

CONTRIBUTION TO THE CALCULATION OF THE MOBILITY AND TEMPERATURE OF CHARGED PARTICLES IN AN ELECTRIC FIELD¹⁾

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The value of the mobility and temperature of charged particles in an electric field dependent on a mass ratio of charged and neutral particles and on an interaction potential type which is considered in the form of $r^{-\nu}$ are computed. The solution of the Boltzmann equation has been made possible by a conversion into the algebraic equation system by extending the distribution function to the series of the Sonin and Legendre polynomials. Higher orders of integrals $\Omega^{(n, \nu)}$, which appear in higher approximations, are computed by means of a numerical calculation of the orbital integral.

О ВЫЧИСЛЕНИИ ПОДВИЖНОСТИ И ТЕМПЕРАТУРЫ ЗАРЯЖЕННЫХ ЧАСТИЦ В ЭЛЕКТРИЧЕСКОМ ПОЛЕ

В работе рассчитаны значения подвижности и температуры заряженных частиц в электрическом поле, которые зависят от отношения масс заряженных и нейтральных частиц и типа потенциала взаимодействия, выбранного в виде $r^{-\nu}$. Уравнение Больцмана решено посредством его преобразования в систему алгебраических уравнений при помощи разложения функции распределения в ряд по полиномам Сонина-Лежандра. Вышние порядки интегралов $\Omega^{(n, \nu)}$, которые появляются в высших приближениях, вычислены на основе численного расчета орбитального интеграла.

1. INTRODUCTION

Many attempts have already been made in literature to solve equations which describe the dependence of distribution function moments on an external force represented by the electric field strength (see e. g. the review [1]). The common shortcomings of all the published works are difficulties in obtaining higher matrix elements of the collision operator, necessary for the approximation of the originally

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infinite equation system through a finite, sufficiently large one. However, the derivation of the general generating function of the collision operator in [7] and the derivation of the explicit form of its matrix elements and the respective calculation algorithm in [8] have made it possible to include also the subprogram of the calculation of necessary matrix elements into the calculation program of coefficients of the distribution function series.

Next the values of the collision integrals $\Omega^{(s,r)}$ must be specified. In the present work we restrict ourselves to potentials of the type r^{-r} . The calculation of the effective cross section from the classical orbital integral has been possible by a suitable geometric substitution.

II. THE EQUATION FOR THE CALCULATION OF THE MOBILITY AND TEMPERATURE OF CHARGED PARTICLES

Let us consider the mixture of two kinds of particles: Charged particles with the charge e , mass m , instant velocity v and temperature T and neutral particles with the mass m_1 , velocity v_1 and temperature T_1 . Let us suppose that all collisions of particles are binary and elastic and that the only external force which is the electric field E affects the charged particles and at the same time the neutral particles have the distribution function of the Maxwell type. The behaviour of the system can then be described by the only Boltzmann integrodifferential equation

$$\frac{e}{m} E \nabla_v f = \iint (f' f'_1 - f f_1) g b \, db \, d\epsilon \, d\epsilon_1 \quad (1)$$

where

$$f_1 = n_1 \left(\frac{m_1}{2\pi k T_1} \right)^{3/2} \exp \left(- \frac{m_1 v_1^2}{2k T_1} \right) \quad (1a)$$

It is possible to solve this equation by expanding the distribution function to the series of the Sonin and Legendre polynomials.

$$f = \sum_m a_{lm} S_{l+1/2}^{(m)}(\gamma^2) P_l \left(\frac{E \cdot \gamma}{|E| \cdot |\gamma|} \right) \quad (2)$$

where γ is the dimensionless velocity. On the basis of this extension the equation system for the calculation of the coefficients a_{lm} has been derived by the variational method. The derivation is detailed in [6] (cf. also [1], [5]).

$$\frac{4(1 - \delta_{0m} \delta_{0l})}{(2l+1) \sqrt{\pi}} \sum_{n=0}^{m+l} M'_{mn} a_{ln} + (1 - \delta_{0m}) \left[E^{*2} a_{l+1,m} \left(\frac{l+5}{m-1} \right) - \right] \quad (3)$$

$$- (1 - \delta_{0l}) a_{l-1,m} \left(\frac{l+3}{m-1} \right)] = \delta_{0m} \delta_{0l}$$

where δ_{ij} is a Kronecker δ .

The coefficients M'_{mn} are the matrix elements of the linearized isothermal Boltzmann collision operator and they depend on a particle interaction model through the collision integrals

$$M'_{mn} = 8 \sum_s \sum_r V_{lmn}^{sr} \Omega^{(s,r)} \quad (4)$$

The integrals $\Omega^{(s,r)}$ are defined as usual (see [2], [3]), and the coefficients V_{lmn}^{sr} have been gained by the expansion of the generating function $V(x, y, t)$ of the collision operator

$$V(x, y, t) = \sum_{l_1, m_1, n_1, s_1, r_1} x^{l_1} y^{m_1} t^{n_1} (\cos \lambda)^{s_1} V_{l_1 m_1 n_1}^{s_1 r_1} \quad (4a)$$

The derivation and the form of this generating function are described in [7]. In [8] the explicit form of the coefficients V_{lmn}^{sr} is derived.

The parameter of the equation system (4) is the relative electric field strength

$$E^* = \frac{eE}{2 \sqrt{2} \pi m k T_1 n_1 \Omega^{(1,1)}} \quad (4b)$$

where the collision integral $\Omega^{(1,1)}$ is defined by Chapman [2]. The solution of the system are the coefficients a_{lm} in the distribution function expansion (2). By means of this distribution function we obtain through adequate integrations of the series (2) the expression for the dependence of the relative mobility of charged particles

$$\frac{K}{[K]_{E^*=0}} = \frac{a_{10}}{[a_{10}]_{E^*=0}} \quad (5)$$

and of their relative temperature

$$\frac{T}{T_1} = 1 - a_{01} \quad (6)$$

on a relative electric field strength (for more detail see [5], [6], [9], [10]).

III. CALCULATION OF COLLISION INTEGRALS $\Omega^{(s,r)}$ FOR THE INTERACTION POTENTIAL r^{-r}

The effective cross section can be expressed in the usual way [3]

$$Q^{(s)}(\theta) = 2\pi \int_0^\infty (1 - \cos^s \chi) b \, db \quad (7)$$

by means of the deflection angle χ of the trajectory of a particle flying on. This angle can be expressed in the quasiclassical approximation through the orbital integral

$$\chi = \pi - 2b \int_{r_m}^{\infty} \frac{dr/r^2}{\sqrt{1 - \left(\frac{b}{r}\right)^2 - \frac{2\varphi(r)}{\mu g^2}}} \quad (8)$$

where r_m is a root of the expression under the radical sign (compare e. g. [3]), μ is the reduced mass. Let us now restrict ourselves to potentials of the type

$$\varphi(r) = U_0 r^{-p}. \quad (9)$$

By substitution (cf. [4])

$$\frac{r_m}{r} = \sin \alpha; \quad \frac{b}{r_m} = \sin \beta \quad (10)$$

into equation (8) we set after rearrangement the relation for the angle χ dependent on the parameter β only:

$$\chi(\beta) = \pi - 2 \sin \beta \int_0^{\pi/2} \left[1 + \frac{\cos^2 \beta}{\cos^2 \alpha} (\sin^2 \alpha - \sin^2 \alpha') \right]^{-1/2} d\alpha. \quad (11)$$

Then we express the effective cross section $Q^{(e)}(\vartheta)$ as

$$Q^{(e)}(\vartheta) = 2\pi \left(\frac{pU_0}{1} \right)^{2/p} A_p^{(e)}. \quad (12)$$

Through substitution (10) we obtain for $A_p^{(e)}$ the expression

$$A_p^{(e)} = p^{-(2/p)} \int_0^{\pi/2} [\cos^2 \beta \sin \beta + \frac{2}{p} \sin^3 \beta] (\cos \beta) \left(-\frac{4}{p} - 1 \right) \times [1 - \cos^2 \chi(\beta)] d\beta. \quad (13)$$

Expressions (11) and (13) have been used for the machine computation of $A_p^{(e)}$. The integrals $Q^{(e, \nu)}$ can then be expressed through the integral $Q^{(e, 1)}$ (which is a part of expression (4b)) for the relative electrical field strength as

$$\frac{Q^{(e, \nu)}}{Q^{(e, 1)}} = \frac{A_p^{(\nu)} \Gamma \left(r + 2 - \frac{2}{p} \right)}{A_p^{(1)} \Gamma \left(3 - \frac{2}{p} \right)}. \quad (14)$$

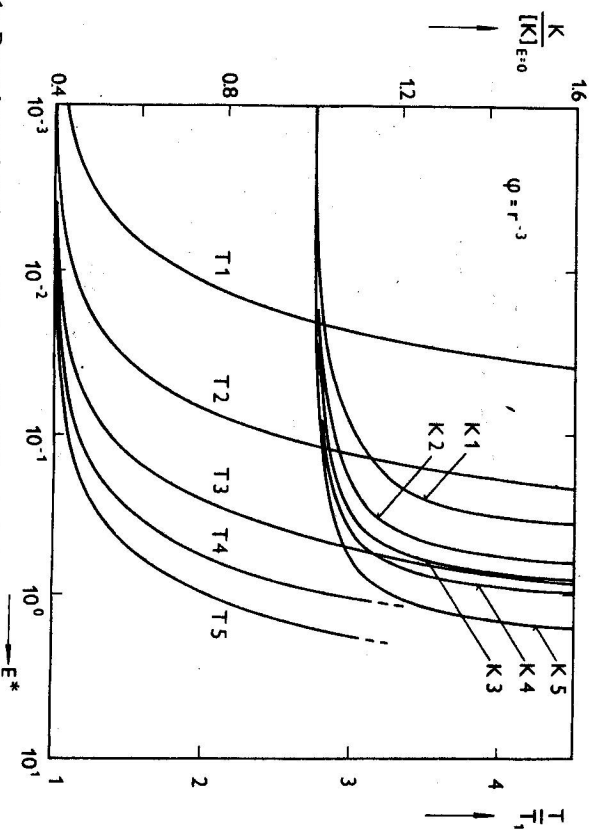


Fig. 1a. Dependence of relative mobility (curves K1—K5) and relative temperature (curves T1—T5) of charged particles on a relative electric field strength at the potential $\varphi(r) = r^{-3}$ for different ratios of relative masses of charged and neutral particles: K1, T1— $M = 10^{-2}$; K2, T2— $M = 0.25$; K3, T3— $M = 0.5$; K4, T4— $M = 0.75$; K5, T5— $M = 0.9$. Here $M = m/(m + m)$.

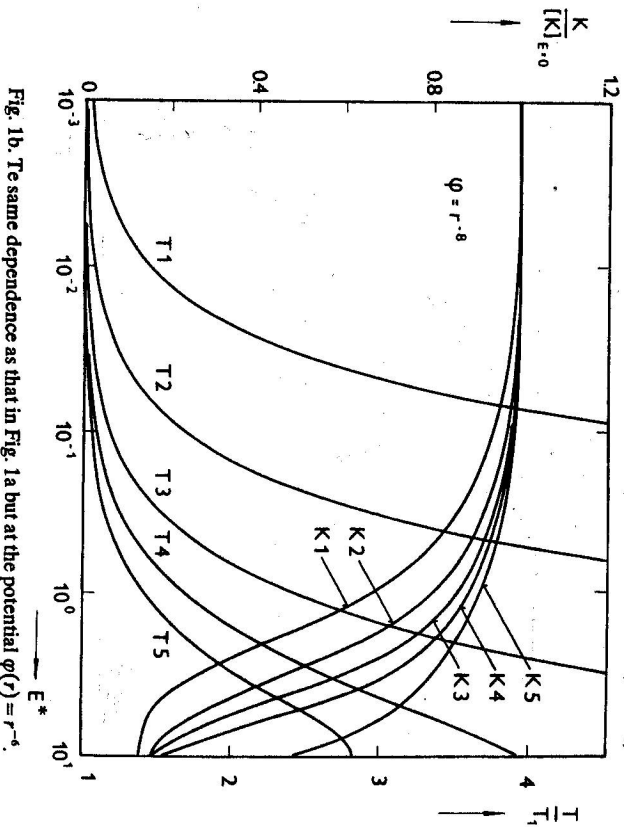


Fig. 1b. The same dependence as that in Fig. 1a but at the potential $\varphi(r) = r^{-6}$.

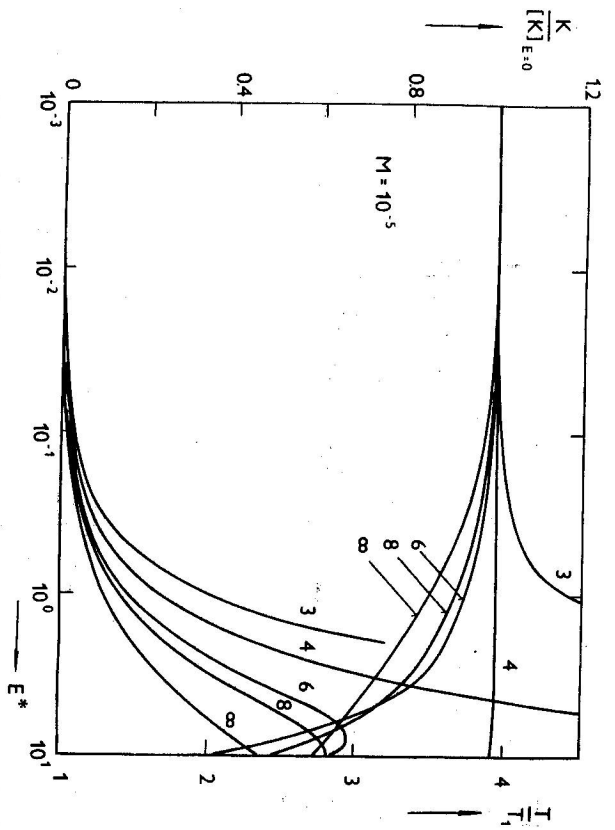


Fig. 2a. The same dependence as in Fig. 1a but with the relative mass of charged particles $M = 10^{-5}$ for different powers of the potential.

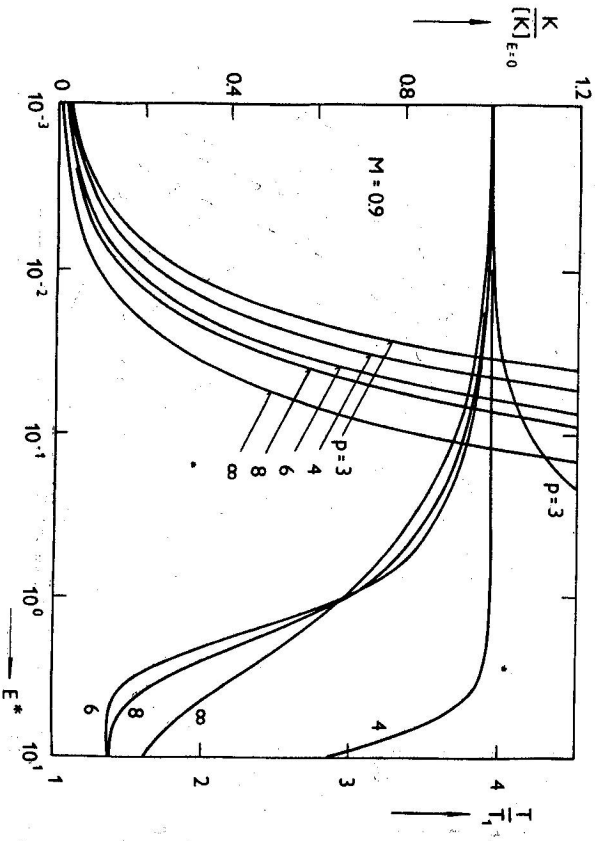


Fig. 2b. The same dependence as that in Fig. 2a but with the relative mass of charged particles $M = 0.9$.

IV. RESULTS AND DISCUSSION

The solution of equation (4) with the computation algorithm of the necessary coefficients M'_{min} (see [9]) has been computed for $l_{max} = 3$ with the calculator HP 9845 for the potentials $\varphi(r)$ of the type r^{-3} , r^{-4} , r^{-6} , r^{-8} and for rigid spheres. For each of the potentials five typical ratios $m : m_1$ have been chosen. In Figs. 1a, b and 2a, b we can follow the courses of the dependences of the relative mobility and temperature of the charged particles on a relative electric field strength E^* . Generally it can be said that the heavier the charged particles are, compared with neutrals, the larger the mobility change and temperature increase. In the region of lower E^* the mobility decreases with the potential p . The temperature increases with p for all E^* .

The results of the numerical solution of integrals of Lorentzian approximation (see e.g. [9]) are in good agreement with the results of the present paper for $m/m_1 = 10^{-5}$.

In the region of $E^* = 5 \div 10$ the convergence of the solution usually disappears because the solution represents in fact a finite series of power of E^* . In that case it could be possible to solve a larger equation system for higher l_{max} .

REFERENCES

- [1] McDaniel, E. W., Mason, E. A.: *The Mobility and Diffusion of Ions in Gases*. John Wiley and Sons, New York 1973.
- [2] Chapman, S.: Cowling, T. G.: *The Mathematical Theory of Nonuniform Gases*. Cambridge University Press 1952.
- [3] Hirschfelder, J. O., Curtiss, C. F., Bird, R. B.: *Molecular Theory of Gases and Liquids*. John Wiley and Sons, New York 1954.
- [4] De Boer, J., Van Kranendonk, J.: *Physica XIV* (1948), 442.
- [5] Neníčka, V.: Report ÚE 662, Praha 1979.
- [6] Kírenek, P.: Report ÚE 702, Praha 1979.
- [7] Neníčka, V.: Report ÚE 725, Praha 1980.
- [8] Kírenek, P.: report ÚE 726, Praha 1980.
- [9] Kírenek, P.: *Cand. degree thesis*, Praha 1981.
- [10] Neníčka, V., Kírenek, P.: *Matcové prvky lineárnizovaného izotermického Boltzmannova srážkového operátoru*. Studie ČSAV, (in print).

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