ON THE VALIDITY OF THE TWO–TERM APPROXIMATION OF THE ELECTRON DISTRIBUTION FUNCTION

By R. E. Robson* and Kailash Kumar*

Abstract

The Boltzmann equation for electrons moving in a neutral gas under the influence of an externally applied field is solved by expanding the electron distribution function in terms of Legendre and Sonine polynomials. The solution is given in terms of infinite matrices which have elements ordered by the Sonine polynomial index, and which are dependent upon the field strength. From the structure of the formulae, it is possible to infer that truncation of the Legendre polynomial expansion after two terms is a good approximation at all field strengths. This is supported by calculations of the electron drift velocity at low field strengths, which show that the error introduced by making the two-term approximation is small, even when the deviation from equilibrium is significant. The convergence of the Sonine polynomial expansion is shown to be strongly dependent upon field strength, and large matrices are required in the drift velocity formula at even small field strengths.

I. Introduction

Theoretical analyses of the mobility and diffusion of electrons in neutral gases under the influence of an applied electric field have traditionally relied upon the so-called two-term approximation (Lorentz 1916; Davydov 1935; Morse, Allis, and Lamar 1935; Margenau 1946; Allis 1956), in which the distribution function is approximated by the first two terms of an expansion in Legendre polynomials,

$$f(c) = \sum_{l=0}^{\infty} f^l(c) \, P_l(\cos\theta), \qquad \cos\theta = (E.c)/Ec, \tag{1}$$

$$\approx f^0(c) + f^1(c)\cos\theta. \tag{1a}$$

The Boltzmann equation appropriate to this case, namely

$$(e/m)E.\partial f/\partial c = J(ff_0) \tag{2}$$

with

$$J(ff_0) \equiv \int \{f(c)f_0(c_0) - f(c')f_0(c_0')\} g\sigma(g,\chi) \, d\Omega \, dc_0, \tag{3}$$

is thus reduced to two coupled differential equations for $f^0(c)$ and $f^1(c)$. In equations (2) and (3) the 0 subscripts refer to the neutral gas while the other notation is standard. Solving for $f^0(c)$ gives the Davydov distribution, which in the limiting case of rigid-sphere interaction and high fields becomes the Druyvesteyn distribution (Allis 1956).

* Department of Theoretical Physics, Research School of Physical Sciences, Australian National University, P.O. Box 4, Canberra, A.C.T. 2600.

This approximation is usually justified on physical grounds (Chapman and Cowling 1970): because of their small mass, electrons suffer relatively large directional changes in velocity but lose only a small fraction ($\sim 2\ m/m_0$) of their energy in collisions with the neutral atoms. (Collisions are assumed here to be elastic.) Thus, while the distribution of velocities may be non-Maxwellian, it would be expected to be nearly spherically symmetric in velocity space, that is, f^0 would be the dominant term in (1). Although, as is shown in Section II below, the smallness of m/m_0 provides the basic justification for using the two-term approximation, these arguments and others (Ginzburg and Gurevich 1960) do not fully justify the omission of higher order terms from (1).

In view of the accuracy of present day experiments (Crompton, Elford, and Robertson 1970), it is of interest to estimate the importance of $f^2, f^3, \ldots$. A systematic method of approximating these terms is presented here and it is shown that they are insignificant. The amount of numerical work required increases with the field strength, but the structure of the formulae and the results for low fields, which are presented below, suggest that for the electrons the two-term approximation remains valid for all values of field strength.

II. Theory and Discussion

The neutral gas is assumed to be in equilibrium at temperature T_0,

$$f_0(\boldsymbol{c}_0) = n_0\,\bar{w}(\alpha_0, c_0)\,, \tag{4}$$

and $f^l(c)$ is expanded further in terms of Sonine polynomials as

$$f^l(c) = n\,\bar{w}(\alpha, c)\frac{4\pi}{2l+1}\sum_{\nu=0}^{\infty} f^{\nu l}\,R_{\nu l}(\alpha c)\,, \tag{5}$$

where

$$\bar{w}(\alpha, c) \equiv (\alpha^2/2\pi)^{3/2}\exp(-\tfrac{1}{2}\alpha^2 c^2)\,, \quad \alpha^2 \equiv m/kT_0\,, \quad \alpha_0^2 \equiv m_0/kT_0\,,$$

$$R_{\nu l}(c) \equiv N_{\nu l}\,(c/\sqrt{2})^l\,S_{l+\frac{1}{2}}^{(\nu)}(\tfrac{1}{2}c^2)\,, \quad N_{\nu l}^2 \equiv 2\pi^{3/2}\nu!/\Gamma(\nu+l+\tfrac{3}{2})\,.$$

The present paper follows the earlier work of Kumar (1967) in notation and in the transformation to matrix form. Substituting for $f(c)$ and $f_0(\boldsymbol{c}_0)$ in (2), we obtain an (infinite) homogeneous matrix equation for the expansion coefficients $f^{\nu l}$. The existence of a summational invariant, corresponding to conservation of electron number, results in the vanishing of the determinant of the matrix of coefficients (Kumar 1967), and a non-trivial solution is assured. Using the normalization condition

$$f^{00} = \sqrt{(4\pi)}\,, \tag{6}$$

the homogeneous matrix equation is then reduced to a solvable inhomogeneous matrix equation of the form

$$[\mathbf{J} - \epsilon\mathbf{D}]\mathbf{f} = -\epsilon\mathbf{d}\,, \tag{7}$$

where $\mathbf{f}$ is the unknown column vector, $\mathbf{d}$ is a known (constant) vector, and $\mathbf{J}$ and $\mathbf{D}$ are matrices labelled by ν and l with $\nu, l = 0, 1, \ldots$, except that $\nu = 0 = l$ terms

do not occur. The field parameter ϵ is defined in equation (9) below. Equation (7) may be written as a series of coupled equations for matrices labelled by ν only,

$$J^0 f^0 - \epsilon D_+^0 f^1 = 0, \tag{8a}$$

$$J^1 f^1 - \epsilon D_+^1 f^2 - \epsilon D_-^1 f^0 = -\epsilon d, \tag{8b}$$

$$J^2 f^2 - \epsilon D_+^2 f^3 - \epsilon D_-^2 f^1 = 0, \tag{8c}$$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

$$J^L f^L - \epsilon D_-^L f^{L-1} = 0, \qquad L \to \infty, \tag{8d}$$

where f^l is a column vector with entries $f^{\nu l}$, d is a fixed vector, and J^l and $D_\pm^l$ are matrices labelled by ν. These equations are directly comparable with the recurrence relations of Kihara (1953) and also have the same formal structure as the coupled integro-differential equations for $f^l(c)$ of equation (1) (Ginzburg and Gurevich 1960). The above matrix form allows calculations of the higher l corrections (dependence on $\cos\theta$) to be made more easily, although perhaps has some disadvantage as far as the determination of c-dependence is concerned.

The quantities appearing in equations (7) and (8) have been made dimensionless by introducing the scale factor r which characterizes the range of the electron–atom interaction; their definitions are:

$$\epsilon \equiv \{m_0/(m+m_0)\}^{\frac{1}{2}} eE/\pi r^2 n_0 kT_0, \tag{9}$$

$$d \equiv d_\nu = (4\pi/3)^{\frac{1}{2}} \delta_{\nu 0},$$

$$D_+^l \equiv (D_+^l)_{\nu_1 \nu_2} \equiv \{(l+1)/(2l+1)\}(2\nu_1)^{\frac{1}{2}} \delta_{\nu_2, \nu_1 - 1}, \tag{10a}$$

$$D_-^l \equiv (D_-^l)_{\nu_1 \nu_2} \equiv -\{l/(2l+1)\}(2\nu_1 + 2l+1)^{\frac{1}{2}} \delta_{\nu_2 \nu_1}, \tag{10b}$$

$$J^l \equiv J_{\nu_1 \nu_2}^l,$$

where, for small m/m_0,

$$J_{\nu_1 \nu_2}^0 \approx (2m/m_0)(\nu_1 \nu_2)^{\frac{1}{2}} V_{\nu_1 - 1, \nu_2 - 1}^1 \tag{11a}$$

and

$$J_{\nu_1 \nu_2}^l \approx V_{\nu_1 \nu_2}^l, \qquad l \geqslant 1, \tag{11b}$$

with

$$V_{\nu_1 \nu_2}^l \equiv \frac{\gamma}{\pi r^2} \int_0^\infty \bar{w}(\gamma, g) R_{\nu_1 l}(\gamma g) R_{\nu_2 l}(\gamma g) \{\sigma_0(g) - \sigma_l(g)\} g^3 \, dg, \tag{12}$$

$$\gamma^2 \equiv \alpha^2 \alpha_0^2 / (\alpha^2 + \alpha_0^2),$$

and

$$\sigma_l(g) \equiv 2\pi \int P_l(\cos\chi) \sigma(g, \chi) \sin\chi \, d\chi. \tag{13}$$

Equation (8d) indicates that in practical situations the series has to be terminated at some maximum value, L, of l (equivalent to approximating the right-hand side of

(1) by the first $L+1$ terms). The first three terms in the formal solution may be written as

$$f^0 = \epsilon(J^0)^{-1} . D^0_+ f^1 , \tag{14a}$$

$$f^1 = -\epsilon M_L^{-1} . d , \qquad L \geqslant 1 , \tag{14b}$$

$$f^2 = \epsilon N_L^{-1} . D^2_- f^1 , \qquad L \geqslant 2 , \tag{14c}$$

where

$$M_L \equiv J^1 - \epsilon^2 \{ D^1_- (J^0)^{-1} D^0_+ + D^1_+ N_L^{-1} D^2_- \} \tag{15}$$

and, for successive truncations,

$$N_1 = 0 , \tag{16a}$$

$$N_2 = J^2 , \tag{16b}$$

$$N_3 = J^2 - \epsilon^2 D^2_+ (J^3)^{-1} D^3_- , \tag{16c}$$

. . . .

It should be noted that as $\epsilon \to 0$, $M_L \to J^1$ so that high l contributions are not important in this situation. Furthermore, because of the smallness of m/m_0, in the second term of (15) the contribution from J^0 (defined in equation (11a)) always overshadows the higher l contributions which enter through N_L. Hence, even for high fields, the contributions from $l \geqslant 2$ will not be important. Then, from (11a) and (14a), we may conclude that $|f^0|$ is always much larger than $|f^1|$. The validity of the two-term expansion is thus seen to derive from the smallness of the mass ratio m/m_0 and the form of the solutions (equations (14) and (15)).*

In numerical calculations with the above equations, it is also necessary to truncate the infinite matrices J^l and $D^l_\pm$ at some upper value, N, of ν. The corrections introduced by increasing N are affected in a different way by the small mass ratio. They are found to be strongly dependent on the field strength, i.e. the parameter ϵ, although they do decrease if N is taken to be sufficiently large. The dimension of the matrices (determined by N) required to obtain convergence to a given accuracy increases rapidly with the field strength. (This is similar to previous experience in matrix calculations of related problems (Pekeris *et al.* 1962; Hochstim and Massel 1969).) The physical reason behind this is the well-known non-Maxwellian nature of the distribution function in this situation; although it is nearly isotropic, a large number of Sonine polynomials are required for a good representation of the velocity dependence.

In the numerical example considered in Section III, because of the slow convergence the whole experimentally available range of energy was not covered, but it appears that results of any accuracy could be obtained provided one were prepared to use sufficiently large matrices.

* This conclusion is expected to be valid for the types of cross sections encountered in the present problem. The hard-sphere interaction considered in Section III has been used in a case where it agrees most satisfactorily with experiment and the results may be considered typical for this type of problem.

III. Numerical Example

The drift velocity W and the effective electron temperature T, as conventionally defined, are given here by

$$W = (3/4\pi)^{\frac{1}{2}}\{f^{01}(E)/\alpha E\}\, E \qquad (17)$$

and

$$T/T_0 = 1 - f^{10}(E)/(6\pi)^{\frac{1}{2}}. \qquad (18)$$

The neutral gas was taken to be helium and a hard-sphere interaction potential of radius r was assumed. In this case, the partial cross sections (13) simplify to

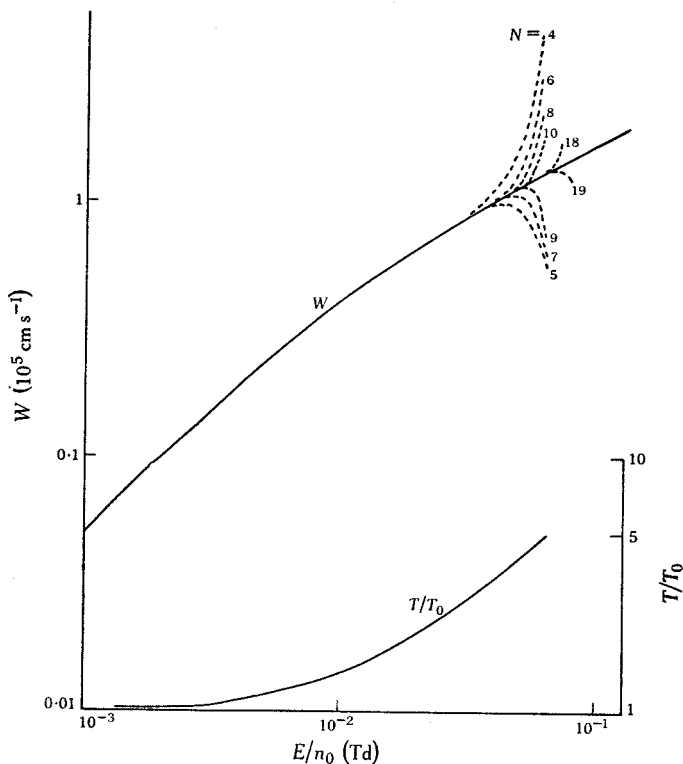$$\sigma_l(g) = \pi r^2.\,\delta_{l0}. \qquad (19)$$

Fig. 1.—Drift velocity W of electrons in helium at $T_0 = 77$ K calculated from truncated matrices for the indicated values of N (dashed curves) and compared with the usual two-term differential equation calculation (solid W curve). All curves coincide for low values of E/n_0. The calculated values of electron temperature T for $N = 19$ are also shown. (Note that 1 townsend (Td) $= 10^{-17}\,\mathrm{V\,cm^2}$.)

The values of parameters chosen were $\pi r^2 = 5\cdot4\times10^{-16}$ cm^2, $m/m_0 = 1\cdot371\times 10^{-4}$, and $T_0 = 77$ K. Figure 1 shows the effect of increasing the order N of the ν truncation in the two-term approximation $(L = 1)$ and also provides a comparison with the usual two-term calculation by numerical solution of differential equations. Clearly, the convergence becomes worse for higher values of E/n_0, indicating that very large matrices would be required to cover the whole of the experimental range. Also shown in Figure 1 is a plot of the ratio of the electron temperature to the gas temperature for $N = 19$. It shows that with increasing field strengths the electron distribution must deviate strongly from the Maxwellian appropriate to T_0.

Because of the slow convergence with N, the present work was limited to low values of E/n_0 in calculations showing the effect of convergence with L. Table 1 shows the variation of the drift velocity with $L = 1, 2$, and 3 for fixed N and different E/n_0 in a region where the deviation from equilibrium is significant. It is seen that the relative magnitude of the correction from higher l terms is even smaller than may have been anticipated, i.e. less than m/m_0. The values change somewhat for different values of N but the pattern remains the same. Similar results have been obtained for many different sizes of matrices and for different parameters. On this basis, it can be conjectured that, although very large matrices in the Sonine polynomial index ν are needed at high fields, as far as the Legendre polynomial expansion (equation (1)) is concerned, inclusion of terms beyond the first two produces corrections of a relative order of magnitude not exceeding m/m_0.

TABLE 1

VARIATION OF DRIFT VELOCITY WITH SUCCESSIVE ORDERS OF TRUNCATION
IN LEGENDRE POLYNOMIAL INDEX

Values are for $N = 10$

Order of Truncation L	Drift Velocity W (10^5 cm s^{-1})		
	$E/n_0 = 0 \cdot 01$	$0 \cdot 02$	$0 \cdot 04$ Td
1	$0 \cdot 4080835$	$0 \cdot 6643601$	$1 \cdot 017357$
2	$0 \cdot 4080756$	$0 \cdot 6643437$	$1 \cdot 017330$
3	$0 \cdot 4080756$	$0 \cdot 6643437$	$1 \cdot 017330$

IV. ACKNOWLEDGMENTS

V. REFERENCES

ALLIS, W. P. (1956).—*In* "Handbuch der Physik". (Ed. S. Flügge.) Vol. 21, p. 383. (Springer-Verlag: Berlin.)
CHAPMAN, S., and COWLING, T. G. (1970).—"The Mathematical Theory of Non-uniform Gases." (Cambridge Univ. Press.)
CROMPTON, R. W., ELFORD, M. T., and ROBERTSON, A. G. (1970).—*Aust. J. Phys.* **23**, 667.
DAVYDOV, B. I. (1935).—*Phys. Z. SowjUn.* **8**, 59.
GINZBURG, V. L., and GUREVICH, A. V. (1960).—*Soviet Phys. Usp.* **3**, 115.
HOCHSTIM, A. R., and MASSEL, G. (1969).—*In* "Kinetic Processes in Gases and Plasmas". (Ed. A. R. Hochstim.) p. 141. (Academic Press: New York.)
KIHARA, T. (1953).—*Rev. mod. Phys.* **25**, 844.
KUMAR, K. (1967).—*Aust. J. Phys.* **20**, 205.
LORENTZ, H. A. (1916).—"Theory of Electrons." (2nd Ed.) (Teubner: Leipzig.)
MARGEEAU, H. (1946).—*Phys. Rev.* **69**, 508.
MORSE, P. M., ALLIS, W. P., and LAMAR, E. S. (1935).—*Phys. Rev.* **48**, 412.
PEKERIS, C. L., ALTERMANN, Z., FINKELSTEIN, L., and FRANKOWSKI, K. (1962).—*Phys. Fluids* **5**, 1608.