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On the Ion Drift in Cold Gas

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Abstract—The problem of ion drift in such a strong electric field that the ion drift velocity significantly exceeds the thermal velocity of atoms is considered. In the case where the ion mass is identical to the gas particle mass, scattering is isotropic in the center-of-mass system and the ion scattering cross section is independent of the collision velocity (hard sphere model). The ion velocity distribution function is calculated by the Monte Carlo method, its characteristics and diffusion coefficient are determined. A comparison with known numerical and analytical solutions is performed. It is found that average characteristics (drift velocity, longitudinal and transverse temperatures) are in very good agreement with the values obtained from integral relations for the two-temperature Maxwellian distribution; however, the ion velocity distribution itself differs significantly from the shifted two-temperature Maxwellian distribution.

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The ion flux characteristics can be determined by solving the Boltzmann kinetic equation for the ion distribution function

$$\frac{\partial f}{\partial t} + v\Delta f + \frac{eE}{m}\frac{\partial f}{\partial v} = I_{\rm st}(f), \tag{1}$$

where e and m are the ion charge and mass, $I_{\rm st}(f)$ is the collision integral.

Let us consider the problem of the ion drift in a strong electric field, so that the ion drift velocity greatly exceeds the thermal velocity of atoms, $W \gg (T_{\rm atom}/m)^{1/2}$. We restrict the analysis to the case where the ion mass is identical to the gas particle mass, scattering is isotropic in the center-of-mass system, and the ion scattering cross section is independent of the collision velocity (hard sphere model).

In the known solution to this problem [1], the ion velocity distribution function was set as the shifted two-temperature Maxwellian distribution

$$f_0(\bar v) = \left(\frac{m}{2\pi T_i}\right)^{3/2} \exp\left(-\frac{m(u-W)^2}{2T_\parallel} - \frac{m(v^2+w^2)}{2T_\perp}\right), \tag{2}$$

where $T_i = (T_\parallel T_\perp^2)^{1/3}$, and $T_\parallel$ and $T_\perp$ are the temperatures along and across the field, respectively. The parameters entering the expression for the ion distribution function (2) were found from integral relations for average ion characteristics [1] and are written as

$$W = 1.07(eE\lambda/m)^{1/2},\ T_\parallel = 0.555eE\lambda,\ T_\perp = 0.294eE\lambda, \tag{3}$$

where $\lambda = 1/\sigma n$ is the mean free path, σ is the cross section of ion—atom collisions, and n is the numerical atomic density.

Table 1 lists the results of Monte Carlo calculations of the drift velocity, longitudinal and transverse temperatures, the average ion energy, and diffusion coefficients in longitudinal and transverse directions. We choose the quantities $u_\lambda = (eE\lambda/m)^{1/2}$ and $\varepsilon_\lambda = eE\lambda$ as characteristic velocities and energies,

Table 1. Dimensionless values of the drift velocity, average energy, temperatures, and diffusion coefficients in the directions along and across the field

	W/u_λ	$\langle\varepsilon\rangle/\varepsilon_\lambda$	$T_\parallel/\varepsilon_\lambda$	$T_\perp/\varepsilon_\lambda$	$D_\parallel/D_\lambda$	$D_\perp/D_\lambda$
[1], approximate solutions	1.07		0.555	0.294		
[1], exact solution	1.14	1.170	0.454	0.293		
Monte Carlo	1.1467	1.1723	0.4431	0.2933	0.324	0.477

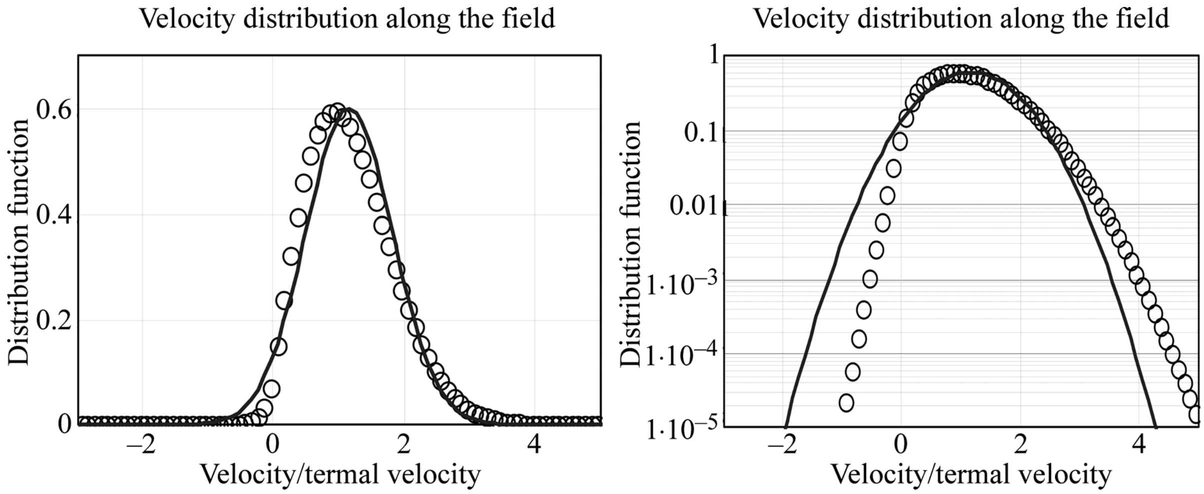

Fig. 1. Ion distribution functions over the longitudinal velocity on linear and logarithmic scales. Solid curves are the Maxwellian distributions (2) at the parameters of distribution (4), circles are Monte Carlo calculations.

respectively. As a characteristic value of the diffusion coefficient, we choose $D_\lambda = \lambda(eE\lambda/m)^{1/2}$, then the diffusion coefficient for hard spheres to a first approximation by Chapman–Enskog in the dimensionless form is written as $D_{C-E}/D_\lambda = 3\sqrt{\pi}/8 \approx 0.66466$. The numerical coefficients in Eq. (3) are the dimensionless drift velocities and longitudinal and transverse temperatures; they are given in the first line of Table 1. The exact solution according to [1] yields the following values

$$W/u_\lambda = 1.14,\ \ T_\parallel/\varepsilon_\lambda = 0.454,\ \ T_\perp/\varepsilon_\lambda = 0.293, \tag{4}$$

and they are given in the second line of Table. 1. The difference in drift characteristics (3) found from integral relations for average ion drift characteristics and the exact solution, according to [1], characterizes the method accuracy.

Monte Carlo simulation is a direct method for solving the problem in which the assumption about the functional form of the distribution function is not used. Accordingly, this simulation makes it possible to obtain a solution to the problem at hand with any accuracy; the average ion drift characteristics resulted from such simulation are given in the third line of Table 1.

An analysis of the Monte Carlo simulation data (lines 2 and 3 in Table 1) shows that the average ion drift characteristics in cold gas are in very good agreement with the results of the accurate solution to the problem within the model of the two-temperature shifted Maxwellian distribution.

However, it is of interest to compare the calculated ion velocity distributions with the Maxwellian distribution. Figures 1 and 2 show the results of calculations of the ion distribution functions over longitudinal and transverse velocities. Solid curves are the Maxwellian distributions (2) at the parameters of distribution (4). To demonstrate the differences in the distribution function body (region of thermal energies) and in tails, the distribution function values are presented on both linear and logarithmic scales.

It turns out that, despite the very good agreement of average characteristics, the distribution functions in the region of thermal energies differ very strongly, and different asymptotic behaviors take place in tails. Discussion of causes of this phenomenon is beyond the scope of this short communication,

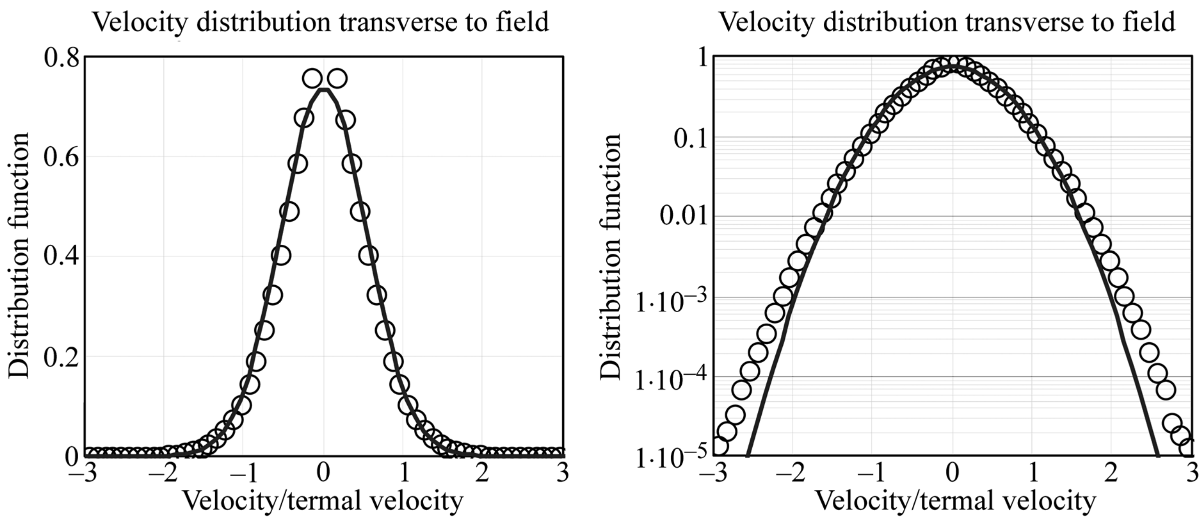

Fig. 2. Ion distribution function over the transverse velocity on linear and logarithmic scales. Solid curves are Maxwellian distributions (2) at the parameters of distribution (4), circles are Monte Carlo calculations.

we only refer to [3—15] where various aspects of the problem of the ion velocity distribution in gas discharges is mentioned. It is an unexpected and surprising result.

Table 2. Results of calculations of the 4-amu ion flux characteristics during the drift in the gas of atoms of the same mass at a temperature of 293 K, density $n_a = 10^{16}$ cm^{-3}, and reduced electric field strength $E/N = 1$ Td. The average ion energies, drift velocities, diffusion coefficients along and across the field, longitudinal and transverse temperatures are given

	$\langle\varepsilon\rangle$, meV	W, m/s	D_l, cm^2/s	D_t, cm^2/s	$T_\parallel$, K	$T_\perp$, K
[2]	42.71	336.8	8.84	8.94	322.0	307.4
Monte Carlo	42.68	336.6	8.63	8.77	321.5	307.5

In [2], the Boltzmann kinetic equation was solved for ions and atoms with a mass of 4 amu at atomic density $n_a = 10^{16}$ cm^{-3}, a temperature of 293 K, and a reduced electric field strength $E/N = 1$ Td. Table 2 lists the average ion drift characteristics [2] and, for comparison, the results calculated in the present work by Monte Carlo simulation. The diffusion coefficient for hard spheres in the first Chapman—Enskog approximation in this case is $D_{C-E} \approx 8.645$ cm^2/s.

As in the previous problem, there is very good agreement between average characteristics (see lines 2 and 3 in Table 2); slightly larger errors in the diffusion coefficient determination are caused by certain features whose consideration is beyond the scope of this short communication, and will be considered elsewhere.

Thus, let us consider the average ion drift characteristics. It seems that the most important characteristic of the ion flux is the average ion kinetic energy, which is related to the effective ion temperature as

$$\langle\varepsilon\rangle = \frac{1}{2}m\langle v^2\rangle = \frac{3}{2}T_{\text{eff}}. \tag{5}$$

Exactly the effective ion temperature of ions should be taken into account when determining macroscopic characteristics of plasma, e.g., the Debye length.

If the average energy of chaotic motion of ions along and across the field are significantly different and the ion velocity distribution function is given in the form of the shifted two-temperature Maxwellian distribution (2), the average energy is written as

$$\langle\varepsilon\rangle = \frac{1}{2}mW^2 + \frac{3}{2}T_i = \frac{1}{2}mW^2 + \frac{1}{2}T_\parallel + T_\perp. \tag{6}$$

Accordingly, the thermal spread of ion velocities is characterized by the temperature $T_i = \frac{1}{3}T_\parallel + \frac{2}{3}T_\perp$ and thermal ion velocity $V_T = (T_i/m)^{1/2}$. In this case, the average ion energy consists of the directional motion energy and thermal energy.

Finally, we draw the following conclusions

(i) The average ion drift characteristics can be determined very accurately (better than 1%) based on the hydrodynamic model with temperatures different in the directions along and across the fields.

(ii) In this case, the ion velocity distribution functions differ significantly from the Gaussian (Maxwellian) distribution not only in the region of thermal energies, but also in tails where the asymptotic behaviors differ from the normal distribution.

(iii) The Mach number defined by the ratio of the drift velocity to the thermal velocity is of the order of unity ($M = W/V_T \approx 1.96$); therefore, the ion flux cannot be strongly supersonic even in cryogenic discharges since the polarization interaction and resonant charge transfer will exist in addition to the interaction considered in the hard sphere model.

(iv) The Townsend energy coefficient defined by the ratio of diffusion and mobility coefficients differs significantly both from the transverse temperature and the longitudinal and effective ones determined by the average ion energy.

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