

Effect of Elastic Collisions on the Ion Distribution Function in Parent Gas Discharge Plasma

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Abstract—An analytical solution is obtained for the Boltzmann kinetic equation for ions in the plasma of its gas with allowance for the processes of resonant charge exchange and elastic ion scattering on the atom. The cross section of differential elastic scattering was assumed to be isotropic in the system of the mass center, and the resonant charge exchange process is independent of the elastic scattering. It is shown that the ion velocity distribution function is determined by two parameters and differs significantly from the Maxwellian one. The allowance for elastic scattering with these assumptions leads to a change in the ion angular distribution and also to a decrease in the average ion energy due to the transfer of part of the ion energy to atoms upon elastic collisions. The calculated values of the drift velocity, the average energy, and the coefficient of transverse diffusion of He⁺ ions in He, Ar⁺ ions in Ar are compared with the known experimental data and the results of Monte Carlo calculations; they show good agreement.

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INTRODUCTION

The study of the ion distribution function (IDF) over velocity is of interest in the study of plasmachemical reactions involving ions, the determination of the mobility ions in a plasma object, the heating of the neutral plasma component, and other cases. The technical applications include modern plasma nanotechnologies, fine-ion cleaning of product surfaces, the technology of selective etching, and the creation of specific reliefs on the surface by ion beam bombardment [1].

The ion drift in direct-current gas discharge plasma has been theoretically studied by a number of authors [2–15], but they are most fully represented in [5–8, 14, 15]. In all of these works, when the IDF was calculated, only the resonant charge exchange was taken into account.

A series of papers considered various aspects of the ion drift in low-pressure capacitive discharge plasma [16–18], ionization in the near-cathode layer of a glow discharge in argon [19], the distribution function of molecular nitrogen ions in a direct-current glow discharge, and the microwave discharge on a mixture of nitrogen with hydrogen [20].

In [21–23], a probe method was developed to measure the electron distribution function in anisotropic plasma with a flat probe, which was modified and successfully applied for IDF measurement in a strong

field in Hg vapors [14] and in an arbitrary field for He⁺ and Ar⁺ ions [24]. It was shown that, in the plasma of inert gases and Hg vapors at low pressures, when there are no processes for the formation of molecular ions with the participation of atomic ions, the IDF for its ions in a wide range of the parameter E/P (where E is the electric field strength and P is the pressure) variation is determined exclusively by resonant charge exchange. The parameters of ion drift (mobility, drift velocity) can be calculated with high accuracy, and elastic collisions can be disregarded.

At the same time, it is known [25, 26] that the elastic scattering cross section of the ion on its own atom at the energies of the relative motion on the order of thermal values for a series of elements is comparable with the cross sections of the resonant charge exchange, and one could expect that elastic scattering will have a certain effect on IDF, even in its gas. In particular, elastic collisions can lead to IDF isotropization. The ion diffusion coefficient across the electric field and the ion mobility were measured experimentally [27–29]. It is well known that, according to these measurements, one can estimate the average energy in the drift direction [30]. In [30–33], the effect of elastic scattering on such characteristics of the IDF as the drift velocity along the field and the mobility, the diffusion coefficients, the average energy along and across the field, etc., was studied by the IDF

decomposition method over time. It was shown that the average ion energy in the plane orthogonal to the direction of the electric field differs significantly from that calculated from the gas temperature and increases with an increase in the parameter E/N , where N is the concentration of neutral atoms). At the same time, with only the process of resonance charge exchange taken into account and without the resulting heating of the gas, the average ion energy in the plane orthogonal to the electric field at any value of the parameter E/N is close to the corresponding value calculated from the gas temperature. It should also be borne in mind that the coefficient of the proportionality between the ratio of the diffusion coefficient to the mobility and the average energy in the direction of drift depends on the form of IDF [30–33], which is determined by the parameter E/N ; at large values, it differs drastically from the Maxwellian parameter [14].

When ion beams are used in the technologies of selective etching and the creation of reliefs on the surface due to ion beam bombardment, IDF over velocities in the plane orthogonal to the direction of the pulling field is of importance, since it determines the spatial resolution of the given technology.

Thus, the goal of this paper is to solve the relevant problem of estimating the effect of elastic collisions of ions with atoms on the form of IDF in gas-discharge plasma in strong and moderate fields.

THEORETICAL STUDY. BASIC RELATIONS

Let us consider the steady-state ion velocity distribution under the following conditions:

- the velocity distribution of gas atoms is Maxwellian;
- the motion of ions occurs in their gas with a low ionization degree;
- the dominant processes forming IDF over velocities are resonant charge exchange and elastic scattering of ions on atoms;
- there are no spatial gradients of the plasma parameters.

The last condition is necessary, since otherwise the coordinates will depend on the IDF.

In steady-state plasma under these assumptions, the Boltzmann equation has the form [3]

$$\frac{e\mathbf{E}}{m}\nabla_v(f_i) = S_i, \quad (1)$$

where e and m are the charge and mass of the ion; \mathbf{E} is the electric field strength; f_i is the IDF over velocities; S_i is the collision integral, which can be divided into two terms S_{ci} and S_{ei} , the first of which corresponds to the charge exchange and the second term is the elastic scattering of the ion on its atom. We consider first the quantity S_{ci} . Considering that the ion arising as a result of the charge exchange has the velocity of the atom, we define the collision integral as follows [14, 15]:

$$S_{ci}(\mathbf{v}_i) = n_a \left\{ f_a(\mathbf{v}_i) \int \sigma_c v_r f_i(\mathbf{v}'_i) d\mathbf{v}'_i - f_i(\mathbf{v}'_i) \int \sigma_c v_r f_a(\mathbf{v}'_a) d\mathbf{v}'_a \right\} \equiv S_{1ci} - S_{2ci},$$

where \mathbf{v}'_i is the velocity of the ion, \mathbf{v}'_a is the velocity of the atom; $f_a(\mathbf{v}'_a)$ is the Maxwellian velocity distribution of atoms (normalized to unity), v_r is the absolute value of the relative velocity of the ion and atom before collision, σ_c is the cross section of the resonant charge exchange; IDF is normalized to the concentration. It is known that the resonant charge exchange cross section σ_c in the energy range of up to several electron volts weakly depends on the relative energy of the ion and atom. In addition, it was shown in [14, 15] how one can obtain the solution of the Boltzmann equation by taking into account such a dependence on IDF with the constant σ_c . Therefore, we first solve the posed problem for the constant section and then formulate the rules for taking into account the dependence of σ_c on the energy of the relative motion of the colliding particles.

It was shown in [15, 34] that the expression for $S_{2ci}(\mathbf{v}_i)$ has the form

$$S_{2ci}(\mathbf{v}_i) = n_a \sigma_c f_i(\mathbf{v}_i) w_{0e}(v_i), \quad (2)$$

$$w_{0e}(v_i) = \left(v_i + \frac{1}{2\beta v_i} \right) \operatorname{erf}(\sqrt{\beta} v_i) + \frac{\exp(-\beta v_i^2)}{\sqrt{\pi\beta}}.$$

Here, $\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2) dt$; $\beta = 1/2kT_a$, $w_{0e}(v_i)$ is the relative velocity of the ion and atom averaged over the distribution function of atoms; k , T_a are the Boltzmann constant and temperature of atoms, respectively. We note that, in limiting cases $\sqrt{\beta} v_i \rightarrow \infty$, $\sqrt{\beta} v_i \rightarrow 0$ for the absolute value of the relative velocity of the ion and atom from (2), we have $\bar{V}_r(v_i) \rightarrow v_i$ and $\bar{V}_i(v_i) \rightarrow 2/\sqrt{\pi\beta}$, respectively. The first of these relations corresponds to the case of the strong field, when the ion velocity before the collision is much higher than the atom thermal velocity; the second is close to the inverse case of the weak field, when the relative velocity of the atom and ion is determined by the average atom thermal velocity.

The following relation holds for $S_{1ci}(\mathbf{v}_i)$ with an accuracy on the order of 10% [15]

$$S_{1ci}(\mathbf{v}_i) = \varphi(v_i) n_a n_i \bar{V}_i \sigma_c f_a(\mathbf{v}_i), \quad \varphi(v_i) = \sqrt{v_i^2 + \bar{V}_i^2}. \quad (3)$$

In (3), \bar{V}_i^2 is the square of the average ion velocity, which depends on the desired distribution function; n_i is the ion concentration. We note that the following condition holds for \bar{V}_i^2

$$\lim_{\alpha_0/\beta \rightarrow \infty} \bar{V}_i^2 = \frac{8kT_a}{\pi m}.$$

We now consider the collision integral S_{ei} corresponding to the elastic scattering of the ion on its atom. It is known that this process is described well by the scattering indicatrix isotropic in the coordinate system of the center of mass in the energy range of up to several tens of electron volts [26, 35, 36]. Collisions with the deviation of the ion by small angles due to the interaction of the ion charge with the induced electric moment of the atom occurring at large impact parameters weakly affect the IDF, since they occur with a small change in the velocity [37], so we will disregard them. In addition, polarization capture can occur at low ion energies [38]. At the same time, the corresponding differential cross section is apparently also close to the isotropic one in the system of the center of mass.

Then, since the atom moves before the collision with the arbitrary velocity \mathbf{v}_a , the probability density $g_e(\mathbf{v}'_i \rightarrow \mathbf{v}_i; \mathbf{v}_a)$ of the fact that an ion having velocity \mathbf{v}'_i will acquire velocity \mathbf{v}_i as a result of collision with the atom can be written in the following form [34]:

$$g_e(\mathbf{v}'_i \rightarrow \mathbf{v}_i; \mathbf{v}_a) = \frac{v_r(v'_i)}{2\pi} \delta\left(\boldsymbol{\xi}\mathbf{v}_a - \frac{\xi^2}{2} - \frac{v_i^2 - v_i'^2}{2}\right),$$

where $\boldsymbol{\xi} = \mathbf{v}_i - \mathbf{v}'_i$, $\xi = |\mathbf{v}_i - \mathbf{v}'_i|$.

For S_{ei} , we have

$$\begin{aligned} & S_{ei}(\mathbf{v}_i, \mathbf{v}_a) \\ &= n_a \int \sigma_e(v_r(v'_i)) v_r(v'_i) g_e(\mathbf{v}'_i \rightarrow \mathbf{v}_i; \mathbf{v}_a) f_a(\mathbf{v}_a) f_i(\mathbf{v}'_i) d\mathbf{v}'_i \quad (4) \\ &- n_a \int \sigma_e(v_r(v_i)) v_r(v_i) g_e(\mathbf{v}_i \rightarrow \mathbf{v}'_i; \mathbf{v}_a) f_a(\mathbf{v}_a) f_i(\mathbf{v}_i) d\mathbf{v}_i. \end{aligned}$$

Integrating (4) over \mathbf{v}_a with account for the weak dependence of the section $\sigma_e(v_r(v'_i))$ on the velocity in comparison with the Maxwellian function [34], we obtain

$$\begin{aligned} \bar{S}_{ei}(\mathbf{v}_i) &= n_a \int \sigma_e(w_{0e}(v_i)) w_e(\mathbf{v}'_i - \mathbf{v}_i) f_i(\mathbf{v}'_i) d\mathbf{v}'_i \\ &- n_a \sigma_e(w_{0e}(v_i)) w_{0e}(v_i) f_i(\mathbf{v}_i), \end{aligned}$$

$$\text{where } w_e(\mathbf{v}'_i - \mathbf{v}_i) = \frac{\beta}{\pi^{1.5}} \frac{\exp\left[-\beta\left(\frac{v_i^2 - v_i'^2}{2\xi} + \frac{\xi}{2}\right)^2\right]}{\xi}.$$

Thus, equation (1) can be written in the form

$$\begin{aligned} & \frac{\partial f_i}{\partial v_{iz}} + 2\alpha_0 w_{0e}(v_i) \left[1 + \frac{\sigma_e(w_{0e}(v_i))}{\sigma_c}\right] f_i \\ &= \mathcal{V}_a(\mathbf{v}_i) \varphi(v_i) + \frac{2\alpha_0}{\sigma_c} \quad (5) \\ &\times \int \sigma_e(w_{0e}(v'_i)) w_e(\mathbf{v}'_i - \mathbf{v}_i) f(\mathbf{v}'_i) d\mathbf{v}'_i, \end{aligned}$$

where $\gamma = 2\alpha_0 n_i$, $2\alpha_0 = \left(\frac{m}{eE}\right) n_a \sigma_c$, $v_{iz} = v_i \mu$, $\mu = \cos \theta$, θ is the angle between the ion velocity and the vector of the axial electric field. It was shown in [14, 15] that, at the approximation of the charge exchange cross section by formula [38]

$$\sigma_c(E_c) = \sigma_{0c} [1 + a \ln(E_c(eV))]^2,$$

where E_c is the energy of the relative motion of the ion and atom, the allowance for the weak dependence of the charge-exchange cross section on the relative velocity of the ion and atom with a sufficient degree of accuracy is reduced to the replacement of the parameter α_0 by $\alpha_0 \kappa(v_i)$, where

$$\kappa(v_i) = \left[1 + a \ln\left(\frac{v_0^2}{w_{0e}(v_i)^2}\right)\right]^2,$$

and the velocity v_0 corresponds to the relative energy of the ion and atom of 1 eV.

In the collision integral, the ionization and electron-ion recombination processes are disregarded, because their characteristic time under these assumptions is large in comparison with the time of the resonant charge exchange.

The elucidation of the effect of elastic collisions on IDF is mainly interesting in medium and strong fields, since this is the situation that is implemented in different plasma technologies. With small fields, the allowance for elastic collisions apparently leads to IDF isotropization and a decrease in the average energy, i.e., the IDF becomes closer to the Maxwellian functions with the atom temperatures. Analysis of the second term on the right-hand side of Eq. (5) leads to the conclusion that the main contribution in these conditions is made by ions, the velocity of which significantly exceeds the average atom velocity. In [15, 24], the IDFs measured by a flat one-sided probe and those calculated without consideration of elastic collisions were compared at moderate fields ($E/P < 20$ V/cm Torr.) It turned out that the calculated and measured IDFs coincide within the measurement error limits estimated by the authors of approximately 10%. The weak effect of elastic collisions on the IDF type at the motion of the ion in its gas is also confirmed by the data of [26, 37]. In this case it is possible to find a solution to Eq. (5) (normalized to unity) by the method of successive approximations

$$f_{ni} = \frac{F_{0i}(x, \mu) + \tilde{F}_{ni}(x, \mu)}{2\pi \int_{-1}^1 [F_0(x, \mu) + \tilde{F}_{ni}(x, \mu)] d\mu dx}, \quad n > 0.$$

As $F_{0i}(\mathbf{v}_i)$ we take the IDF satisfying the equation

$$\begin{aligned} \frac{\partial F_{0i}}{\partial v_{iz}} + 2\alpha_0 w_{0e}(v_i) \left[1 + \frac{\sigma_e(w_{0e}(v_i))}{\sigma_c} \right] F_{0i} \\ = \gamma f_a(\mathbf{v}_i) \Phi(v_i), \end{aligned} \quad (6)$$

and the function \tilde{F}_{ni} at $n \geq 1$ is found as the solution of the following differential equation:

$$\begin{aligned} \frac{\partial \tilde{F}_{ni}}{\partial v_{iz}} + 2\alpha_0 w_{0e}(v_i) \left[1 + \frac{\sigma_e(w_{0e}(v_i))}{\sigma_c} \right] \tilde{F}_{ni} \\ = \frac{2\alpha_0}{\sigma_c} \int \sigma_e(w_{0e}(v_i')) w_e(\mathbf{v}'_i \rightarrow \mathbf{v}_i) \\ \times \sum_{k=0}^{n-1} \tilde{F}_{ki}(\mathbf{v}'_i) d\mathbf{v}'_i. \end{aligned} \quad (7)$$

As can be seen from the following, the first approximation of the above method describes fairly well the exact solution that is in agreement with that noted earlier about the weak effect of elastic collisions on the IDF type in the consideration situation.

The solution of Eq. (6) F_{0i} is taken in the form obtained for the IDF in the case of resonant charge exchange [15] but it takes into account that, on the left-hand side of this equation, the second term, in addition to the resonance charge-exchange cross section, also contains the elastic scattering cross section (see Appendix 1). The solutions of Eqs. (6) and (7) are also given in Appendix 1.

Since, from the point of view of the effect of elastic collisions, we are interested in large values of the parameter E/P , we consider this situation separately. The condition $w_{0e}(v_i) \approx v_{iz}$ is then fulfilled, and $F_{0i}(\mathbf{v}_i)$ is determined by relations [14]

$$\begin{aligned} \tilde{F}_{0i}(\mathbf{v}_i) = A \exp[-\beta v_i^2 + \beta a_-(v_i) v_{iz}^2] \\ \times \operatorname{erfc}(-\sqrt{\beta a_-(v_i)} v_{iz}) \left\{ 1 + O\left(\frac{\alpha_0}{\beta}\right) \right\} \text{ at } v_{iz} \geq 0; \\ \tilde{F}_{0i}(\mathbf{v}_i) = A \exp[-\beta v_i^2 + \beta a_+(v_i) v_{iz}^2] \\ \times \operatorname{erfc}(-\sqrt{\beta a_+(v_i)} v_{iz}) \left\{ 1 + O\left(\frac{\alpha_0}{\beta}\right) \right\} \text{ at } v_{iz} \leq 0; \end{aligned} \quad (8)$$

where $A = \frac{\gamma \beta \bar{V}_i}{2\pi}$ is the constant factor and \bar{V}_i is the average ion velocity, $a_-(v_i) = 1 - \varepsilon_0 \left[1 + \frac{\sigma_e(w_{0e}(v_i))}{\sigma_c} \right] > 0$,

$$a_+(v_i) = 1 + \varepsilon_0 \left[1 + \frac{\sigma_e(w_{0e}(v_i))}{\sigma_c} \right], \operatorname{erfc}(x) = 1 - \operatorname{erf}(x).$$

In addition, in the strong-field approximation, the expression for functions $w_e(\mathbf{v}'_i \rightarrow \mathbf{v}_i)$ is [34]

$$w_e(\mathbf{v}'_i \rightarrow \mathbf{v}_i) = \frac{1}{\pi v_i v_i'^2} \delta\left(\mu_0 - \frac{v_i}{v_i'}\right), \quad (9)$$

where the cosine of the scattering angle is

$$\mu_0(\mu, \eta, \varphi) = \frac{(\mathbf{v}_i, \mathbf{v}'_i)}{v_i v_i'} = \mu \eta + \sqrt{1 - \mu^2} \sqrt{1 - \eta^2} \cos(\varphi),$$

φ is the difference of azimuthal angles of vectors $\mathbf{v}_i, \mathbf{v}'_i$ and μ, η are cosines of polar angles of velocities $\mathbf{v}_i, \mathbf{v}'_i$, respectively.

One can then obtain the solutions of Eqs. (6) and (7) in a simpler form (see Appendix 1).

In the conclusion of this part of the paper, we obtain formulas for calculation of the ion diffusion coefficient in the plane orthogonal to the electric field in the plasma D_{ir} . This value is largely determined by the elastic collisions of ions with atoms, and there are presently extensive arrays of experimental data, including those in inert gases [27–29]. Under conditions in which the ion collision frequency does not depend on its velocity or in which the IDF is the Maxwellian, the Einstein relation $eD_{ir}/K = kT_{ir}$, where T_{ir} is the ion temperature in the plane XY and K is the mobility of ions, holds. In the general case, the inequality $eD_{ir}/K \leq T_{ir}$ occurs [32, 33].

To find the diffusion coefficient D_{ir} , one can apply the described method (e.g., in [39, 40]). We consider the situation in which there is a small ion concentration gradient in steady-state plasma. We represent the IDF in the form of the expansion

$$f_i(\mathbf{r}, \mathbf{v}) = \sum_{j=0}^{\infty} \mathbf{f}^{(j)}(\mathbf{v}) \left(-\frac{\partial}{\partial \bar{r}}\right)^j n(\mathbf{r}),$$

where $f^{(0)}(\mathbf{v})$ is a scalar and $\mathbf{f}^{(j)}(\mathbf{v})$ at $j > 0$ are vectors.

The function $f^{(0)}(\mathbf{v})$ is normalized to unity, and $\mathbf{f}^{(1)}(\mathbf{v})$ has the dimension s^3/m^2 . Substituting this expansion into the Boltzmann equation, we obtain the equations for the first two coefficients $f^{(0)}(\mathbf{v})$ and $\mathbf{f}^{(1)}(\mathbf{v})$ [40]:

$$\begin{aligned} \left(\frac{eE}{m} \frac{\partial}{\partial v_{iz}} + \hat{S}_i\right) f^{(0)}(\mathbf{v}) = 0, \\ \left(\frac{eE}{m} \frac{\partial}{\partial v_{iz}} + \hat{S}_i\right) \mathbf{f}^{(1)}(\mathbf{v}) = (\mathbf{v} - \mathbf{v}_d) f^{(0)}(\mathbf{v}), \end{aligned} \quad (10)$$

where \hat{S}_i is the operator of the collision integral and $\hat{S}_i \mathbf{f}^{(j)}(\mathbf{v}) = \mathcal{S}_i$.

The diffusion coefficient D_{or} is expressed by the relation [39]

$$D_{ir} = \int v_x \mathbf{f}^{(1)}(\mathbf{v}) d\mathbf{v} = \int v_y \mathbf{f}^{(1)}(\mathbf{v}) d\mathbf{v}. \quad (11)$$

As the solution of the first of Eqs. (10), we can take the function $f_{ni}(\mathbf{v})$. The solution of the second equation (10) for the most interesting case of the strong field is given Appendix 2. If we disregard the elastic scattering of ions on atoms, then, in the limiting case of the strong field (at $\varepsilon_0 \rightarrow 0$), the following relation is

obtained from formulas (10) and (11) with allowance for formula (14) from Appendix 2

$$D_{ir} = \lambda_c \sqrt{\frac{2kT_a \epsilon_0}{\pi m}} [1 + O(\epsilon_0)] \approx kT_a \sqrt{\frac{2\lambda_c}{\pi m e E}},$$

which coincides with the result given in [40] for the case of the resonant charge exchange of an ion on its own atom.

Thus, a solution of the equation for IDF in its gas that takes into account elastic scattering ions on atoms is obtained, as are the relations for calculation of the quantities characterizing the motion of the ion in its gas with allowance for elastic collisions.

DISCUSSION OF RESULTS AND COMPARISON WITH DATA OF OTHER AUTHORS

We note that the obtained formulas for IDF at $\sigma_e(v_i) \rightarrow 0$ coincide identically with the corresponding expressions [14, 15], where only the resonance charge exchange process was taken into account. Calculations according to the obtained formulas were carried out for Ar^+ in Ar and He^+ in He, since namely for these ions it was possible to find reliable data on the elastic scattering cross sections of ions on their atoms [25, 26, 41]. Data on the resonance charge exchange cross sections of Ar^+ in Ar were taken from [26, 42, 43], and those for He^+ in He are from [42, 43]. Note that the sections from the last two works differ slightly for Ar^+ in Ar and for He^+ in He, while the cross section of resonant charge exchange given in [26] for Ar^+ in Ar is noticeably lower. This leads to a significant difference in the dependences of the ratio of the elastic scattering cross section of the ion on the atom to the resonant charge exchange cross section on the relative energy of ion and atom for Ar^+ in Ar calculated from data [42, 43] and [26], particularly in the low-energy region (Fig. 1). As seen below, the ion energy distribution function values calculated from these sections differ markedly.

To verify the obtained formulas, the following calculated motion characteristics were compared with experimental data and the results of numerical simulation: plasma ions, the drift velocity; the average energy; and the ratio of the diffusion coefficient in the plane orthogonal to the electric field vector to the ion mobility. Figures 2 and 3 show such a comparison for the drift velocity of Ar^+ in Ar and for He^+ in He in a wide range of parameter E/N values with data from [44–46] and [44, 38, 46, 47], respectively. It can be seen that the experimental and calculated values of the drift velocity are in good agreement. Figures 4 and 5 show the comparison of the calculated dependence of the average ion energy on the parameter E/N for Ar^+ in Ar and for He^+ in He, respectively, with the results of the numerical Monte Carlo simulation [47, 26]. Analytical and numerical computations coincide sat-

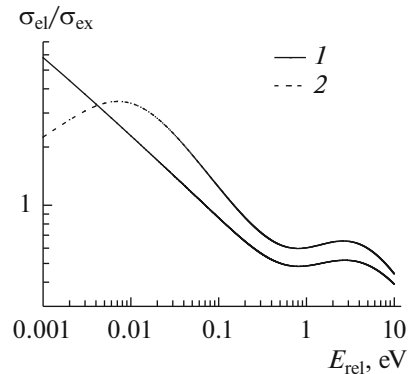


Fig. 1. Dependence of the ratio of total cross sections σ_{el} and of resonance charge exchange σ_{ex} for Ar^+ in Ar with the use of data on the elastic scattering cross-section from [26], and the resonance charge exchange cross-section from [43] (1) and [26] (2).

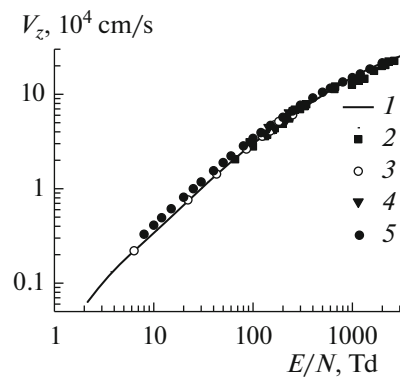


Fig. 2. Comparison of the experimental data on the drift velocity of Ar^+ in Ar with calculations by the elaborated theory: (1) calculations of the authors; (2, 5) experiment [44, 46], respectively; (3, 4) experiment on the determination of mobility [38, 45].

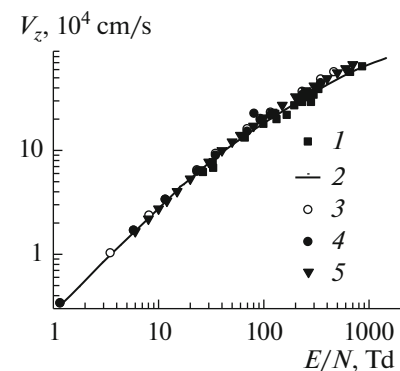


Fig. 3. Comparison of the experimental data on the drift velocity of He^+ in He with calculations by the elaborated theory: (1, 5) experiment [44, 47]; (2) calculations by the authors; (3, 4) calculation and measurement of the mobility [48], respectively.

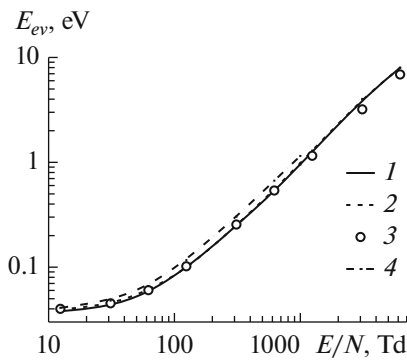


Fig. 4. Dependence of the average energy of the Ar^+ ion in Ar on parameter E/N at $T_a = 300$ K: (1) calculation by analytical formulas with allowance for elastic collisions [26], (2) disregarding elastic collisions [43], (3) Monte Carlo calculation by the authors with allowance for elastic collisions, (4) calculation according to [26].

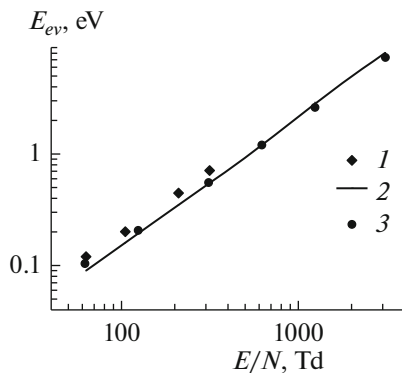


Fig. 5. Calculations of dependence with allowance for elastic collisions of the average energy of the He^+ ion in He on parameter E/N at $T_a = 300$ K: (1) Monte Carlo method according to data [26], (2) according to the elaborated theory with cross sections from [41, 43], (3) Monte Carlo calculation by the authors.

isfactorily. The average energy of the Ar^+ ion calculated in this work is somewhat lower (by 10–15%) than that obtained by numerical simulation [26], although the course of curves coincides. Analogous features of the difference of the average He^+ ion energy are also seen in Fig. 5, where calculations by analytical formulas are compared with numerical data [47]. The difference from the case of Ar^+ is that the same sections of resonant charge exchange and elastic scattering for argon were used in the numerical and analytical calculations [26], but the author [47] took sections from his own calculations for helium. In this work, the resonance charge exchange cross sections are taken from [43], and those for elastic scattering are from an experimental work [41]. This may have led to differences in the calculations of the average He^+ ion energy.

Figures 6 and 7 show a comparison of the quantity eD_{tr}/K with experimental data [28, 29, 48], numerical

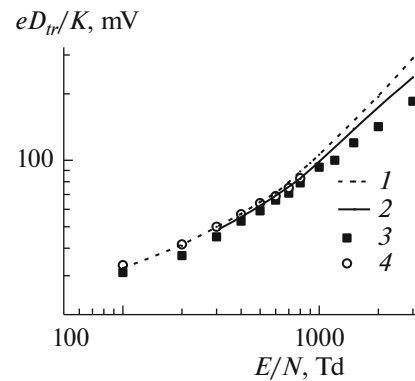


Fig. 6. Dependence of the ratio eD_{tr}/K for Ar^+ in Ar on the parameter E/N at $T_a = 294$ K: (1) Monte Carlo calculation according to data [26]; (2) calculation according to the given theory with cross sections from [26]; (3, 4) experiments [28, 48], respectively.

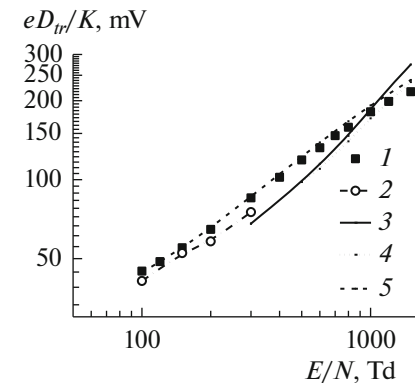


Fig. 7. Dependence of the ratio eD_{tr}/K for He^+ in He on the parameter E/N at $T_a = 294$ K: (1) experiment [29]; (2) Monte Carlo calculation according to [26]; 3—calculation according to the elaborated theory with cross sections from [41, 43]; (4) with the elastic scattering cross section reduced by 1.5 times; (5) calculation by the method of momenta [49].

Monte Carlo calculations [47, 26] and momenta method [49] for cases Ar^+ in Ar and for He^+ in He. As already noted, the most interesting is the effect of elastic collisions on IDF at large fields, and the formula (14) was applied in calculations in this work (see Appendix 2), which, in the considered cases, Ar^+ in Ar and for He^+ in He, holds at $E/N > 200$ – 300 Td. It is seen from the data in Fig. 6 that the authors' calculations correlate well with the Monte Carlo calculations [26] and experimental data [48]. At the same time, both curves in the region of large values of the parameter E/N lie above the experimental points [28]. In the authors' opinion, this may indicate a certain inadequacy of the used expression for the energy dependence of the relative motion of the elastic scattering cross section of the Ar^+ ion on the Ar atom taken in both calculations from [26]. As for the data in Fig. 7, the authors unfortunately did not find Monte Carlo

calculations of the quantity eD_{tr}/K for He^+ in He at $E/N > 300$ Td. However, it can be seen that numerical and analytical calculations yield an underestimated result as compared with experiments.

Let us now turn to the IDF calculations. They show that the ion energy distribution function upon inclusion with consideration of elastic collisions becomes less high-energy (Fig. 8), although the differences between both IDFs are small. Thus, at the same normalization of both functions (without elastic collisions and with allowance for with them) in the low-energy region, the IDF becomes higher, and it becomes lower in the high-energy region. These features are true at any value of the parameter ϵ_0 , since the IDF is Maxwellian with the atom temperature in the absence of the field, and the presence of the electric field only increases the average ion energy, such that it always exceeds the atom temperature. Thus, the energy flux upon elastic collisions of the ion with the atom is directed toward the atoms: the atoms are heated, and the ions are cooled. In addition, it can be noted that the IDF difference calculated with allowance for elastic collisions and without them increases with a decrease in ion energy. This is obviously related to the fact that the cross section of elastic collisions falls relatively rapidly upon an increase in the relative energy of the colliding particles. However, at a decrease in the electric field, this difference will also decrease starting with some value, since the IDF is close to Maxwellian in the absence of the field, regardless of the allowance for the elastic collisions.

Let us consider how the IDF changes along the motion directions at $\epsilon_0 < 1$ (this, as already mentioned, is the most interesting situation, which corresponds to moderate and strong fields). It is seen from the data in Fig. 9, which shows calculations for Ar^+ in Ar at $E/P = 200$ V/cm Torr for the ion energy $\epsilon = 0.03$ eV, that the IDF at low energies becomes more elongated upon the inclusion of elastic collisions, and it is less elongated in the direction of the field at high energies (much higher than the average atomic thermal energy). Moreover, it follows from the same data that at the deviations low energies are maximal at ion motion along the field. With an increase of the angle between the vector of the electric field and the ion velocity, the IDF difference rapidly falls; at an angle on the order of 35° – 40° , it is almost invisible. Let us consider the physical origin of this IDF behavior.

In the absence of elastic collisions in strong and moderate fields, the IDF is strongly elongated at high energies (on the order of several electron volts) and weakly anisotropic at energies in the region of the IDF maximum [14, 15, 24] (i.e., at the thermal energies of the atoms). The latter is due to the fact that this group is formed by ions that were just born as a result of resonance charge exchange and did not have time to accelerate in the electric field. With allowance for elastic collisions, the angular distribution of ions at low

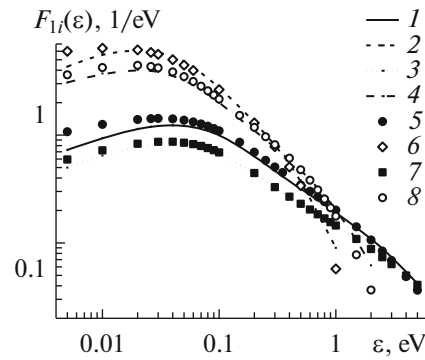


Fig. 8. Ion energy distribution function for Ar^+ in Ar and He^+ in He for different gas temperatures and values of parameter E/P calculated without elastic collisions of ions with atoms (1–4) and with allowance for them (5–8): cross sections of resonant charge exchange from [42], cross section of the elastic scattering for Ar^+ from [26], for He^+ from [41]; (1, 5) He, $T_a = 600$ K, $\frac{E}{P} = 200 \frac{\text{V}}{\text{cm Torr}}$; (2, 6) Ar, 300, 100; (3, 7) He, 600, 400; (4, 8) Ar, 300, 200.

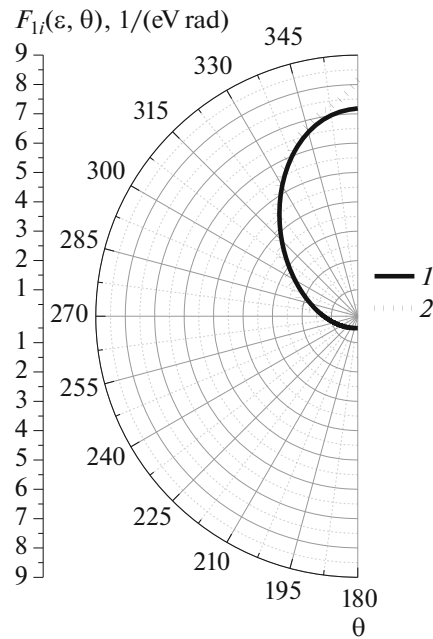


Fig. 9. IDF of Ar^+ ions in Ar over the motion directions at the ion energy $\epsilon = 0.03$ eV, $E/P = 200 \frac{\text{V}}{\text{cm Torr}}$, $T_a = 300$ K calculated without elastic collisions of ions with atoms (1) and with allowance for them (2).

energies is formed first by the creation of slow ions at charge exchange (which has a weak anisotropy) and, second, due to the energy relaxation of ions at elastic collisions. Since the losses of the energy are significant in collisions with their own atoms (the mass ratio is equal to unity), ions quickly relax over the energy (upon a shock close to the central one, the ion loses almost all energy and becomes thermal). As a result,

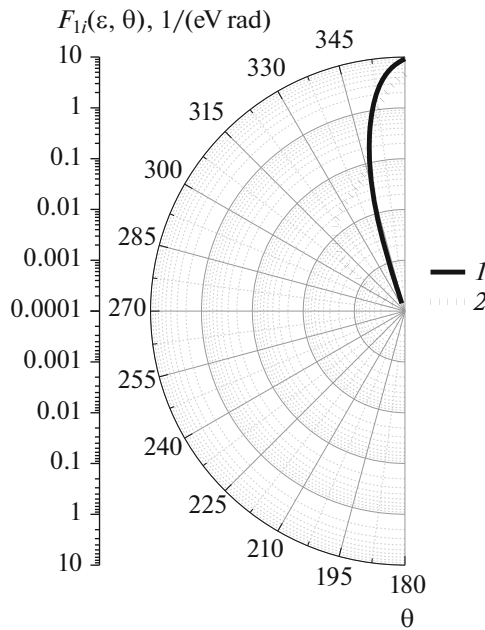


Fig. 10. IDF of Ar^+ ions in Ar over the motion directions at $\epsilon = 2$ eV, $E/P = 200 \frac{\text{V}}{\text{cm}}$ Torr, $T_a = 300$ K: (1, 2) the same as in Fig. 9.

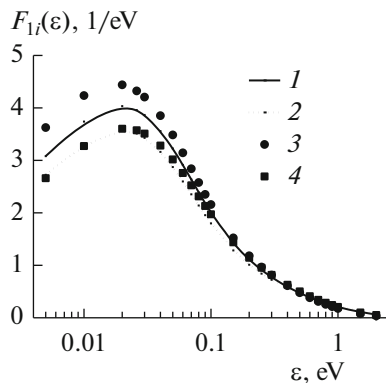


Fig. 11. Comparison of the IDF of Ar^+ in Ar calculated from different cross sections of resonant charge exchange at $E/P = 200 \frac{\text{V}}{\text{cm}}$ Torr; $T_a = 300$ K: (1, 2) disregarding elastic collisions; (3, 4) with allowance for them; cross sections of resonant charge exchange from [42] (1), [26] (2, 4) and [43] (3).

their angular distribution is less elongated than that before the collision (when they had much higher energy) but remains more elongated than that of those of the ions at the low energy. If we consider the angular distribution of ions at high energies, then this effect of energy relaxation is less pronounced, since, as can be seen from data in Fig. 2, the elastic scattering cross section rapidly (in comparison with the cross section of the resonance charge exchange) decreases with an increase in the relative energy of the ion and the atom. At relatively high energies, the IDF isotropization effect is dominated by elastic collisions, since the

arrival of ions with a more anisotropic distribution due to energy relaxation is inhibited by a rapid decrease in the cross section of elastic scattering with an increase in ion energy. This is confirmed by the data in Fig. 10, which shows the IDF for Ar^+ in Ar at $E/P = 200 \text{ V/cm Torr}$ for ion energy $\epsilon = 2$ eV. The same figure shows that, at large angles (larger than 45°) between the direction of the electric field and the ion velocity, the IDF calculated with elastic collisions exceeds the IDF without them. This is also a consequence of the isotropization at elastic collisions; however, this excess is insignificant (the data scale in Fig. 10 is logarithmic). Thus, a more elongated ion distribution along the direction of the motion at low energies is formed and less elongated at high ones.

Finally, the data given in Fig. 11 illustrate the effect of the charge exchange cross section on the IDF type. Here, we present functions of the Ar^+ ions in Ar calculated with elastic collisions and without them for sections of resonant charge exchange taken from [26, 42, 43]. It is seen that the IDF, which was calculated with the cross section from [26], is higher energy one. This is obviously connected with the fact that this cross section is smaller than the analogous ones given in [42, 43] (which are close), and, hence, the ion energy, which it receives by accelerating in the electric field, is higher.

CONCLUSIONS

An analytical theory has been developed for calculation of the total IDF in its own gas with allowance for processes of resonant charge exchange and elastic collisions of ions with atoms. The theory describes well the known experimental data on the drift of ions in the plasma of inert gases. The calculations based on the obtained formulas at different values of the parameter E/N of such quantities as the average ion energy and the ratio of the diffusion coefficient in the plane orthogonal to the field to the mobility are in agreement with data of the numerical Monte Carlo simulation.

The energy dependences of the IDF for Ar^+ in Ar and He^+ in He were calculated, and a series of features was revealed. Namely, in comparison with the IDF without elastic collisions, this function is less high-energy due to losses of the energy upon the elastic collisions of ions with atoms, although the IDF differences are small.

An analysis of IDF changes along the directions of motion at large fields was carried out:

- at low energies comparable with the thermal energy, the energy distribution becomes less isotropic due to the fast relaxation of ions from the region, where the distribution over the directions is strongly elongated in the direction of the field;
- at high energies, on the contrary, the IDF over directions with allowance for elastic scattering becomes less elongated, since the effect of the energy relaxation

decreases due to the relatively fast decrease in the elastic scattering cross section with an increase in ion energy.

APPENDIX 1

To solve Eqs. (6) and (7), we use the method proposed in [15]. Passing to the dimensionless variable $x = v_i \sqrt{\beta}$, with allowance for the dependence of the parameter α_0 on the ion energy (see above), we can obtain

$$\begin{aligned}
 F_{0i}(x, \mu \geq 0) &= \exp[-x^2(1 - \mu^2) - 2\varepsilon_{el}(x)\eta(x, \mu)] \\
 &\times \int_0^\infty \exp[-y^2 - 2\varepsilon_{el}(x, y, \mu)\eta_1(x, y, \mu)] \bar{\varphi}(y, x, \mu) dy \\
 &\quad + \exp[-x^2(1 - \mu^2) - 2\varepsilon_{el}(x)\eta(x, \mu)] x^2 \\
 &\times \int_0^{x\mu} \exp[-y^2 + 2\varepsilon_{el}(x, y, \mu)\eta_1(x, y, \mu)] \bar{\varphi}(y, x, \mu) dy, \\
 F_{0i}(x, \mu < 0) &= \exp[-x^2(1 - \mu^2) - 2\varepsilon_{el}(x)\eta(x, \mu)] \\
 &\times \int_{-x\mu}^\infty \exp[-y^2 - 2\varepsilon_{el}(x, y, \mu)\eta_1(x, y, \mu)] \bar{\varphi}(y, x, \mu) dy,
 \end{aligned}$$

where

$$\begin{aligned}
 \eta(x, \mu) &= \int_0^{x\mu} \{ [y^2 + x^2(1 - \mu^2)]^{0.5} \\
 &\quad + \frac{2}{\sqrt{\pi}} \exp[-\sqrt{y^2 + x^2(1 - \mu^2)}] \\
 &\quad \times [1 + 0.5[y^2 + x^2(1 - \mu^2)]^{1.25}] dy, \\
 \eta_1(x, y, \mu) &= \int_0^y \{ [z^2 + x^2(1 - \mu^2)]^{0.5} \\
 &\quad + \frac{2}{\sqrt{\pi}} \exp[-\sqrt{z^2 + x^2(1 - \mu^2)}] \\
 &\quad \times [1 + 0.5[z^2 + x^2(1 - \mu^2)]^{1.25}] dz, \\
 \bar{\varphi}(x, y, \mu) &= \frac{\sqrt{y^2 + x^2(1 - \mu^2)} + \beta \bar{V}_i^2}{\sqrt{\beta}}, \\
 \varepsilon_{el}(x) &= \varepsilon_0(x) \left[1 + \frac{\sigma_e(w_{0e}(x))}{\sigma_c(w_{0e}(x))} \right], \\
 \varepsilon_{el}(x, y, \mu) &= \varepsilon_0(\sqrt{x^2(1 - \mu^2) + y^2}) \\
 &\times \left[1 + \frac{\sigma_e(w_{0e}(\sqrt{x^2(1 - \mu^2) + y^2}))}{\sigma_c(w_{0e}(\sqrt{x^2(1 - \mu^2) + y^2}))} \right], \quad \varepsilon_0(x) = \frac{\alpha_0 \kappa(x)}{\beta}. \\
 F_{ni}(x, \mu \geq 0) &= \exp[-2\varepsilon_{el}(x)\eta(x, \mu)] \\
 &\times \int_0^\infty \exp[-2\varepsilon_{el}(x, y, \mu)\eta_1(x, y, \mu)] \Phi_{n-1}(x, y, \mu) dy \\
 &\quad + \exp[-2\varepsilon_{el}(x)\eta(x, \mu)] \\
 &\times \int_0^{x\mu} \exp[2\varepsilon_{el}(x, y, \mu)\eta_1(x, y, \mu)] \Phi_{n-1}(x, y, \mu) dy;
 \end{aligned}$$

$$F_{ni}(x, \mu < 0) = \exp[-2\varepsilon_{el}(x)\eta(x, \mu)]$$

$$\times \int_{-x\mu}^\infty \exp[-2\varepsilon_{el}(x, y, \mu)\eta_1(x, y, \mu)] \Phi_{n-1}(x, y, \mu) dy,$$

where

$$\begin{aligned}
 \Phi_{n-1}(x, y, \mu) &= 2\varepsilon_{el}(x, y, \mu) \\
 &\times \iiint \sigma_e(w_{0e}(z)) w_{el}(\sqrt{y^2 + x^2(1 - \mu^2)}, z, \mu, \eta, \varphi) \\
 &\quad \times \sum_{k=0}^{n-1} \tilde{F}_{k-li}(z, \eta) dz d\eta d\varphi, \\
 &\quad w_{el}(x, z, \mu, \eta, \varphi) \\
 &= \frac{\beta^{3/2} \exp \left[- \left\{ \frac{x^2 - z^2}{2S(x, z, \mu, \eta, \varphi)} + \frac{S(x, z, \mu, \eta, \varphi)}{2} \right\}^2 \right]}{\pi^{1.5} S(x, z, \mu, \eta, \varphi)}, \\
 &\quad S(x, z, \mu, \eta, \varphi) \\
 &= \sqrt{x^2 + z^2 - 2xz[\mu\eta - \sqrt{1 - \mu^2}\sqrt{1 - \eta^2} \cos(\varphi)]}.
 \end{aligned}$$

In the case of the strong field, when $\bar{V}_r(v_i) \approx v_{iz}$ and $\sqrt{\varepsilon_0} \ll 1$, and relations (8) and (9) are satisfied for $F_{0i}(x, \mu)$ and $w_e(\mathbf{v}'_i \rightarrow \mathbf{v}_i)$, respectively, we have

$$\begin{aligned}
 \Phi_{n-1}(x, y, \mu) &= \frac{2}{\pi} \varepsilon_{el}(x, y, \mu) x \\
 &\times \int_{-1}^1 \int_0^{2\pi} \sigma_e \left(w_{0e} \left(\frac{\sqrt{y^2 + x^2(1 - \mu^2)}}{\mu_0(\mu, \eta, \varphi)} \right) \right) \\
 &\quad \times \sum_{k=1}^{n-1} \tilde{f}_{n-li} \left(\frac{\sqrt{y^2 + x^2(1 - \mu^2)}}{\mu_0(\mu, \eta, \varphi)}, \eta \right) \\
 &\quad \times \frac{d\varphi d\eta}{\mu_0(\mu, \eta, \varphi)^3} \\
 \eta(x, \mu) &= 0.5x^2\mu^2, \quad \eta(x, y, \mu) = 0.5y^2\mu^2.
 \end{aligned} \tag{12}$$

APPENDIX 2

As before, we first consider the case of constant charge-exchange cross sections, and then, to account for this dependence, we use the rule formulated above.

We write the projection of the second of equations (10) on the x (or y) axis:

$$\left(\frac{eE}{m} \frac{\partial}{\partial v_z} + S_i \right) f_x^{(1)}(\mathbf{v}) = v_x f^{(0)}(\mathbf{v}).$$

We introduce the dimensionless ion velocity $\mathbf{w} = \sqrt{\beta} \mathbf{v}_i$, multiply the equation by v_x , and integrate over v_x . Taking into account that, in the strong field $w_z \gg w_x, w_y$ and after integration over w_x the terms in the collision integral corresponding to the ion arrival in the phase space element as a result of charge exchange and elastic scattering vanishes, since the atom velocity distribution function and the indicatrix of elastic scattering are even functions of w_x , we obtain

$$\begin{aligned} \frac{\partial \tilde{\Psi}(w_z)}{\partial w_z} + 2\varepsilon_0 \left[1 + \frac{\sigma_e(w_{0e}(w_z))}{\sigma_c} \right] w_z \tilde{\Psi}(w_z) \\ = 2\varepsilon_0 \lambda_c \sqrt{\beta} \tilde{\Phi}(w_z), \end{aligned} \quad (13)$$

where $\lambda_c = 1/n_a \sigma_c$ is the ion run length before charge exchange, the parameter ε_0 is determined above,

$$\begin{aligned} \tilde{\Psi}(w_z) = \Psi(v_{iz} \sqrt{\beta}), \quad \Psi(v_{iz}) = \int \int_{-\infty}^{\infty} v_x f_x^{(1)}(\mathbf{v}) dv_x dv_y, \\ \tilde{\Phi}(w_z) = \Phi(v_{iz} \sqrt{\beta}), \quad \Phi(v_{iz}) = \int \int_{-\infty}^{\infty} v_x^2 f^{(0)}(\mathbf{v}) dv_x dv_y. \end{aligned}$$

Equation (13) has the solution satisfying zero conditions at $|w_z| \rightarrow \infty$:

$$\begin{aligned} \Psi_+(w_z \geq 0) = 2\varepsilon_0 \lambda_c \sqrt{\beta} \exp[-\varepsilon_0 \omega(w_z)] \\ \times \left[\int_0^{\infty} \exp[-\varepsilon_0 \omega(y)] \Phi(-y) dy \right. \\ \left. + \int_0^{w_z} \exp[\varepsilon_0 \omega(y)] \Phi(-y) dy \right], \quad (14) \\ \Psi_-(w_z < 0) = 2\varepsilon_0 \lambda_c \sqrt{\beta} \exp[\varepsilon_0 \omega(w_z)] \\ \times \int_{|w_z|}^{\infty} \exp[-\varepsilon_0 \omega(y)] \Phi(y) dy, \end{aligned}$$

where $\omega(w_z) = \int_0^{w_z} \left[1 + \frac{\sigma_e(w_{0e}(y))}{\sigma_c} \right] dy$. We recall that, during the derivation $\Phi(v_{iz})$ one should take the solution f_{ni} as $f^{(0)}$ using formulas (8) and (12) for the case of the strong field.

The dependence of the cross section of the resonant charge exchange on the energy of the relative motion of the ion and atom is taken into account by substituting the parameter ε_0 for the function $\varepsilon_0 \kappa(v_i)$ and the substitution of the cross section σ_c for $\sigma_c \kappa(y)$ under the integral sign in the formula for $\omega(w_z)$.

Using the well-known formula for the drift velocity of ions in their own gas at high fields [38] and the determination of mobility, one can obtain from (14) with allowance for the dependence of charge exchange and elastic scattering cross sections on the relative velocity of the colliding particles,

$$\begin{aligned} \frac{eD_{or}}{K} = \pi \kappa(w_{ev}) \int_0^{\infty} \exp[\varepsilon_0 \omega(y)] \\ \times \operatorname{erfc}(\sqrt{\varepsilon_0 \omega(y)}) \Phi(y) dy, \end{aligned}$$

where w_{ev} is the average dimensionless ion velocity. In the derivation of this relation, it is also taken into account that, in the presence of elastic collisions, the formula for the drift velocity in the strong field is

transformed corresponding to the increase in the total collision cross section of the ion with the atom.

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