Calculation of the Drift Velocity of Ions in the Electric Field in Their Gas

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(Submitted to JEPT editor February 6, 1956)
J. Exptl. Theoret. Phys. (U.S.S.R) **32**, 526-533 (March, 1957)

On the basis of the "pure overcharge" model proposed by L. A. Sena, the drift velocity of ions moving in the respective gas under the influence of an electric field is calculated as a function of the ratio of the work done by the field over the length of a free path to the mean thermal energy of the atoms. The results of the calculations are in good agreement with the experimental data for inert gases.

1. STATEMENT OF THE PROBLEM. THE KINETIC EQUATION

THE problem of the motion of positive ions in a gas is divided into two main parts. The first part consists of the determination of the differential effective cross-section for collision of an ion with an atom and must be solved by the methods of quantum mechanics. The differential effective cross-section of collision being know, the second part consists in determining the velocity distribution function for the ions and mean values, of which the most important is the drift velocity of the ions in the direction of the electric field.

At the present time, it can be considered established that the chief process of interaction with neutral atoms in the motion of positive atomic ions in the respective gas is resonance overcharge [1-6].

Calculations of the drift velocity of ions moving in a gas of the same nature under the influence of a constant homogeneous electric field, based on the model of pure overcharge proposed by Sena, give values which agree well with experimental data [1,4,5]. These calculations, however, were carried out strictly only for two limiting cases: for the case of a strong electric field, when it is possible to neglect the thermal motion of atoms of the gas[4], and for the case of a weak electric field, when the energy acquired by an ion over the length of a free path under the action of the field is much smaller than the mean energy of thermal motion of a neutral atom[5]. The results obtained in Ref. 4 for intermediate cases are based on the replacement of the real velocity distribution of the atoms by two opposite fluxes. The possibility of such a consideration requires substantiation. Furthermore, the velocity of the two fluxes remains undetermined, their being know only that it must be of the order of the mean velocity of the gas atoms.

In the present work, a method of successive approximations is put forward which permits one to solve the second kinetic part of the problem on the drift velocity of ions, on the basis of the model of "pure overcharge", for any ratio of the work done by the field over the length of a free path of an ion to the mean thermal energy of the atoms of the gas.

In the calculation, the concentration of charged particles is assumed so small that their interaction with one another and also the effect of their motion on the velocity distribution function of the atoms can be disregarded.

The calculation is carried out under the assumption that the effective cross section of overcharge does not depend on velocity, however the proposed method of successive approximations is applicable also in the case where the cross section can not be considered constant.

The kinetic equation for the velocity distribution function of ions moving in the respective gas under the influence of a constant electric field E under the assumptions indicated above, has the form[4]:

$$a\lambda \frac{\partial f}{\partial v_z} = n(v) \int f(\mathbf{v}') |\mathbf{v} - \mathbf{v}'| d\mathbf{v}' - f(\mathbf{v}) \int n(v') |\mathbf{v} - \mathbf{v}'| d\mathbf{v}', \quad (1)$$

where $a = eE/m$ is the acceleration of an ion in the electric field, e and m are the charge and mass of an ion, $\lambda = 1/Nq$ its mean free path, N the concentration of gas atoms, q the effective cross section of overcharge, $f(\mathbf{v})$ the velocity distribution function of the ions, $n(v)$ the velocity distribution function of the neutral atoms and $d\mathbf{v}' = dv_x' dv_y' dv_z'$. The direction of the field is taken along the direction of the

axis OZ*. We introduce the notation

$$u_0 = \sqrt{2kT/m}, \quad \gamma = \pi e E \lambda / 4kT,$$

u_0 is the most probable speed for atoms of the gas and the dimensionless quantity γ characterizes the ratio of the work done by the field over a free path length of an ion to the mean thermal energy of the atoms.

Taking account of the cylindrical symmetry of the problem, we introduce cylindrical coordinates in velocity space and transform to dimensionless variables:

$$z = v_z/u_0, \quad \rho = \sqrt{v_x^2 + v_y^2}/u_0; \tag{2}$$

$\varphi$is the angle which the projection of the velocity on the plane XOY makes with the axis OX. Then for the velocity distribution function of the atoms we obtain

$$n(v)\, dv_x\, dv_y\, dv_z = W_1(z)\, W_2(\rho^2)\, dz\, d\rho^2\, d\varphi/2\pi, \tag{3}$$

$$W_1(z) = \pi^{-1/2} e^{-z^2}; \quad W_2(\rho^2) = e^{-\rho^2}. \tag{4}$$

Considering Eq. (1) as a non-homogeneous differential equation it is easy to obtain.

$$f(\rho, z) = 2W_2(\rho^2) \int_{-\infty}^{z} W_1(u)\, F(\rho, u)\, G(\rho, u, z)\, du,$$

$$f(\rho, z)\, \rho\, d\rho\, dz\, d\varphi = f(\mathrm{v})\, dv_x\, dv_y\, dv_z, \tag{5}$$

$$G(\rho, u, z) = \frac{1}{\gamma} \exp\left[-\frac{1}{\gamma}\int_u^z F_0(\rho, u')\, du'\right], \tag{6}$$

$$F(\rho, z) = \iint f(\rho', z')\, g(\rho', \rho, z - z')\, \rho'\, d\rho'\, dz', \tag{7}$$

$$F_0(\rho, z) = \iint 2W_2(\rho'^2)\, W_1(z')\, g(\rho', \rho, z - z')\, \rho'\, d\rho'\, dz', \tag{8}$$

$$g(\rho', \rho, t) = \frac{1}{4}\int_0^{2\pi} \sqrt{\rho^2 - 2\rho\rho'\cos\varphi + \rho'^2 + t^2}\, d\varphi. \tag{9}$$

The function $g(\rho', \rho, t)$ can be expressed through a complete elliptic integral of the second type:

$$g(\rho', \rho, t) = \sqrt{\rho\rho'}\, \frac{1}{k} E(k), \quad k^2 = \frac{4\rho\rho'}{(\rho + \rho')^2 + t^2}. \tag{10}$$

We note that the function $g(\rho', \rho, t)$ is symmetrical with respect to interchange of the variables ρ' and ρ and is an even function of t.

2. METHOD OF SUCCESSIVE APPROXIMATIONS FOR SOLUTION OF THE KINETIC EQUATION

For an approximate solution to Eq. (5) we use the Gaussian type quadrature formulas

$$\int_{-\infty}^{\infty} W_1(z)\, \varphi_1(z)\, dz = \sum_{n=1}^{N} a_n \varphi_1(z_n), \tag{11}$$

$$\int_0^{\infty} W_2(t)\, \varphi_2(t)\, dt = \sum_{m=1}^{M} b_m \varphi_2(t_m), \tag{12}$$

where $W_1(z)$ and $W_2(t)$ are determined by Eqs. (4), z_n are the roots of the Hermite polynominal of degree N, t_m are the roots of the Laguerre polynominal of degree M, a_n and b_m are the corresponding Christoffel numbers. The values of a_n and z_n for $N \leqslant 9$, and of b_m and t_m for $N \leqslant 5$ were calculated by Reiz[8]. We observe that the coefficients a_n and b_m satisfy the condition

$$\sum_{m=1}^{M}\sum_{n=1}^{N} a_n b_m = 1. \tag{13}$$

Later, we shall have to evaluate approximately integrals of the form

$$\int_{-\infty}^{\infty} \frac{d\varphi_1}{dz}\left\{\int_{-\infty}^{z} W_1(z')\, \varphi(z')\, dz'\right\} dz.$$

Integrating by parts and applying Eq. (11) we find

$$\int_{-\infty}^{\infty} \frac{d\varphi_1}{dz}\left\{\int_{-\infty}^{z} W_1(z')\, \varphi(z')\, dz'\right\} dz =$$

$$-\int_{-\infty}^{\infty} W_1(z)\, \varphi_1(z)\, \varphi(z)\, dz = -\sum_{n=1}^{N} a_n \varphi_1(z_n)\, \varphi(z_n).$$

*V. A. Fock solved the problem of the motion of ions in a gas in an electric field under the assumption that they emerge with a Maxwellian velocity distribution and disappear as a result of overcharge. It is not difficult to obtain Equation (21) of Fock's work[7] from Eq. (1) if one regards the integral in the first term on the right as independent of velocity.

It is easy to verify the same result is obtained if we set

$$\int_{-\infty}^{z} W_1(z')\,\varphi(z')\,dz' = \sum_{n=1}^{N} a_n(z)\,\varphi(z_n), \qquad (14)$$

$$a_n(z) = 0 \quad \text{when } z < z_n, \qquad a_n(z) = a_n \quad \text{when } z > z_n. \qquad (15)$$

The primary argument in favor of a method based on the utilization of quadrature formulas is that to each mathematical approximation here, there corresponds a completely distinct physical model.

Actually it is not difficult to see that utilization of Eqs. (11), (12) and (14) is equivalent to the replacement of the functions $W_1(z)$ and $W_2(\rho^2)$ by the functions:

$$W_1^N(z) = \sum_{n=1}^{N} a_n \delta(z - z_n); \qquad (16)$$

$$W_2^M(\rho^2) = \sum_{m=1}^{M} b_m \delta(\rho^2 - \rho_m^2); \quad \rho_m^2 = t_m. \qquad (17)$$

The physical meaning of the quadrature equations (11) through (13) consists in the fact that the real motion of the atoms with a Maxwellian distribution Eq. (14) is replaced by motion with distribution corresponding to Eqs. (16) and (17).

The Gaussian method applied for a choice of points of subdivision likewise permits of a simple interpretation. Let us examine, for example, Eq. (11). For points of subdivision chosen according to the Gaussian method we obtain, using this equation, explicit values for the integrals

$$\int_{-\infty}^{\infty} W_1(z)\,z^k\,dz$$

with $k = 0, 1, 2 \ldots (2N-1)$. These integrals represent the mean values of the various powers of z, i. e., of the projection of the velocity of an atom on the direction of the field. The more points of subdivision we take, the better will the distribution of Eqs. (16) and (17) convey the actual character of the motion of the atoms.

The method of successive approximations used by us is analogous to a method developed by Chandrasekhar[9] for the solution of a radiative transfer equation. In Chandrasekhar's method, however, use of quadature formulas is equivalent to the prior introduction of an approximate expression for an unknown function (the radiation density), while in the method set forth here, the physical model itself is approximate. Within the framework of this approximate model the problem is solved explicitly.

We note that in the case where the work done by the field over the length of the free path of the ions is much larger than the mean energy of thermal motion of the atoms, all the approximations lead to one and the same exact result. Actually, the various approximations differ one from another in the character of the motion of the atoms in the corresponding physical models, but if the field is large, the atoms can in general be regarded as immobile.

Using the quadrature equations (11) through (13), in other words, replacing W_1 and W_2 in the expressions under the integrals by the functions (16) and (17), we obtain [instead of Eqs. (5) and (8)]:

$$f(\rho, z) = 2W_2(\rho^2) \sum_n a_n(z)\,F(\rho, z_n)\,G(\rho, z_n, z), \qquad (18)$$

$$F_0(\rho, z) = \sum_{n,m} g(\rho_m, \rho, z - z_n)\,a_n\,b_m. \qquad (19)$$

Here and further on, the summation over n is carried from 1 to N, and the summation over m from 1 to M.

In Eq. (18) we replace ρ and z by ρ' and z', multiply both parts of the equation by $g(\rho', \rho, z - z')\,\rho'\,d\rho'\,dz'$ and carry out integration over ρ' and z'. Then using Eqs. (12) and (7), we obtain

$$F(\rho, z) = \sum_{m,n} F(\rho_m, z_n)\,b_m \times \int_{-\infty}^{\infty} a_n(z')\,G(\rho_m, z_n, z')\,g(\rho_m, \rho, z - z')\,dz'. \qquad (20)$$

Taking account of Eq. (15), we introduce the notation

$$b_m\,a_n\,F(\rho_m, z_n) = x_{mn}, \qquad (21)$$

$$a_s\,b_k \int_{z_n}^{\infty} G(\rho_m, z_n, z')\,g(\rho_m, \rho_k, z_s - z')\,dz' = c_{ks}^{mn}. \qquad (22)$$

Assigning now the values ρ_k and z_n to ρ and z in Eq. (20) ($k = 1, 2, \ldots M$; $n = 1, 2 \ldots N$), we arrive at a system of equations for the quantities x_{mn}:

$$x_{ks} = \sum_{m,n} c_{ks}^{mn}\,x_{mn},$$

which in a given approximation replaces the integral equation (5).

The homogeneous system Eq. (23) can have non-zero solutions only if the determinant of its coefficients is equal to zero. Using Eqs. (19) and (22) and the properties of the function $g(\rho', \rho, t)$ we find:

$$\sum_{ks} c_{ks}^{mn} = \int_{z_n}^{\infty} G(\rho_m, z_n, z') F_0(\rho_m, z')\, dz',$$

whence, if Eq. (6) is considered:

$$\sum_{ks} c_{ks}^{mn} = 1. \tag{24}$$

From the relation Eq. (24) it follows at once that the determinant of the system Eqs. (23) is equal to zero and, consequently, non-zero solutions exist.

From Eqs. (23) the quantities x_m are determined, obviously, explicit up to an arbitrary common factor. This factor is found from the normalization condition:

$$\int_{-\infty}^{\infty}\int_{0}^{\infty} f(\rho, z)\, \rho\, d\rho\, dz = 1, \tag{25}$$

which, according to Eq. (18) takes the form:

$$\sum_{m, n} A^{mn} x_{mn} = 1; \tag{26}$$

$$A^{mn} = \int_{z_n}^{\infty} G(\rho_m, z_n, z)\, dz. \tag{27}$$

If one determines x_{mn} through Eqs. (23) and (26), then it is possible by means of Eqs. (18) and (12) to obtain the mean values of the various quantities which characterize the motion of the ions. For example, for the drift velocity we obtain:

$$\bar{z} = \int_{-\infty}^{\infty}\int_{0}^{\infty} f(\rho, z)\, z\rho\, d\rho\, dz = \sum_{m, n} B^{mn} x_{mn}, \tag{28}$$

$$B^{mn} = \int_{z_n}^{\infty} zG(\rho_m, z_n, z)\, dz. \tag{29}$$

In order to obtain an idea of the closeness of the various approximations, we examine the limiting cases of small and large fields. In the case of large fields ($\gamma \gg 1$), as has already been pointed out above, all the approximations give one and the same precise[4] result:

$$\bar{v}_z = \sqrt{2a\lambda/\pi}. \tag{30}$$

Equation (30) differs from the formula derived by Sena[1] by a numerical factor. This is related to the fact that in Ref. 1 the difference in duration of the free paths of various lengths was not taken into account. If this circumstance is considered, then the method used by Sena also leads to Eq. (30).

For small fields ($\gamma \ll 1$), the coefficients c_{ks}^{mn}, A^{mn}, B^{mn} can be expanded in powers of γ and restricted to terms of first degree in γ. By such means, we obtain for the drift velocity:

In the approximation $M=1$, $N=2$, $\bar{v}_z = 0.452\, a\lambda/u_0$,
In the approximation $M=1$, $N=3$, $\bar{v}_z = 0.496\, a\lambda/u_0$,
In the approximation $M=1$, $N=4$, $\bar{v}_z = 0.481\, a\lambda/u_0$,

For comparison, we quote values of $\bar{v}_z$ obtained in Ref. 5 for the case of small fields by the method of Chapman and Enskog:

In the first approximation $\bar{v}_z = 0.470\, a\lambda/u_0$,
In the second approximation $\bar{v}_Z = 0.481\, a\lambda/u_0$.

The case of small fields is the most unfavorable for the application of the method of successive approximations based on quadrature formulas inasmuch as the smaller the field the larger must be the effect of the motion of the atoms on the drift velocity of the ions. Even in the case of small fields, however, the approximation $M=1$, $N=2$ already gives a fair result for the drift velocity of the ions.

3. THE APPROXIMATION $N=2$, $M=1$. COMPARISON WITH EXPERIMENT

Let us examine in more detail the approximation $N=2$, $M=1$. The velocity distribution of the atoms corresponding to this approximation is determined by the formulas:

$$W_1^{(2)}(z) = {}^1/_2 [\delta(z - z_1) + \delta(z + z_1)];$$

$$W_2^{(1)}(\rho^2) = \delta(\rho^2 - \rho_1^2),$$

$$z_1 = -z_2 = 1/\sqrt{2}; \quad \rho_1 = 1; \quad a_1 = a_2 = {}^1/_2;$$

$$b_1 = 1. \tag{31}$$

The mean energy of the atoms and the portions of it which come from motion along and transverse to the field calculated by means of Eqs. (31) coincide with the exact values of these quantities.

In the approximation $M=1$, $N=2$, the integrals which enter in Eqs. (22), (27) and (29) were evaluated for different values of γ and the drift velocity of the ions was calculated. The dependence of $\bar{z}$ on γ in

this approximation is depicted in Fig. 1 on a logarithmic scale. Points for which calculations were

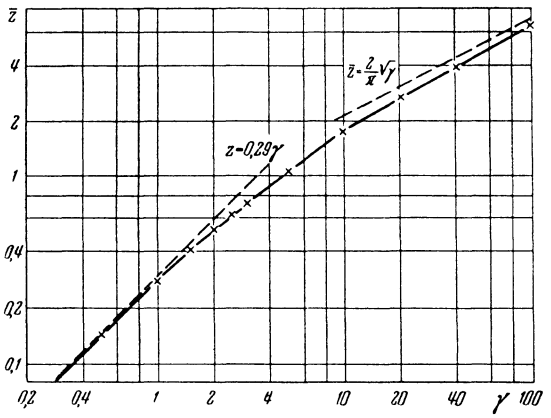

FIG. 1

carried out are marked with x's. For comparison there are included in Fig. 1 the lines which give the dependence of $\bar{z}$ on γ in the limiting cases of small and large fields. The values of the drift velocity calculated from the graph presented in Fig. 1 are close to the values calculated by Eq. (7) of Ref. 4. The maximum difference occurs for the case of small fields and amounts to about 10%.

The results of the calculations can be compared with data on the drift velocity of ions, obtained in the experiments of Hornbeck[10] for He^+ in He, Ne^+ in Ne and A^+ in A and in the experiments of Varney[11] for Kr^+ in Kr, and Xe^+ in Xe. Such a comparison is given in Figs. 2 and 3, where the points indicate the

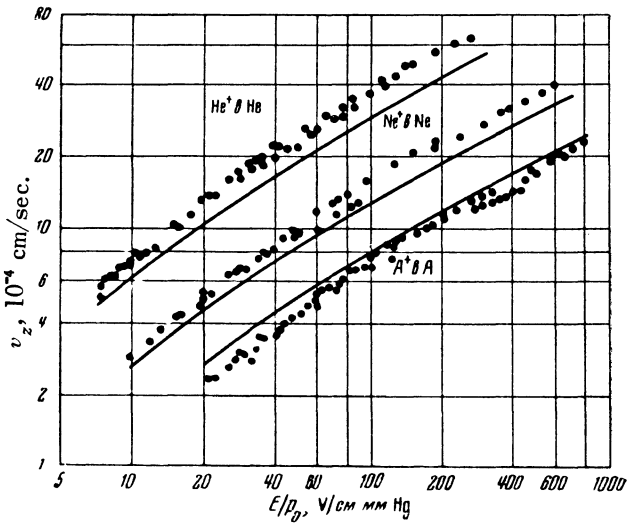

FIG. 2

experimental data and the solid curves give the results of calculations according to Fig. 1. The values obtained in Ziegler's experiments[12] (energy of the ions of the order of 1 ev) were taken for the cross-sections of overcharge.

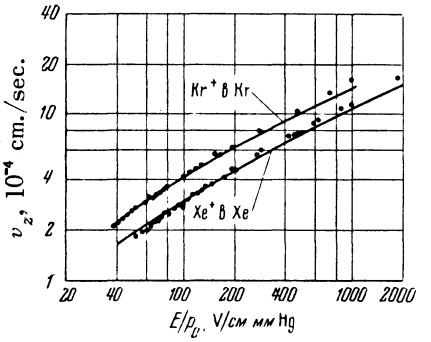

FIG. 3

From Figs. 2 and 3 it is seen that for all of the investigated gases, with the exception of He, there is good agreement of the results of the calculation with experimental data over the entire interval of values of E/p_0, attained in the experiments** (here $p_0=p\cdot 273/T$ is the reduced pressure of the gas).

The reason for a certain discrepancy between the theoretical and experimental results for the case of He^+ and He (approximately 30%) is not clear. One should note that in this case the theoretical curve correctly conveys the course of the dependence of the drift velocity on E/p_0. In order to achieve complete agreement with experiment, it is sufficient to take 3×10^{-15} cm^2 as the value of the cross-section for overcharge instead of the 4.1×10^{-15} cm^2 value obtained by Ziegler.

On the whole, the comparison of theory with experiment shows that the model of "pure overcharge" with cross-section not depending on velocity is a good approximation for the description of the interaction of an ion with atoms of the same gas over a broad interval of values of E/p_0.

I am genuinely grateful to Dozent Iu. M. Kagan under whose guidance this work was completed, and to Professor L. E. Gurevich for a series of valuable comments.

**In comparing Figs. 2 and 3 of the present work with Figs. 1 and 2 of Ref. 4, one should keep in mind that the difference between them is related for the most part with the fact that in Ref. 4 values were taken for the cross-section of overcharge calculated according to Demkov's formulas[13], while in the present work the direct experimental data of Ziegler is used.

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Translated by R. L. Eisner
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SOVIET PHYSICS JETP VOLUME 5, NUMBER 3 OCTOBER, 1957

Contribution to Field Theory Involving a Cut-off Factor

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(Submitted to JETP editor February 6, 1956)
J. Exptl. Theoret. Phys. (U.S.S.R.) **23**, 534-541 (March, 1957)

A study is made of the question of the uniqueness of quantum field theory involving a cut-off factor, and it is found that even finite (renormalized) expressions depend on the form of the cut-off factor. Examples are given in which the renormalized Green's function of a boson has no pole for finite momenta, but the critical momentum in the charge renormalization can be made arbitrarily large. In this connection difficulties with the vanishing of the charge and the existence of a pole in the Green's function are considered, and also the question of the domain of applicability of meson theory.

1. BECAUSE of the divergence difficulties inherent in quantum field theory, use is often made of cut-off factors, which have the effect of reducing the part played by high-frequency virtual quanta, so as to secure the convergence of the expressions occurring in the theory[1,2]. Upon completion of the intermediate calculations, the cut-off parameters (which play the part of effective limiting momenta) are let go to infinity, the cut-off factor (CF) approaches unity, and, at least formally, the original "not cut-off" theory is recovered. This procedure corresponds to regarding a point interaction as the limit of a smeared-out interaction.

In such an approach to the problems of quantum field theory there inevitably arises the question as to its uniqueness, i.e., as to the dependence of the results obtained on the form of the CF used. The most important aspect of this question is considered in the present paper: do the finite (renormalized) expressions depend on the CF?

This question has been given partial consideration in Refs. 2 and 3, where it was answered in the negative; but it will be shown that this conclusion was essentially based on the use of CF's that approached unity sufficiently rapidly with increase of the cut-off parameter. We consider below a wider class of CF's, for which the problem of lack of uniqueness takes on primary significance.

The study will be carried out in the framework of the asymptotic theory of Landau, Abrikosov, and Khalatnikov[2] (cf. also Ref. 4), with a single modification — replacement of the plateau-shaped cut-off factor by a CF of more general type (but still very close to the plateau-shaped). The basic relationships of the theory are the integral equations connecting the Green's functions G and D and the vertex part Γ, the integrands being certain combinations of G, Γ, D, and the CF. In the calculation of the asymptotic forms at large momenta it turns out that essential parts are played not only by the prin-