a . \quad (6)$$

In the following we use for the self-energy the random-phase approximation (RPA). Further, in nonideal plasmas the two-particle energies and the wave functions $\Psi_{P\nu}$ for bound states ($\nu = j$) and for scattering states ($\nu = p$) are given by an effective wave equation [12, 18]

$$\left(\frac{p_e^2}{m_e} + \frac{p_p^2}{m_p} + \Delta_{ep}^{\mathrm{eff}}(p_e p_p z) - z\right) \Psi_{P\nu}(p_e, p_p, z) - [1 - f_e(p_e) - f_e(p_e)] \int V_{ep}^{\mathrm{eff}}(p_e p_p q z) \Psi_{P\nu}(p_e + q, p_p - q, z) d^3q = 0. \quad (7)$$

The explicit expressions of these quantities can be found in [18]. If the nondegenerate case is considered, the dynamically screened effective potential is given by

$$V_{ab}^{\mathrm{eff}}(p_a p_b q z) = V_{ab}(q) \left[1 + \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \mathrm{Im}\epsilon^{-1}(q, \omega + i0) \times \left(\frac{n_B(\omega) + 1}{z - \omega - \varepsilon_a(p_a) - \varepsilon_b(p_b - q)} + \frac{n_B(\omega) + 1}{z - \omega - \varepsilon_a(p_a + q) - \varepsilon_b(p_b)} \right)\right] . \quad (8)$$

The dynamical self-energy and the effective potential are connected by

$$\Delta_{ab}^{\mathrm{eff}}(p_a p_b z) = \int \frac{d^3q}{(2\pi\hbar)^3} [V_{ab}^{\mathrm{eff}}(p_a p_b q z) - V_{ab}(q)] . \quad (9)$$

The dynamical screening can be evaluated [18] and yields an effect of around 8% to transport properties. The kinetic features considered in this paper are of greater value as can be seen below, so that we can neglect the influence of dynamics in (9). In the static limit the effective potential simplifies to

$$V_{ab}^{\mathrm{eff}}(p_a p_b q, 0) = \frac{V_{ab}(q)}{\epsilon(q,0)} , \quad \epsilon(q,0) = \left(\frac{q^2}{q^2 + \kappa^2}\right)^{-1} ,$$

where V_{ab} is the Coulombic potential and ϵ the static dielectric function. From the effective wave equation the quasiparticle energies of the electron-proton pairs can be calculated. We have for the scattering states

$$E_{Pp} = \frac{P^2}{2m_{\mathrm{H}}} + \frac{p^2}{2m_e} + \Delta_e + \Delta_p$$

and for the bound states

$$E_{Pj} = \frac{P^2}{2m_{\mathrm{H}}} + E_j^0 + \Delta_j .$$

Here E_j^0 is the binding energy of an isolated hydrogen atom and Δ_j is the atomic energy shift due to the surrounding plasma. Therefore we obtain the following expression for the lowering of the ionization energy:

$$\Delta I_j = \Delta_e + \Delta_p - \Delta_j .$$

Let us come back to the ionization coefficient α_a^j. Because of the large mass difference between electrons and ions the adiabatic approximation can be applied. Further, we use a modified first Born approximation [13]

$$\langle p_a p_e p_p | T^{02} | j \bar{P} \bar{p}_a \rangle = \langle p_a | \langle + p_e p_p \, | V_{ee}^{\mathrm{eff}} | \, j \bar{P} \rangle | \bar{p}_a \rangle$$

where $|p_e p_p +\rangle | Pj\rangle$ are scattering and bound-state solutions of the effective wave equation.

It follows for the ionization coefficient of electron impact:

$$\alpha_e^j = \frac{8\pi m_e}{(2\pi\hbar)^3 n_e} \int_{|E_j| + \Delta I}^{\infty} d\varepsilon \, f(\varepsilon, E) \varepsilon \sigma_j^{\mathrm{ion}}(\varepsilon, E) . \quad (10)$$

In the following E denotes the electric field. Further on we have introduced the ionization cross section by

$$\sigma_j^{\mathrm{ion}} = \frac{8\pi\hbar^2}{p_e^2 a_0^2} \int_0^{\bar{p}_{\max}} d\bar{p} \, \bar{p}^2 d\Omega_{\bar{p}} \int_{q_{\min}}^{q_{\max}} q \, dq \left| V_{ee}^{\mathrm{eff}}(q) P_{j\mathbf{p}}(q) \right|^2 . \quad (11)$$

Here $\hbar\mathbf{q} = \mathbf{p}_e - \bar{\mathbf{p}}_e$ denotes the momentum transfer of the projectile and

$$\bar{p}_{\max} = \left(p_e^2 - 2m_e I^{\mathrm{eff}}\right)^{1/2} ,$$
$$\bar{p}_e = \left(p_e^2 - 2m_e I^{\mathrm{eff}} - \bar{p}^2\right)^{1/2} ,$$
$$\hbar q_{\min} = p_e - \bar{p}_e ,$$
$$\hbar q_{\max} = p_e + \bar{p}_e$$

follow from energy conservation where the effective ionization energy is given by $I_j^{\mathrm{eff}} = |E_j| + \Delta I_j$.

With $P_{j\bar{p}}$ we denote the atomic form factor

$$P_{j\mathbf{p}}(q) = \int d^3r \, \Psi_j^*(\mathbf{r}) \Psi_{\mathbf{p}}^+(\mathbf{r}) e^{\frac{i}{\hbar}\mathbf{q}\cdot\mathbf{r}} . \quad (12)$$

For the determination of α_e^j we have to solve two problems: (i) the calculation of σ_j^{ion} on the basis of the effective Schrödinger equation and (ii) the determination of the electron distribution function f_e in a strong electric field.

Let us consider the first problem. The simplest approximation for $\sigma_j^{\rm ion}$ follows if we restrict ourselves to ground-state ionization. Using the effective wave equation (7) the wave functions $\Psi_j^*(\mathbf{r})$ $\Psi_{\mathbf{p}}^+(\mathbf{r})$ and with (11) the ionization cross section can be calculated [13]. The result for the ionization cross section as a function of the electron-impact energy for different screening parameters is shown in Fig. 1. One can see that the threshold energy moves down to zero with increasing screening as well as the maximum of ionization-coefficient increases.

Using the Coulomb potential for $V_{ee}^{\rm eff}$ and Coulombic wave functions but taking into account quasiparticle energies, the following modified Bethe formula is a good approximation [6]:

$$\sigma_1^{\rm ion} = 2.5\pi a_0^2 \frac{|E_1|}{\varepsilon} \ln \frac{\varepsilon - \Delta_e - \Delta_p + \Delta_1}{|E_1|} \tag{13}$$

with $\varepsilon = p_e^2/2m_e$.

Next we look at the distribution function in an external field. The determination of f_e in a strong electric field starting from a kinetic equation is a well-known problem. To account for anisotropy in a first approximation we write

$$f_e = f_e^0 + f_e^1 \cos\vartheta \ , \tag{14}$$

where f_e^0 is the isotropic part which includes the field dependence explicitly. If we insert (14) in the electron kinetic equation assuming the diffusion approximation and the stationary case we arrive at

$$\frac{1}{p^2}\frac{\partial}{\partial p}\left\{p^2\left(\frac{eE}{3}f_e^1 - \frac{m_e}{m_{\rm H}}\frac{1}{\tau_e}\left[pf_e^0 + mkT\frac{\partial}{\partial p}f_e^0\right]\right)\right\} = 0, \tag{15}$$

$$eE\frac{\partial}{\partial p}f_e^0 + \frac{1}{\tau_p}f_e^1 = 0 \ . \tag{16}$$

Here the contributions of collisions are included in the energy- and momentum-relaxation time [14, 15]

$$\tau_e^{-1} = \left(\nu_a + \nu_p + \nu_{ao} + \frac{m_{\rm H}}{m_e}\nu_e\right),$$

$$\tau_p^{-1} = (\nu_a + \nu_p + \nu_{a1}),$$

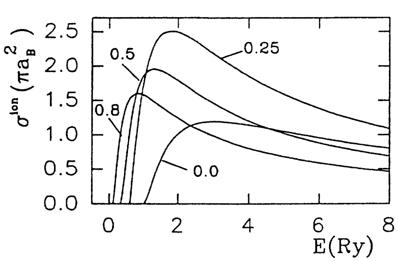

FIG. 1. Total ionization cross section $\sigma_1^{\rm ion}$ for electron impact vs impact energy for different screening parameters κa_o.

where the collision frequencies ν are connected with the quantum-mechanical cross section σ by

$$\nu_a = \frac{p}{m_a} n_a \sigma_a^T \ .$$

We want to solve Eqs. (15) and (16) under the usual boundary condition. The result is the well-known Dawydow expression

$$f_e^0 = C \exp\left(-\int_0^\varepsilon \frac{d\varepsilon}{kT + \frac{m_{\rm H} e^2 E^2 \tau_p \tau_e}{3m_e^2}}\right) \ . \tag{17}$$

In order to determine f_e^0 from (17) the cross sections must be known. In the case of electron-proton collisions the scattering phase shifts were calculated by a numerical solution of Schrödinger's equation assuming the statically screened Debye potential. The elastic scattering of electrons on hydrogen atoms in the ground state was treated using the adiabatic-exchange model taking into account a screened polarization potential [16]. For the excited processes we have used a semiempirical formula given by Drawin [17].

Now let us return to the ionization and recombination processes. First we consider the stationary solution of the rate equation (1). In this case we have for atoms in the ground state

$$\frac{n_H}{n_e n_p} = \frac{\beta_e^1}{\alpha_e^1} \ . \tag{18}$$

This is a mass-action law which determines the plasma composition. But, if a significant number of electrons exceeds the threshold energy due to the strong field and due to the lowering of ionization energy, this equation is no longer the thermodynamic mass-action law. We have a nonequilibrium Saha equation caused by the strong electrical field. Therefore the rate coefficients have to be determined by the distribution function (17), which depends on the plasma composition itself. We solved this problem by an iteration procedure introducing an effective temperature at each step which enters the self-energy shifts,

$$T(E) = \frac{2}{3k}\langle E_{\rm kin}(E)\rangle \ .$$

This effective temperature is just defined in order to reproduce the field dependence of the mean kinetic energy and the particle flux determined by the distribution function (17). With the help of this effective electron temperature we can calculate all many-particle shifts by a displaced Maxwellian distribution. This procedure ensures the main features of the distribution function (17) as well as the self-consistent solution to the plasma composition and does not change the result compared with using the Dawydow expression itself. The results for the distribution function which follows from (17) together with the ionization cross section can be seen in Fig. 2. In the low-density regime we observe a fine splitting of the ionization cross section due to the applied electric

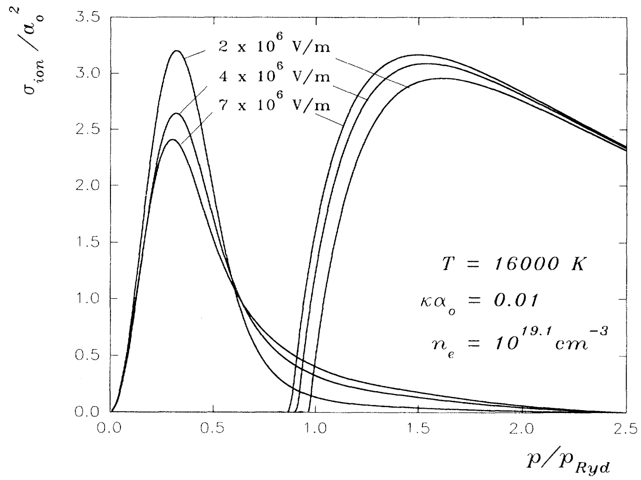

FIG. 2. The self-consistent distribution functions for different field strengths (arbitrary units) in comparison with the field-dependent ionization cross section vs momentum for a constant screening parameter of $0.01\kappa a_o$.

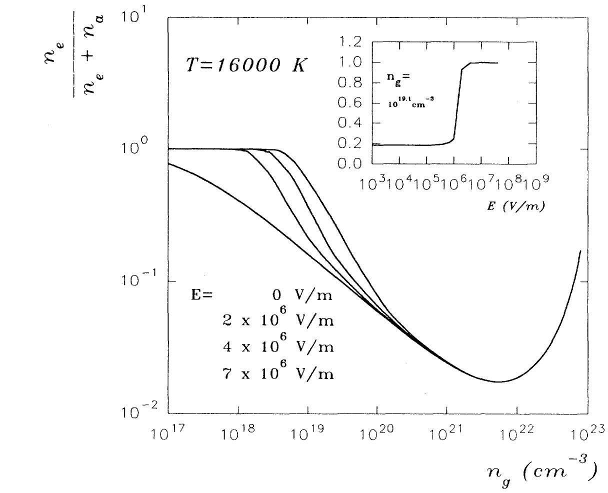

FIG. 4. The ionization degree vs total electron density for different applied electric fields and for one density selected over the field.

field. Further on the high energetic tail of the distribution function increases and both effects contribute to an enhancement of ionization processes. The situation is very different at high densities, as we can see in Fig. 3. Whereas at zero electric field and neglecting many-body effects ($\Delta I_1 = 0$) a very small fraction of electrons is sufficiently high energetic for impact ionization, the fraction of electrons capable for impact ionization is strongly increased by the lowering of threshold due to screening effects at higher densities (with a large ΔI_1). Here the electric fields of Fig. 2 have no remarkable influence.

In the same manner we have used (18) in order to determine the degree of ionization $\alpha = n_e/(n_e + n_{\rm H})$. The result is shown in Fig. 4. The sharp drop of the number of atoms at higher densities is due to the lowering of the ionization energy ΔI_1 , the so-called Mott transition. On the other hand, we observe deviations from the equilibrium mass-action law at lower densities. Here the drop in the number of atoms is the result of impact ionization by field-excited electrons, as it is to be seen in the figure. Finally let us consider the density dependence of the ionization coefficient which follows from (10) using the impact-ionization cross section (13) and the distribution function (17) in Fig. 5. Again two density regions can be observed with a different behavior of α_1. In the low-density case the electrons are strongly accelerated by the field and therefore we have higher ionization rates in

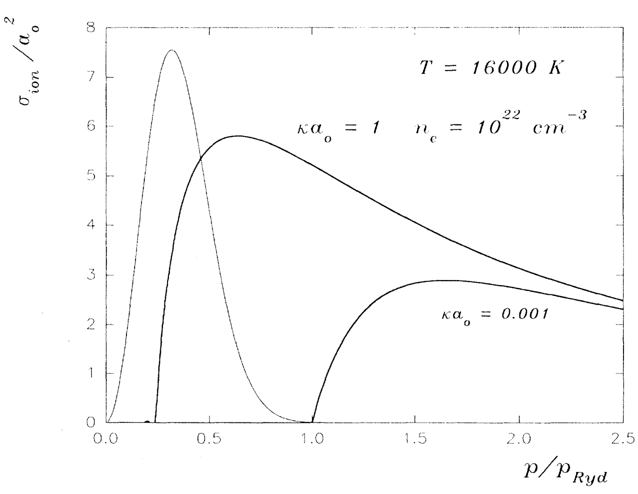

FIG. 3. The self-consistent distribution functions for same field strengths (arbitrary units) with the corresponding ionization cross section vs momentum for a constant screening parameter of $1\kappa a_o$ as well as for a vanishing screening of $0.001\kappa a_o$.

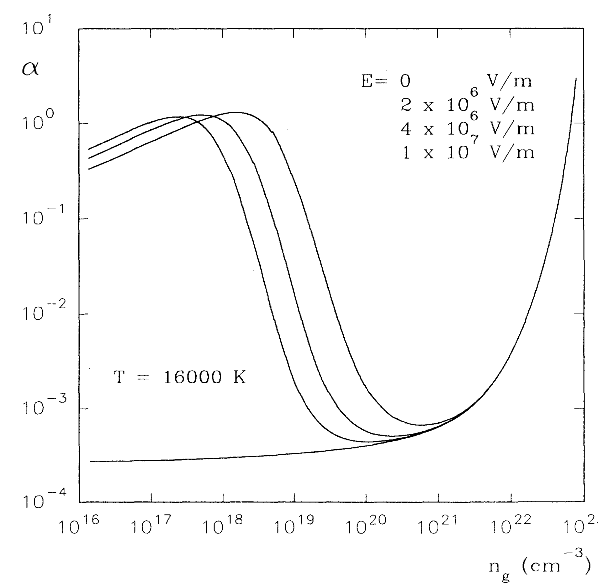

FIG. 5. Ionization coefficient vs total electron density for three different applied electric fields.

comparison to the zero-field case. At high densities the many-particle effects dominate which leads to an exponential increase of α. In dependence of the field strength a separation of these two effects is observed in the region of moderate densities. The result is a minimum behavior of the ionization coefficient. The minimum vanishes at strong fields because of the overlap of field and plasma medium effects. In a forthcoming paper we will present some details of the calculation and we will discuss the influence of strong fields on the recombination coefficient.

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