Distribution Function and Transport Properties of the Ions Moving in a Neutral Gas under External Electric Field

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Abstract. The moment method is used to describe a behavior of ions at the electric field. The authors of the present paper have been obtained the new results which permit to calculate the matrix elements of the collision integral at large indices. Applying these results, the moment system is calculated. The non-stationary problem concerning the behavior of ions under sharp switch-on of the electric field is solved. For the first time, the distribution function is built up for this process. A number of the analytical results are obtained to be compared with the calculated ones.

INTRODUCTION

At the strong electric field, ions' mobility depends on the field intensity, the velocity distribution function (DF) turns out to be strongly anisotropic, and a diffusion coefficient depends on direction.

The main method in calculating the transport coefficients in ionized gas under the electric (and magnetic) field turns out to be the moment method (see, review [1]), the Boltzmann equation being substituted with the equivalent system of equations for the expansion coefficients (moments) of DF. To build up the strongly nonequilibrium DF, the large number of its moments should be known. We developed a new method to build up the matrix elements (ME) of the collision integral [2, 3]. Based on the invariance principle of the collision integral relative to a basis choice, the recurrence relationships relating the MEs of different indices were built up. As a result, the MEs of large indices and arbitrary mass ratios of colliding particles could be found. And, hence, generally, the method was developed to calculate the nonlinear MEs, it is suitable for the linear MEs needed in solving the problems under consideration. The linear MEs are proportional to the bracket integrals widely used in calculating the transport coefficients. For these problems, it is sufficient to know only the brackets corresponding to one–three Legendre polynomials. Even in this case, the calculations are cumbersome and complicated resulting often in misleading conclusions. Performing the calculations, we use the MEs corresponding to the number of Legendre polynomials up to 128 in an expansion as well as 128 Sonine polynomials.

It should be noted that, when calculating the transport coefficients of the charged particles in the electric field, the moment method was applied in literature with very small number of the MEs of collision integral, e.g., in [4], it was used no more than 20-30 MEs. So, the power of the moment method has not being expired, but the problems concerning its convergence are far from being studied.

Usually, the moment method is used for obtaining the stationary values of the transport coefficients. We are solving the more complicated problems: building-up the DF via the moment method and to solve the nonstationary problem of DF evolution as well as the transport coefficients after an instant switch-on of the electric field. Studying such transient process is interesting by itself and, specially, gives an opportunity to obtain the stationary solution.

When studying the moment method convergence, it is of importance to have the analytical solutions of the problem under consideration, if in certain cases. It is known that a collision operator of the Boltzmann equation is essentially simplified for the Maxwellian model of particle interaction, in which a scattering cross-section is inversely proportional to a velocity. For ions, moving in their own gas, the main interaction process is resonance charge-exchange, when ion past atom exchanges its electron with it. A differential cross-section with 180^{o}–scattering refers to this process. Consider a model in which a cross-section is reversely proportional to relative velocity and angular part is $\delta(\theta-\pi)$, being named CEM–model. For this model, the collision operator coincides with BGK–model [5].

In this paper, for *CEM*–model, the analytical solutions of the non-stationary problem are built up, the numerical results obtained with the moment method are compared with the analytical ones, and the solutions are built up with the moment method for several other interaction models.

STATEMENT OF THE PROBLEM

Let the DF of atoms to be the equilibrium one of a temperature *T*. The Boltzmann equation for the DF of ions $f(\mathbf{v},t)$ is as follows

$$\frac{\partial f(\mathbf{v},t)}{\partial t}+\frac{e\mathbf{E}}{m}\cdot\frac{\partial f(\mathbf{v},t)}{\partial v}=\hat{I}(f(\mathbf{v},t),M(T,v))\ . \tag{1}$$

Here, e is electron's charge, $\mathbf{E}$ is electric field strength, m is a particle mass, $\hat{I}$ is the collision integral, $M(T,v)$ is the Maxwellian. The ion DF is considered, initially, to coincide with atom DF

$$f(\mathbf{v},0)=M(T,v)\ . \tag{2}$$

Let a field is directed along z -axis, then, arising flow of charged particles is directed along the same axis and the DF is axially symmetric in velocity space. In the standard moment method, the DF is taken as follows

$$f(\mathbf{v},t)=M(\alpha,c)\sum C_{rl}(t)H_{rl}\quad \alpha=m/2kT,\quad \mathbf{c}=\sqrt{\alpha}\mathbf{v}\ . \tag{3}$$

Here, $H_{rl}=S^r_{l+1/2}c^lP_l(c_z/c)$ are the spherical Hermite polynomials (Burnett's functions), $S^r_{l+1/2}$ are the Sonine (Laguerre) polynomials and $P_l(x)$ are the Legendre polynomials.

The left-side part of the system of moment equations was deduced earlier taking into consideration the external forces in the 3D spatially non-uniform case (see, [6]). In the case under consideration, it is essentially simplified, and a full system of moment equations in the dimensionless mode takes a form

$$\frac{dC_{rl}}{dt}+\varepsilon\left(\frac{2}{2l+3}r(l+1)C_{r-1l+1}-\frac{2l}{2l-1}C_{rl-1}\right)=\sum_{r_1}\Lambda^1_{r,r_1,l}C_{r_1l}\ . \tag{4}$$

Here, time is reduced to τ , i.e., intercollision mean time, and $\varepsilon=\frac{eE\tau}{m}\sqrt{\alpha}$. In (4), the linear MEs of the first kind $\Lambda^1_{r,r_1,l}$ are related with a collision integral $\hat{I}$ as follows

$$=\frac{1}{g_{rl}}\int H_{rl}\hat{I}(H_{r_1l},M(\alpha,c))d^3c\ . \tag{5}$$

In the case of *CEM*–model, we have $\Lambda^1_{r,r_1,l}=(\delta_{l0}\delta_{r0}-1)\delta_{rr_1}$, i.e., a matrix Λ at any l is diagonal, and all its eigenvalues equal -1 except $\Lambda_{0,0,0}$.

ANALYTICAL SOLUTIONS

The Boltzmann equation for *CEM*–model takes a form

$$\frac{\partial f}{\partial t}+\varepsilon\cdot\frac{\partial f}{\partial c_z}+f=M\ . \tag{6}$$

A Maxwellian distribution M can be presented as $M(c_z)M(c_\rho)$, where $M(c_z)=(\alpha/\pi)^{1/2}\exp(-\alpha c_z^2)$, and $M(c_\rho)=(\alpha/\pi)\exp(-\alpha c_\rho^2)$ and $c_\rho^2=c_x^2+c_y^2$.

In the stationary case, there is not the derivative with respect to t in (6), and it can be shown that a solution is

$$f(c_\rho,c_z)=\frac{\sqrt{\pi}}{2}M(c_\rho)M(c_z)\frac{1}{\varepsilon}e^{Z^2}\left(1+erfZ\right), \qquad Z=c_z-1/(2\varepsilon)\,. \tag{7}$$

From (7), it is easily found the DF at large negative and large positive c_z

$$f_-(c_\rho,c_z)\approx M(c_\rho)M(c_z)\frac{1}{2\varepsilon\,|\,c_z\,|+1}, \qquad f_+(c_\rho,c_z)\approx\frac{1}{\varepsilon}e^{1/4\varepsilon^2}M(c_\rho)e^{-c_z/\varepsilon}\,. \tag{8}$$

As it is known, for moment method convergence, the DF shoud meet the Grad criterion:

$$\int_{-\infty}^{\infty} f^2(c_\rho,c_z)\exp(c_\rho^2+c_z^2)d^3c<\infty\,. \tag{9}$$

It is easily seen from formulas (8) and (9) that, at arbitrary intensity of the electric field, the Grad criterion is not met as a function f goes too slowly to zero at $c_z\to\infty$.

Consider the non-stationary process at instant switch-on of the electric field when, at $t<0$, the field is zero, and, at $t\geq 0$, it is constant, ε. At taken initial conditions, the DF with respect to a transversal component c_ρ is always the Maxwellian one. To build up the solution of the Boltzmann equation one can use the method of characteristics, passing from variables t, c_z to the variables t, $Y=c_z-\varepsilon t$. Such solution is given below:

$$f(c_zc_\rho,t)=\left(\frac{\sqrt{\pi}}{2}M(c_z)e^{Z^2}\,\frac{1}{\varepsilon}\left(erf(\varepsilon t-Z)+erf(Z)\right)+e^{-t}M(Y)\right). \tag{10}$$

At $t\to\infty$, the second term in (10) turns out to be zero, and the first one transforms into a solution of stationary problem (7), which, as shown above, does not meet the Grad criterion. However, at any finite t, such large c_z is found that $\varepsilon t-(c_z-1/(2\varepsilon))$ becomes a large negative number. Then, the first term in large round brackets (10) tends to -1, but not to +1. At very large positive c_z, we have

$$f_+(c_z,c_\rho,t)\approx\frac{1}{2}M(\alpha,c)\frac{1}{\varepsilon}\left(\frac{e^{2\varepsilon t(c_z-1/(2\varepsilon))-(\varepsilon t)^2}}{c_z-1/(2\varepsilon)-\varepsilon t}-\frac{1}{c_z-1/(2\varepsilon)}\right). \tag{11}$$

A behavior of this DF at large c_z is determined by a term $-c_z^2$ in exponent, but not $-c_z$ as in the stationary solution. Such a fast decrease in DF at $c_z\to\infty$ provides a satisfaction of the Grad criterion. Hence, the moment method must converge at finite t. One question stays unsolved: how many moments should be taken into consideration to build up the distribution function using the moment method at large ε and t.

For *CEM*–model, the analytical solution of the moment system can be build up. A system (4) is solved by recurrence method. Starting with a moment $C_{00}=1$, we obtain easily:

$$C_{01}=2\varepsilon(1-\exp(-t)). \tag{12}$$

Further, the solutions can be found in layers $N = l + 2r = const$, increasing N. It can be shown that the analytical solution of a system (6) is as follows

$$C_{rl} = B_{rl}\varepsilon^N S_N(t), \quad B_{rl} = (-1)^r \frac{(2l+4r)!!(2l+1)}{2^r(2l+2r+1)!!}, \quad S_N(t) = 1 - \exp(-t)\sum_{k=0}^{N-1}\frac{t^k}{k!} \tag{13}$$

A function $S_N(t)$ is unique for all layer N. This function turns out to be zero at $t = 0$ and unity at $t \to \infty$, at large N, it is very small for a long time, and a transfer to unity occurs at sufficiently larger time, the more the N, the large a delay time is.

CALCULATION RESULTS

The numerical calculations of a moment system (4) are carried out with the Runge-Kutta method of 4th order.

The calculations are performed, beside *CEM*–model, with several other models. The systematic calculations are performed for the hard-sphere model (*HS*–model) and a resonance charge-exchange model with a constant free length (*CEHS*–model).

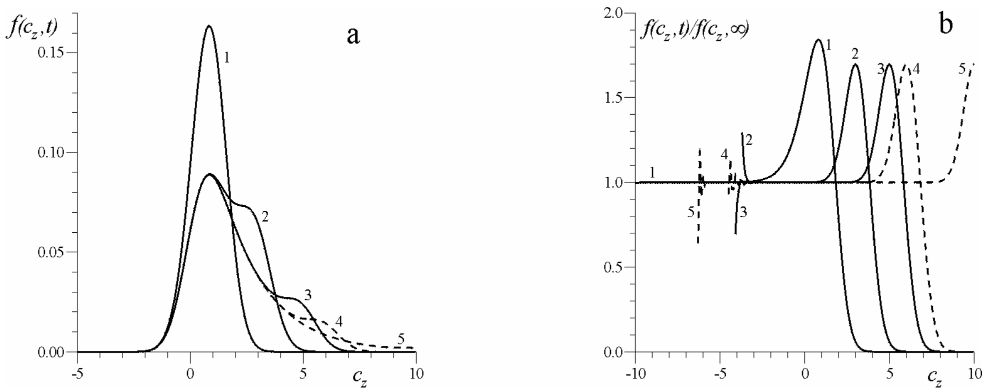

FIGURE 1. Distribution function at axis of symmetry at different time for *CEM* - model at $\varepsilon = 2.0$. **Figure a** refers to $f(c_z, t)$. **Figure b** refers to $f(c_z,t)/f(c_z,\infty)$. Curves 1-5 refer to $t = 0.5$ ($L_0 = 35$, $R_0 = 23$); 1.5 ($L_0 = 30$, $R_0 = 26$); 2.5 ($L_0 = 37$, $R_0 = 70$); 3 ($L_0 = 75$, $R_0 = 100$); 5 ($L_0 = 100$, $R_0 = 280$).

It is shown that, for *CEM*–model, the numerical $C_{rl}(t)$ are well described by the analytical formulas (13), and a good coincidence of the DF with an analytical solution (10) is observed. In Fig. 1, the DF at a symmetry axis ($c_\rho = 0$) is presented at different time at $\varepsilon = 2$. With time increase, the numbers of the Sonine R_0 and Legendre L_0 polynomials increase which should be taken into consideration in expansion (3). In Fig. 1b, the DF is reduced to a stationary solution (7). For $c_z > -4$, a fine coincidence with the corresponding ratio of the analytical solutions (10) and (7) is observed. For $c_z < -4$, a very fast flattening on the stationary solution is observed, but, with time, a solution turns out to be found with more difficulties when using the moment method. Along the electric field, a moving front can be observed in velocity space with a constant velocity ε, behind which there is a stationary state of DF.

It is maintained that, for all models under consideration here, at finite t, the moments $|C_{rl}|$ decrease with an increase in r always at large r. However, if a product εt is sufficiently large, the maximum of $|C_{rl}|(r)$ turns out to be such large that the DF restoration via its moments becomes impossible when summing in (4).

In fig. 2, for *HS*–model, it is shown the origin of maximums of $|C_{r0}|(r)$. If a value of maximum exceeds 10^{16}, to overcome this maximum, when summing in (3), becomes impossible. One succeeds in moving of somewhat far using the procedures with larger number of digits (dashed curves in Fig. 1). On contrary to C_{rl} with the large indices, a mobility $K = C_{01}/(2\varepsilon)$ is never large. The functions $K(t)$ are given in Fig. 3a. At calculations, it is used such a normalization of the ME, that $K = 1$ at a limit of very small ε. The dependences of the stationary K on ε for two models are shown in Fig. 3b.

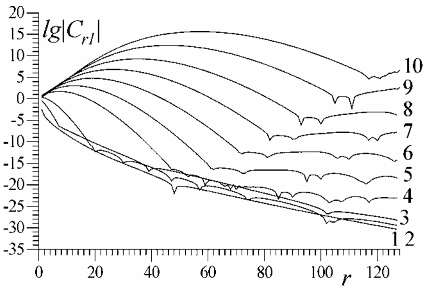

FIGURE 2. Dependences of the moments C_{rl} on r for the hard-sphere model at $l = 0$, $\varepsilon = 2.0$. Curves 1-10 refer to t =0.1, 0.5, 1, 2, 2.5, 3, 3.5, 4, 4.5, and 5, respectively.

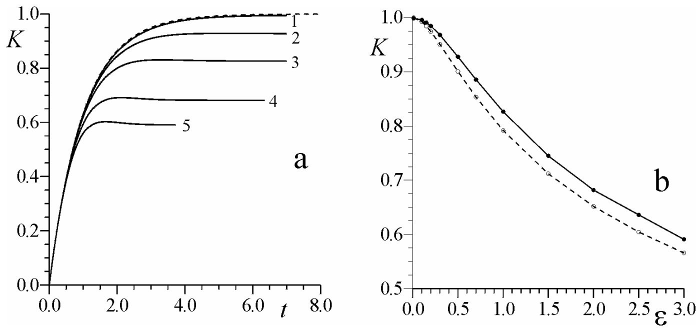

FIGURE 3. Mobility K for the hard-sphere model: (**a**) $K(t)$ at different ε, curves 1-5 refer to ε =0.1, 0.5, 1, 2, end 3, respectively, (**b**) the stationary $K(\varepsilon)$, dashed curve corresponds to *CEHS*–model.

Nevertheless the complications at summation in (3), there is a wide range of ε and t, in which the DF is restored with a very high accuracy. In Fig. 4, the DF evolution is presented for *HS*–model at $\varepsilon = 2$. A function $f(c_z, \infty)$ is built up numerically and refers to $t = 3.5$. The DF flattening with an increase in t proceeds non-uniformly, with a rise in c_z a relaxation process slows down.

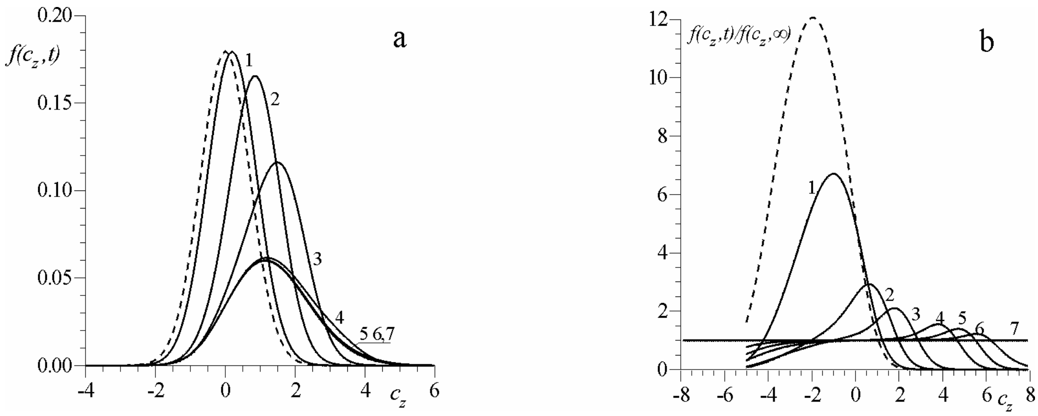

FIGURE 4. Distribution function at axis of symmetry at different time for hard-sphere model at $\varepsilon = 2.0$, $L_0 = 128$, $R_0 = 128$: **a** [$f(c_z,t)$], **b** [$f(c_z,t)/f(c_z,\infty)$]. Curves 1-7 refer to *t*=0.1; 0.5; 1; 2; 2.5; 3; 3.5, respectively.

The calculations being accomplished, it can be secured that, at the stationary state, the DF building-up is successfully obtained via non-stationary system solution with such ε, with which the stationary moment system solution can not be obtained, the DF being restored up to 8–10 times thermal velocity at $\varepsilon < 2$.

Besides the mobility, other moments of physical meaning are built up such as a pressure and heat flow. They are calculated in a reference frame moving with ion drift velocity. In Fig. 5, for HS–model, it is shown a heat flow evolution at different ε. If, at small ε, a heat flow decreases monotonically with time, a non-monotony is observed with a rise in ε as well as a sigh change. One can see how much would the heat flow be in value when increasing the electric field.

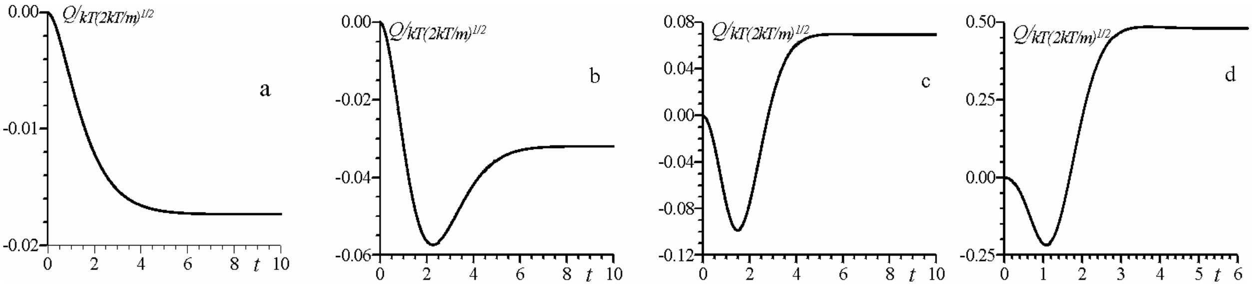

FIGURE 5. A heat flow vs. time for several ε : **a** ($\varepsilon = 0.1$), **b** ($\varepsilon = 0.5$), **c** ($\varepsilon = 1$), **d** ($\varepsilon = 2$).

At $\varepsilon > 3$, the stationary state for a sufficiently large velocity range is out of reach when using the moment method.

The transfer to a new basis, of which temperature is distinct from the atoms ones, opens up good perspectives [4]. In Fig. 6, it is shown that 1.5 times the temperature of a basis results in a decrease in the maximum C_{r0} down to a value of more than 4 orders. Using the results of [2] for the non-linear MEs, the linear MEs in a new basis can be easily found.

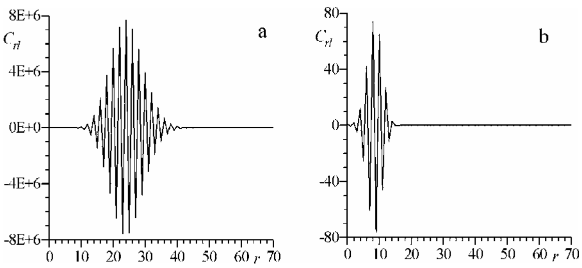

FIGURE 6. The moments $C_{r0}(r)$ in two bases with temperature ratio $T_1/T_0 = 1.5$: **a** (Bas0), **b** (Bas1).

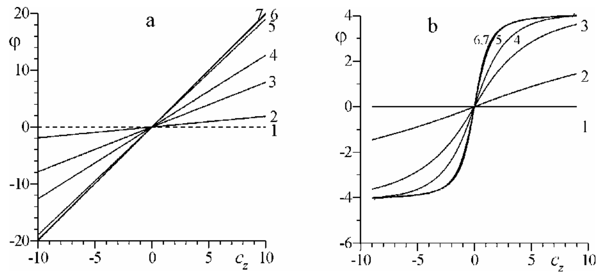

FIGURE 7. Dependence $\varphi(c_z)$ at $c_\rho = 0$: **a** (*CEM*–model), **b** (*CEHS*–model). Curves 1-7 correspond to t =0, 0.1, 0.5, 1, 3, 5, 10, respectively.

At very small ε, the DF takes a form $f(c_z, c_\rho, t) \approx M(\alpha, c)(1 + \varepsilon\varphi(c_z, c_\rho, t))$. In Fig. 7, it is shown the calculations of a function φ for two interaction models via the moment method.

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