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Solution of the non-stationary electron Boltzmann-equation for a weakly ionized collision dominated plasma.

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1. The mathematical problem from the physical point of view

For the kinetic description of a non-isothermal, weakly ionized, collision dominated plasma the knowledge of the behaviour of the electron component is of great importance because via this component the energy from the action of an electric field is transfered to the different degrees of freedom of the neutral gas component. Starting point for such a description is the well known Boltzmann equation for the velocity distribution function of the electrons which presents their probability density in the velocity space. There are many physical viewpoints from which the determination of the behaviour of the electrons is significant particularly under non-stationary conditions. In this case the temporal development of the distribution function is determined by the time dependent Boltzmann equation including the action of a time variable electric field and that of several collision processes of electrons with neutral gas atoms as well as the generation of electrons via ionizing collisions and their loss for example by diffusion.
Appropriate analytical developments of such a Boltzmann equation lead to an equation for the isotropic part $f(U,\bar{t})$ of the distribution function of the electrons, which presents their probability density in the energy space, in the form /1/

$$\frac{1}{n_g}\left(\frac{m}{2e_o}\right)^{1/2} U^{1/2}\frac{\partial}{\partial \bar{t}} f(U,\bar{t}) - \frac{1}{3n_g^2}\left(\frac{E(\bar{t})}{p_o}\right)^2 \frac{\partial}{\partial U}\left[\frac{U}{Q_d(U)}\frac{\partial}{\partial U} f(U,\bar{t})\right]$$

$$- 2\frac{m}{M}\frac{\partial}{\partial U}\left[Q_d(U)\,U^2 f(U,\bar{t})\right]$$

$$+ U\,Q_e(U) f(U,\bar{t}) - (U+U_e)Q_e(U+U_e) f(U+U_e,\bar{t})$$

$$+ U\,Q_i(U) f(U,\bar{t}) - \frac{1}{\beta}\left(\frac{U}{\beta}+U_i\right)Q_i\left(\frac{U}{\beta}+U_i\right) f\left(\frac{U}{\beta}+U_i,\bar{t}\right)$$

$$- \frac{1}{1-\beta}\left(\frac{U}{1-\beta}+U_i\right)Q_i\left(\frac{U}{1-\beta}+U_i\right) f\left(\frac{U}{1-\beta}+U_i,\bar{t}\right) + \frac{1}{n_g}\left(\frac{m}{2e_o}\right)^{1/2}\frac{U^{1/2}}{p_o\tau} f(U,\bar{t}) = 0 . \qquad (1)$$

In the order of occurence the terms in (1) describe the temporal variation of the isotropic distribution function $f(U,\bar{t})$ as

determined by the electric field $E(\bar{t})$, elastic collisions, a lumped excitation process, ionizing collisions and finally by an additional electron loss term, which for example may represent the usual diffusion loss of electrons. U means the momentary electron energy measured in electron volts and $\bar{t} = p_o t$ the time normalized by the pressure p_o of the neutral gas.

Important quantities appearing in the coefficients of this equation are the collision cross sections $Q_d(U)$ for impulse transfer in elastic collisions, $Q_e(U)$ and $Q_i(U)$ for exciting and ionizing collisions which are still dependent on the special kind of neutral gas. U_e and U_i are the threshold energies for the last two inelastic processes mentioned. τ is the given constant life time of the electrons and β a quantity between o.5 and 1 characterizing the partition of the remaining kinetic energy between the two electrons appearing after each ionization process. However, all the other quantities m, M, e_o, n_g are atomic constants. The temporal development of all important macroscopic quantities of the electron component such as the electron concentration $n_e(\bar{t})$, the mean energy $\bar{U}(\bar{t})$ as well as the energy gain and the different energy losses are already determined by the isotropic distribution function via energy averaging over this function multiplied by appropriate weight functions.

2. The numerical method for the solution of the time dependent kinetic equation

Equation (1) is a linear parabolic partial differential equation with additional difference terms at the energies $U + U_e$, $U/\beta + U_i$ and $U/(1-\beta) + U_i$, which arise from the exciting and ionizing collision processes. We sought for the solution in the region $U \geq 0$ and $\bar{t} \geq 0$. To determine the unique solution we applied the appropriate boundary condition /1/, /2/.

$$\lim_{U \to 0} \frac{\partial f}{\partial U} = 0 \quad , \quad \lim_{U \to \infty} f = 0 \qquad (2a,b)$$

for all $\bar{t} \geq 0$ and start at $\bar{t} = 0$ with a suitable initial distribution $\tilde{f}(U)$. For convenient handling we confined the energy region applying the boundary condition (2a) to a quasi-zero point U_{qz} and (2b) to a quasi-infinite point U_∞ instead of the points $U = 0$ and $U = \infty$ respectively.

A finite difference approximation was employed to find the numerical solution of (1) using a grid point representation

$$f_{j,k} = f(U_j, \bar{t}_k)\,;\ 1 \le j \le r\,,\ U_1 = U_{q\ge}\,,\ U_r = U_\infty\,;\ k \ge 0\,,\ \bar{t}_0 = 0$$

of the distribution $f(U,\bar{t})$ with the chosen constant increment sizes ΔU and $\Delta\bar{t}$. According to the Crank-Nicolson method /3/ we transformed the equation (1) at the point U_j, $\bar{t}_{k+1/2}$ with $1 \le j \le r-1$ and $k \ge 0$ where we applied the second-order-correct difference analogs

$$\left(\frac{\partial f}{\partial \bar{t}}\right)_{j,k+\frac{1}{2}} = (f_{j,k+1} - f_{j,k})/\Delta\bar{t}\,,$$

$$\left(\frac{\partial^2 f}{\partial U^2}\right)_{j,k+\frac{1}{2}} = (f_{j+1,k} - 2f_{j,k} + f_{j-1,k} + f_{j+1,k+1} - 2f_{j,k+1} + f_{j-1,k+1})/2(\Delta U)^2\,,$$

$$\left(\frac{\partial f}{\partial U}\right)_{j,k+\frac{1}{2}} = (f_{j+1,k+1} + f_{j+1,k} - f_{j-1,k+1} - f_{j-1,k})/(4\Delta U)\,,$$

$$f_{j,k+\frac{1}{2}} = (f_{j,k+1} + f_{j,k})/2\,. \qquad (3)$$

In this transformation the resulting values $f(U_j + U_e, \bar{t}_\mu)$, $f(U_j/\beta + U_i, \bar{t}_\mu)$, $f(U_j/(1-\beta) + U_i, \bar{t}_\mu)$ with $\mu = k, k+1$ usually do not fit with the chosen grid points for arbitrary values of U_e, U_i and β. With the aid of parabolic interpolations in the distribution function with regard to the energy variable U around all the three energy points $U_j + U_e$, $U_j/\beta + U_i$ and $U_j/(1-\beta) + U_i$ for each time $\bar{t}_k$ and $\bar{t}_{k+1}$ using the neighbouring distribution values at both $\bar{t}_k$ and $\bar{t}_{k+1}$ we could represent these values in the same grid.

Employing additionally

$$\left(\frac{\partial f}{\partial U}\right)_{j,k} = (f_{j+1,k} - f_{j-1,k})/(2\Delta U) \qquad (4)$$

for the boundary condition (2a) we obtained from both boundary relations (2a,b) the conditions $f_{0,k} = f_{2,k}$ and $f_{1,k} = 0$ for $k \ge 0$ and $1 \ge r$; thus it is possible to eliminate the values for the fictitious points outside the considered region.

At the end of this procedure we obtained a closed linear equation system from which the values $f_{j,k+1}$ at the time $\bar{t}_{k+1}$ can be calculated for all energy points from the values $f_{j,k}$ at the time $\bar{t}_k$ or from the initial function $\tilde{f}$ at $\bar{t}_0 = 0$.

This system has a tridiagonal matrix and in the upper part of this matrix there are, resulting from each of the difference terms in (1), three additional neighbouring non-vanishing elements in each row, which are at higher energy points, far away from the diagonal. The latter are due to the exciting and ionizing collisions and the distance to the diagonal in each row is determined by the values of the parameters U_e, U_i and β.

Because of the great efficiency of the inelastic collisions and the resulting depopulation of the distribution it can be presumed that the distribution function decreases rapidly with increasing energy U, particularly in the high energy region, where inelastic collisions are acting. Therefore, if the threshold energies of the inelastic processes are not too small, it is to be expected that the influence on the solution of all additional non-vanishing elements at high energy points is only limited. Thus it is possible to obtain the solution of this equation system by iterative application of the well known algorithm for a tridiagonal matrix /3/. For this purpose the terms of all non-vanishing elements resulting from the inelastic collisions were put on the r.h.s. of the linear equation system. Especially in the first step the values of these terms were assumed to be equal to the already well known values of the distribution at the time step $\bar{t}_k$. This iterative solution process at each time $\bar{t}_{k+1}$ was finished if the absolute deviation of the ratio of two succesive distribution values at each energy point from the value 1 is smaller than 10^{-5}.

In order to guarantee a precise solution at each time step, the fulfilment of the concentration and energy balance of the electron component was controlled. These balances are obtained from equation (1) in the form

$$\frac{d}{d\bar{t}} n_e(\bar{t}) = n_e(\bar{t}) \frac{\nu_i(\bar{t})}{p_0} - n_e(\bar{t}) \frac{1}{p_0 \tau} \quad ,$$

$$\frac{d}{d\bar{t}} [n_e(\bar{t}) \bar{U}(\bar{t})] = n_e(\bar{t}) \left[\frac{\bar{U}^F(\bar{t})}{p_0} - \frac{\bar{U}^{el}(\bar{t})}{p_0} - \frac{\bar{U}^e(\bar{t})}{p_0} - \frac{\bar{U}^i(\bar{t})}{p_0} - \frac{\bar{U}^\tau(\bar{t})}{p_0} \right] \qquad (5a,b)$$

by pertinent analytical averaging of the partial differential equation, using the boundary conditions (2a,b). Here

$$n_e(\bar{t}) = n_e(0) \int_0^\infty U^{1/2} f(U,\bar{t})\, dU,$$

$$\nu_i(\bar{t})/p_0 = \left(\frac{2e_0}{m}\right)^{1/2} n_g \int_0^\infty U Q_i(U)\, f(U,\bar{t})\, dU / n(\bar{t}) \qquad (6a,b)$$

$$\left(n(\bar{t}) \equiv n_e(\bar{t}) / n_e(0) \right)$$

are the still time dependent electron concentration n_e and the ionization frequency ν_i of the electrons. Additionally, the mean energy $\bar{U}$, the energy gain from the electric field $\bar{U}^F$ and the energy losses $\bar{U}^{el}$, $\bar{U}^e$, $\bar{U}^i$, $\bar{U}^\tau$ by elastic, exciting and ionizing collisions as well as by the electron loss term have the representation

$$\bar{U}(\bar{t}) = \int_0^\infty U^{3/2} f(U,\bar{t})\, dU / n(\bar{t}),$$

$$\bar{U}^F(\bar{t})/p_0 = -\frac{1}{3n_g}\left(\frac{2e_0}{m}\right)^{1/2} \int_0^\infty \frac{U}{Q_d(U)} \frac{\partial}{\partial U} f(U,\bar{t})\, dU \left(\frac{E(\bar{t})}{p_0}\right)^2 / n(\bar{t}),$$

$$\bar{U}^{el}(\bar{t})/p_0 = 2\frac{m}{M}\left(\frac{2e_0}{m}\right)^{1/2} n_g \int_0^\infty U^2 Q_d(U)\, f(U,\bar{t})\, dU / n(\bar{t}),$$

$$\bar{U}^e(\bar{t})/p_0 = U_e\left(\frac{2e_0}{m}\right)^{1/2} n_g \int_0^\infty U Q_e(U)\, f(U,\bar{t})\, dU / n(\bar{t}),$$

$$\bar{U}^i(\bar{t})/p_0 = U_i \frac{\nu_i(\bar{t})}{p_0},$$

$$\bar{U}^\tau(\bar{t})/p_0 = \bar{U}(\bar{t}) \frac{1}{p_0 \tau}. \qquad (7a\text{-}d)$$

Using the numerically obtained distribution function $f(U,\bar{t})$ at each given time $\bar{t}_{k+1}$ we calculated all macroscopic quantities (6) and (7) and then checked the fulfilment of the concentration and energy balance (5a,b).

3. Examples illustrating the mathematical procedure

The calculations presented in this section were performed for a neon plasma applying the cross sections Q_d, Q_e and Q_i shown in Fig. 1 with the threshold potentials U_e = 16.6 V and U_i = 21.5 V. Starting with the stationary solution of equation (1) for the undisturbed value of the electric field and the life time τ of the electrons, which is determined by the stationary solution, the non-stationary energy distribution function f was calculated for great perturbations of the field by a rectangular pulse at $\bar{t} = 0$. The parameters of the undisturbed electric field $(E/p_o)_s$, the pulse amplitude $(E/p_o)_a$ and the pulse duration $\bar{t}_E$ of four considered cases are given in the following table.

$(E/p_o)_s$ [V/(cm Torr)]	$(E/p_o)_a$ [V/(cm Torr)]	$\bar{t}_E$ [Torr s]
5	15	$5 \cdot 10^{-7}$, $1 \cdot 10^{-6}$
20	- 15	$5 \cdot 10^{-7}$, $1 \cdot 10^{-6}$

Using appropriate increment sizes such as $\Delta U \approx 10^{-2} \gamma$ and $\Delta \bar{t} \approx 10^{-10}$ Torr s, which led to a system of about 1000 linear equations, the iteration at each time step needed no more than three cycles and the fulfilment of the concentration and energy balance was very precise /1/.

To illustrate the temporal behaviour of the distribution in Figs. 2a,b this quantity is shown as function of U with $\bar{t}$ as parameter. This function is presented for the two field parameter combinations of the table with the pulse duration $\bar{t}_E = 1 \cdot 10^{-6}$ Torr s which characterize a great increase or a great decrease of the electric field during the action of the pulse. From Fig. 2a it can be seen that, due to the jump-like increase of the field by switching on the pulse at $\bar{t} = 0$, a rapid increase of the distribution from its stationary state is effected within very short times, especially at higher energies. Then for all energies a nearly equal factorial increase with the time follows and after switching off the pulse a strong decrease of the high energy part occurs, following which the new stationary state is reached within a short time interval

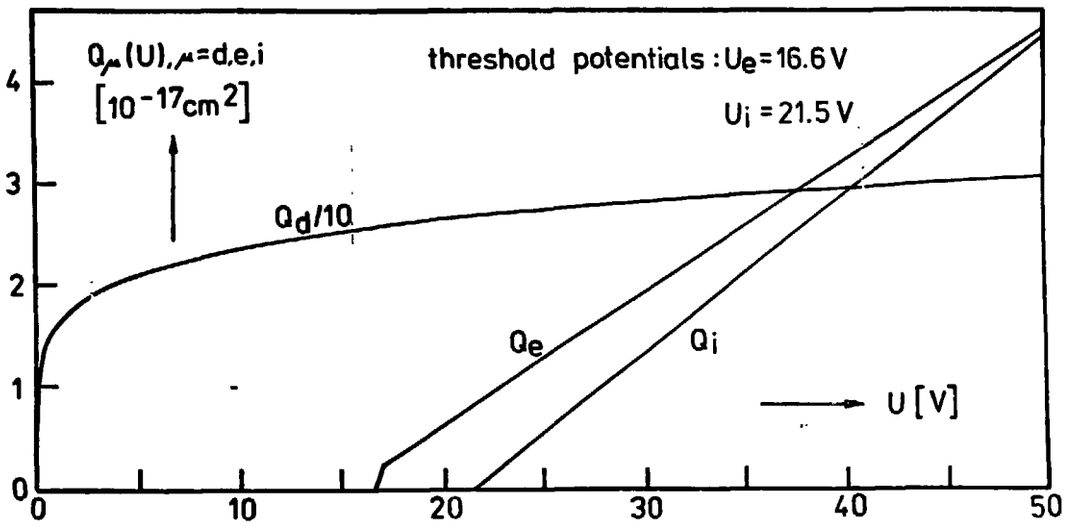

Fig. 1

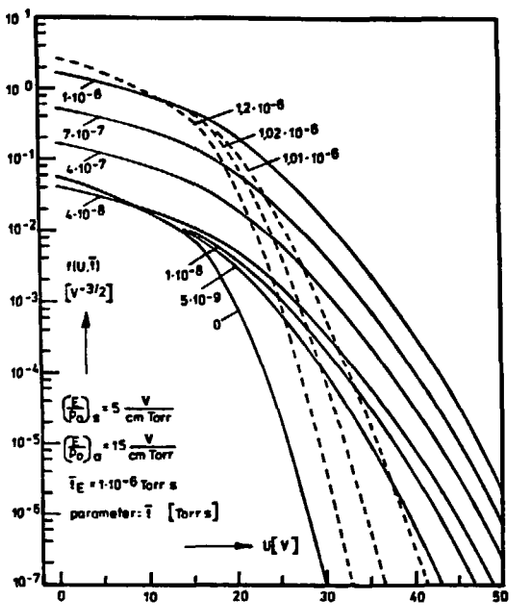

Fig. 2a

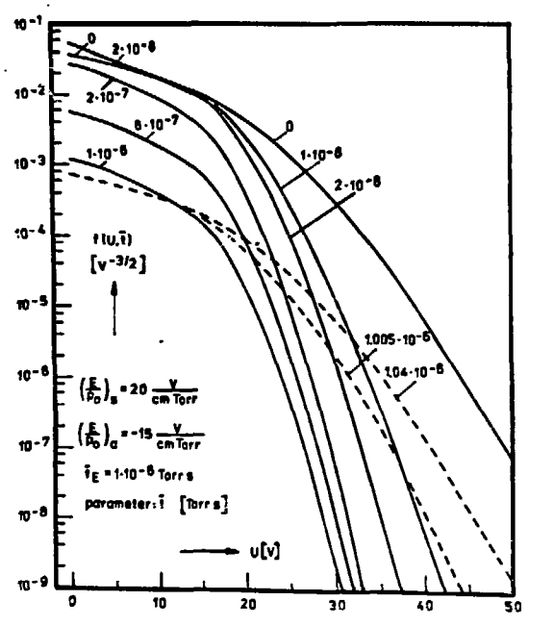

Fig. 2b

after the jump-like return to the undisturbed electric field. Nearly the inverse behaviour is to be observed in the second case (Fig. 2b), where during the action of the pulse the electric field is markedly reduced. To a certain extent already these results demonstrate the great stability of the numerical solution approach because after some

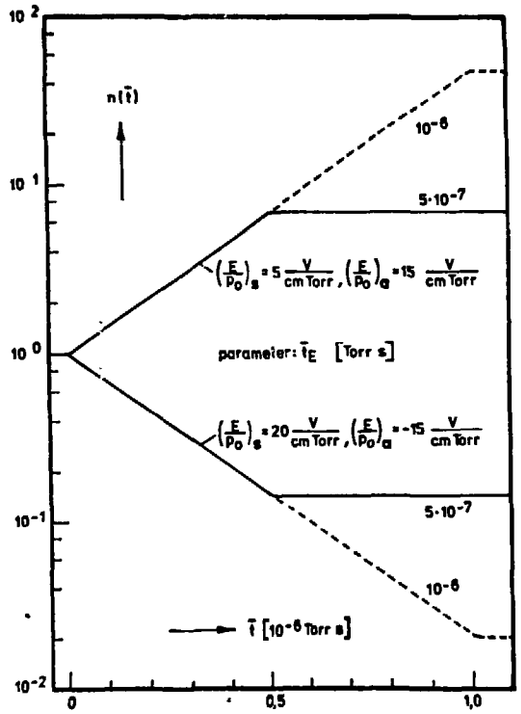

Fig. 3

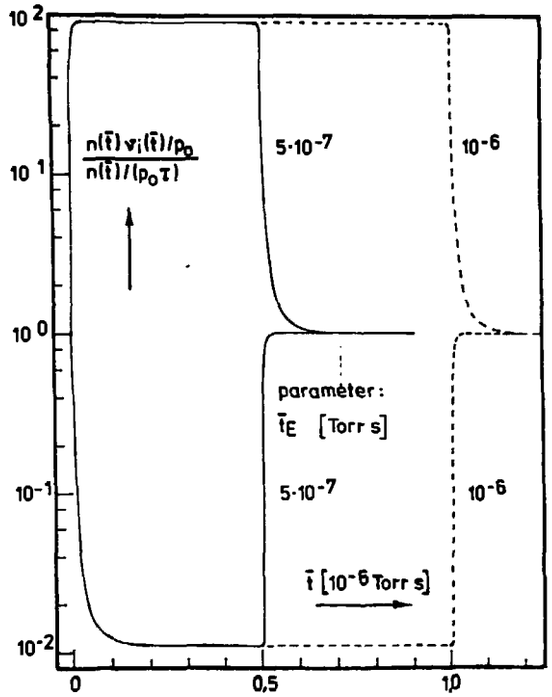

Fig. 4

thousand time steps the new stationary distribution is reached very precisely.

For all four cases the temporal behaviour of the electron concentration is shown in Fig. 3. We notice that the concentration of the electrons related to the initial concentration $n_e(0)$, is strongly changed by the pulse action. For both field parameter combinations it is to be observed that increasing pulse durations lead to increasing alterations of the concentrations. After switch-off of the pulse the new stationary concentration will be established immediately.

Finally in Fig. 4 the temporal dependence of the ratio of the electron gain due to ionizing collisions and the electron loss as described by the electron loss term with the life time τ is indicated for all the cases considered. Starting from the value 1, which characterizes the initial stationary state, this ratio changes by nearly two orders of magnitude during the action of the pulse and then returns to its final stationary value after the switch-off of the pulse.

This figure clearly demonstrates that during the action of the pulse a marked non-stationary behaviour of the electron component results due to the great pulsive perturbation of the electric field. Besides

the results presented here, many other aspects of interest have thus become solvable, for instance the time behaviour of the main energy transfer channels for the field energy to the different degrees of freedom of the neutral component.
Using nearly arbitrary energy dependent collision cross sections according to different kinds of neutral gases employed /4/ the method which we demonstrated here has proved suitable for the investigation of many relaxation problems in different time dependent electric fields. This approach provides a deeper insight into the physical mechanism of temporal relaxation and gives the possibility to solve further generalized problems of the non-stationary electron kinetics.

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