Calculation of the distribution function of small ion admixture in parent gas for arbitrary scattering cross sections by the moment method

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Abstract. The paper is focused on the calculation of the distribution function of a small ion admixture in parent gas in a spatially homogeneous case in the presence of an electric field. The problem is solved by solution of the nonstationary Boltzmann equation by moment method (by expansion in terms of Barnett functions). It is demonstrated that the use of recurrence relations for calculating the matrix elements of the collision integral along with the expansion in \(\Omega\)-integrals allows successfully calculate the distribution functions for arbitrary scattering cross sections.

Introduction
The description of processes in weakly ionized gases is a complex problem that is actively studied. During last years, a number of approaches have been developed which make it possible to obtain a solution with different accuracy. Among these numerical methods of solution, two main approaches can be distinguished: the first is based on the Monte Carlo method, and the second is the so-called deterministic approach that require the solution of the Boltzmann equation. Using the approach based on the Boltzmann equation opens the possibility of describing processes at the level of the ion velocity distribution function (IVDF). Similar studies were carried out earlier in the works of various authors. However, none of the groups succeeded in creating a completely universal methodology that would work successfully with all problem parameters.

So in R. White’s works, a wide range of field values is considered, but the calculation for the case of close ion and atom masses prove to be problematic. In Viehland’s works, it is possible to calculate macro parameters, but the form of the IVDF can not be obtained. Finally, in the works of A. Ender and co-authors, calculations were carried out for equal masses and a wide range of fields, the temporal evolution of the IVDF was studied, but the analysis was carried out only for model interaction potentials. The models of interaction with isotropic scattering by angles and with two velocity dependences (constant and inversely proportional) were considered. These models allowed for some analytical calculations, which in turn made it possible to calculate a large number of matrix elements by means of recurrence relations.

The present paper is the first step in an attempt to apply the so-called moment method (used in Ender’s works [1], as proposed by Barnett [2]) to the calculation of the IVDF for arbitrary interaction potentials. On a global scale, this work is in the trend of developing deterministic methods for solving the Boltzmann equation. These works are conducted in many countries. The
approaches used are somewhat different. Two main directions can be distinguished depending on the method of calculating the matrix elements of the collision integral: the spectral method (Galerkin) and method based on the Talmi coefficients. In our case, a different approach is developed, based on recurrence relations for the calculation of matrix elements using the expansion in terms of Ω*-integrals.

Problem statement
In this paper, we consider a nonstationary spatially homogeneous problem of the motion of a small impurity of ions in a parent gas. We note that this means that we neglect the intrinsic field of the ions and assume that the ion impurity does not affect the parameters of the background gas. This model can describe situations without any inelastic processes and moderate and weak electric fields (up to 500 Td). Despite the seeming simplicity, this problem turns out to be relevant not only for testing the numerical model but also for description of particles drift in experiments.

Under these conditions, the IVDF of the ions is described by the Boltzmann equation in the form

\[ \frac{\partial f(v,t)}{\partial t} + eE \frac{\partial f(v,t)}{\partial v} = \int \sigma(v-v',\theta)(v-v')(f(v,t) - f'(v',t))M(v) \, dv', \]

\[ M(v) = \left( \frac{m}{2\pi kT} \right)^{3/2} \exp\left(-\frac{mv^2}{2kT}\right) \]

We would like to emphasize particularly that we consider the problem in a nonstationary formulation. This approach allows us to track the setting of a stationary solution. The effectiveness of this approach was demonstrated in the work [1].

For the convenience of calculations and presentation of results, we introduce dimensionless variables. The dimensionless velocity \( c = \frac{v}{\sqrt{2kT/m}} \), dimensionless time \( \tilde{t} = t/\tau \), where \( \tau \) is the mean time between collisions. Starting from these units, we can introduce a dimensionless unit characterizing the field \( \epsilon = eE\lambda/(2kT) \), where \( \lambda \) - the ion mean free path.

The moment method, which we use to solve the Boltzmann equation involves transformation of initial integro-differential equation to a system of differential equations. The distribution function is expanded into a system of orthogonal polynomials. In our case, we use the Barnett functions [2].

\[ f(c, r, t) = M(c) \sum C_{\alpha lm} r l m(r, t) H_{\alpha lm}(c), \quad c = \sqrt{\frac{m}{2kT}}(v - u), \]  

\[ M_n = \left( \frac{m_n}{2kT r} \right)^{3/2} e^{-c_n^2}, \quad H_j(c_n) = Y_i^{\alpha}(\Theta, \varphi)c_i^n S_{i+1/2}(c_n^2), \quad \lambda = 0, 1, \]

where \( C_{\alpha lm} r l m(r, t) \) expansion coefficients, \( Y_i^{\alpha}(\Theta, \varphi) \) - spherical harmonics, \( S_{i+1/2}(c_n^2) \) - Sonin–Laguerre polynomials.

After substituting the expansion of the distribution function \( f(c, r, t) \), the equation is multiplied by a polynomial and integrated along the velocities. As a result, an infinite system of differential equations is obtained.

The resulting system of equations takes the form

\[ \frac{\partial C_{r,l}}{\partial t} + \epsilon \left( \frac{2r(l+1)}{2l+3} C_{r-1,l+1} - \frac{2l}{2l-1} C_{r,l-1} \right) = \sum_{r_1} \Lambda_{r,r_1,l} C_{r_1,l}, \]
When solving a particular problem, the system of equations is truncated to certain values of the indices. In the course of numerical calculations, the sufficiency of the number of terms in the expansion of the DF is checked by means of internal convergence control. It should be noted that the most time-consuming and difficult part is the calculation of matrix elements $\Lambda_{r,r_1,l}$. They are calculated using the technique described in the article [3]. It involves the calculation of matrix elements by means of recurrence relations. The starting values of the matrix elements are calculated using the so-called $\Omega_*$-integrals:

$$
\Omega_*(n,m) = \int_0^\infty \exp(-c^2)c^{2m+3}Q_*(n)c\,dc,
$$

$$
Q_*(n) = 2\pi(1 - \delta_{n,0}) \int_0^{\pi} (1 - \cos\theta)^n \sigma(g,\theta) \sin\theta d\theta
$$

This allows calculations for scattering cross sections with arbitrary velocity and angular dependence.

Results

To carry out the calculations, we used well-known model cross sections: hard spheres with isotropic scattering, pseudo-Maxwellian molecules and the velocity-dependent scattering cross section, which was proposed in [4] for Argon, as for the most well-studied gas.

The evolution of the DF of ions for moderate fields was calculated. In such a way it was possible to confine ourselves to a not very large number of matrix elements, which made it possible to shorten the calculation time. In the case of moderate field ($\epsilon = 0.5$), it turns out that it is sufficient to use matrix elements with maximum indices 8 for Legendre and 16 for Sonine to calculate DF and get the stationary solution. Figure 1 shows the time evolution of the distribution function for the isotropic cross section from [4]. It can be seen that at time $t = 4$, a stationary solution is already established in a wide range of velocities.

![Figure 1](image1.png)

**Figure 1.** Time evolution of ion distribution function $f(c_z,0)$ for $Ar^+ - Ar$ at $\epsilon = 0.5$ in the case of isotropic cross section from paper [4]. (1) $t = 0$, (2) $0.5$, (3) $1$, (4) $3$, (5) $4$, (6) $4.5$.

![Figure 2](image2.png)

**Figure 2.** Stationary limit of the ion distribution function time evolution for $Ar^+ - Ar$ at $\epsilon = 0.5$. Solid line (1) - Piscitelli [4] cross section, dashed (2) - hard sphere model, dotted (2) - pseudo-maxwellian molecules model.

Figure 2 shows the successfully calculated stationary ion distribution functions for the three interaction models considered. It can be seen that the distribution functions for hard sphere model and cross section from Piscitelli are quite close (the difference is mainly in the region of DF maximum).
As can be seen from the presented results, the moment method in combination with the calculation of the matrix elements through $\Omega^*_\nu$-integrals makes it possible to calculate the distribution function while solving the problems of ion motion in fields for a scattering cross section with arbitrary velocity dependence. Macroscopic quantities like mobility, ion current and ion energy then could be calculated via obtained IVDF. The calculation of $\Omega^*_\nu$-integrals and matrix elements of the collision integral takes the most time (from several hours up to several days on PC computer). However it should be done only once while perform calculations for particular type of cross section. The solution of the moment system itself for specific conditions turns out to be fast, which makes it possible to do calculations for various field parameters. In the future we are going to use a two-temperature method [2] to perform calculations not only for moderate, but also for strong electric fields.

References
[1] Ender A Ya et al 2010 Tech. Phys. 55 176
[2] Mason E A and McDaniel E W 1988 Transport properties of ions in gases (New York: Wiley)
[3] Ender I A et al 2017 Tech. Phys. 62 1148
[4] Piscitelli D et al 2003 Phys. Rev. E 68 046408