J. Fluid Mech. (1969), *vol.* 36, *part* 3, *pp.* 555–570

Printed in Great Britain

Minimum error solutions of the Boltzmann equation for shock structure

By R. NARASIMHA AND S. M. DESHPANDE

Department of Aeronautical Engineering, Indian Institute of Science, Bangalore 12

(Received 20 August 1968)

'Best' solutions for the shock-structure problem are obtained by solving the Boltzmann equation for a rigid sphere gas by applying minimum error criteria on the Mott-Smith ansatz. The use of two such criteria minimizing respectively the local and total errors, as well as independent computations of the remaining error, establish the high accuracy of the solutions, although it is shown that the Mott-Smith distribution is not an exact solution of the Boltzmann equation even at infinite Mach number. The minimum local error method is found to be particularly simple and efficient. Adopting the present solutions as the standard of comparison, it is found that the widely used v_x^2-moment solutions can be as much as a third in error, but that results based on Rosen's method provide good approximations. Finally, it is shown that if the Maxwell mean free path on the hot side of the shock is chosen as the scaling length, the value of the density-slope shock thickness is relatively insensitive to the intermolecular potential. A comparison is made on this basis of present results with experiment, and very satisfactory quantitative agreement is obtained.

1. Introduction

Recent studies of a model Boltzmann equation (Liepmann, Narasimha & Chahine 1962; Narasimha 1968) have provided some insight into the structure of a shock wave in a simple monatomic gas as described by kinetic theory, but the complexity of the true Boltzmann equation has till now precluded the calculation of reliable quantitative estimates for the shock thickness. An exact solution, even on a computer, has not yet proved possible, although Bird (1967) and Nordsieck & Hicks (1967) have recently reported some very interesting numerical experiments. Many approximate methods have been proposed and estimates of the shock thickness abound in the literature. However, there are considerable differences among these results, and as there is no completely rational theoretical basis for preferring one of these estimates over the rest, the problem is still essentially open.

Most of the approximate methods used so far are direct or indirect developments of a pioneering contribution of Mott-Smith (1951). They usually retain his ansatz for the distribution function containing one space-dependent free parameter, but differ in the methods used for the evaluation of this parameter. The technique employed by Mott-Smith himself was to require that a suitable moment of the error or residual be zero; it has been shown by Gustafson (1960) and Narasimha (1966) that the method of Rosen (1954) belongs to the same class. The choice of the 'moment function' H used in these methods is to a great extent arbitrary, and, as Rode & Tanenbaum (1967) have recently highlighted, the results show an unfortunately strong dependence on the choice. This fact, coupled with uncertainties in our knowledge of the exact intermolecular potential for any given gas, suggests that agreement between experiment and the results of one of the approximate methods is not a sufficient indication of success.

This variability in the results from the moment methods has occasionally prompted the view that what is required is a better basic ansatz for the distribution. On the other hand, a result of Sakurai (1957) has often been quoted in defence of the Mott-Smith (or bimodal) ansatz: namely that for an infinitely strong shock, the ansatz represents an exact solution of the Boltzmann equation. There are, however, two limitations to this result. First, it is not uniformly valid in molecular velocity space, and there is no obvious reason why the regions in which it is not valid can be ignored. Secondly, the result rests on the shock thickness taking on a certain limiting value: this appears as a postulate rather than a consequence. Oberai (1967) has recently shed some light on this question by proving the interesting result that the value assumed is the best in a least squares sense for the ansatz. We will be able to show here that the ansatz in fact does not represent the exact solution.

Apart from its attractive simplicity there are a few other reasons for not abandoning the Mott-Smith ansatz in haste. The exact solutions of the BGK model equation obtained by Chahine & Narasimha (1965) suggest that the true distribution does resemble the form proposed by Mott-Smith although a detailed asymptotic study (Narasimha 1968) shows that it is unlikely to be an exact solution (at least not for all inter-molecular potentials of interest). Bird's (1967) Monte-Carlo calculations also support this belief. Finally, Ananthasayanam & Narasimha (1968) have shown, again for the model, that the bimodal ansatz can give reliable estimates of the density-slope shock thickness provided suitable criteria are employed.

The main object of this paper is to present and discuss results for shock thickness using certain minimum error criteria. Although it may generally be conceded that such criteria are more rational than moment methods, they are not free from a certain arbitrariness either, as the definition of the 'error' is not unique. However, we show here that by investigating the consequences of adopting two such criteria, which we shall call minimization of local and total error respectively (§ 2), we can get a fairly good idea of the accuracy of the final solutions.

The application of minimum error methods to the Boltzmann equation would seem to involve great difficulties in practice (Oberai 1967), but with the knowledge that the collision integrals for the Mott-Smith ansatz can be calculated explicitly in closed form (Deshpande & Narasimha 1969) these difficulties become much less severe. Furthermore, we shall find here (§ 3) that the minimum 'local' error criterion is not only successful in terms of accuracy but is quite simple to apply, and in fact gives results in closed form (although they will be found to be rather complicated). A critical comparison of these results with those obtained by other approximate methods (§ 4) provides an interesting assessment of the latter.

The calculations mentioned above are all strictly valid only for rigid-sphere molecules. However, we show in § 5 that they have much wider relevance embracing more general intermolecular potentials, provided the density-slope shock thickness is scaled with the Maxwell mean free path on the hot side of the shock. The adoption of an equivalent scaling has previously been found useful by Lighthill (1956) for estimating the Navier–Stokes shock thickness, and by Ananthasayanam & Narasimha (1968) for the BGK model. It suppresses to a great extent the importance of the intermolecular potential, and so a comparison of present results with experiments becomes meaningful. In fact, the comparison turns out to be very satisfactory.

2. Description of minimum error methods

For the one-dimensional problem of the flow through a plane shock layer (figure 1), we write the Boltzmann equation in a shock-fixed co-ordinate system as

$$v_x(\partial/\partial x)f(\mathbf{v};x) = \mathscr{J}(f,f), \tag{2.1}$$

where f is the distribution function and $\mathbf{v}$ the molecular velocity vector with a component v_x along the direction of the mean flow. $\mathscr{J}(f,f)$ represents the col-

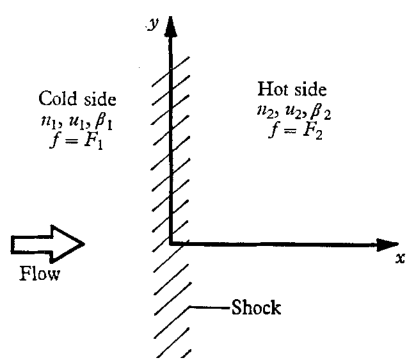

FIGURE 1. Co-ordinate system for shock.

lision integrals; the notation follows that of Deshpande & Narasimha (1969) (referred to as I in the following). Boundary conditions on f are

$$f(\mathbf{v}; -\infty) = F_1(\mathbf{v}), \quad f(\mathbf{v}; +\infty) = F_2(\mathbf{v}), \tag{2.2}$$

where F represents the equilibrium Maxwellian distribution, and subscripts 1 and 2 refer to the far upstream and downstream sides of the shock, the parameters in F being related through the Rankine–Hugoniot conditions. We shall often use the mean free path on the *hot* side of the shock,

$$l = (2^{\frac{1}{2}}\pi n_2 \sigma^2)^{-1}, \tag{2.3}$$

as the basic length scale in the problem. The reason for preferring this to the more usual choice of the cold side mean free path will become apparent later (see § 5).

As in most approximate methods for solving (2.1), we adopt the simple bimodal ansatz for f and write

$$f_0(\mathbf{v};x) = \{1-\nu(x)\}F_1(\mathbf{v})+\nu(x)F_2(\mathbf{v}), \tag{2.4}$$

where $\nu(x)$ is a function to be determined; from (2.2), $\nu(-\infty)=0$ and $\nu(+\infty)=1$. As (2.4) will not in general solve (2.1) exactly, we define a residual or error e as

$$e(\mathbf{v};x) = v_x(\partial f_0/\partial x) - \mathscr{J}(f_0,f_0)$$
$$= v_x(F_2-F_1)(d\nu/dx) - \nu(1-\nu)(\mathscr{J}_{12}+\mathscr{J}_{21}). \tag{2.5a}$$

We further define 'local' and 'total' errors as

$$E(x) = \int e^2(\mathbf{v};x)\,D\mathbf{v}, \quad \bar{E} = \int E(x)\,dx, \tag{2.5b}$$

respectively, the integrations being carried out in each case over the whole range of the relevant variable. Substituting (2.5a) into (2.5b), we can write

$$E = X\nu'^2 - 2Y\nu(1-\nu)\nu' + Z\nu^2(1-\nu)^2, \tag{2.6}$$

where $\nu' \equiv d\nu/dx$ and

$$\left.\begin{aligned} X &= \int v_x^2(F_2-F_1)^2\,D\mathbf{v}, \\ Y &= \int v_x(F_2-F_1)(\mathscr{J}_{12}+\mathscr{J}_{21})\,D\mathbf{v}. \\ Z &= \int (\mathscr{J}_{12}+\mathscr{J}_{21})^2\,D\mathbf{v}. \end{aligned}\right\} \tag{2.7}$$

It proves to be of interest to consider two alternative criteria for determining the 'best' ν'. The first is to minimize the local error, i.e. put $\partial E/\partial\nu' = 0$; this gives

$$\nu' = (Y/X)\,\nu(1-\nu). \tag{2.8}$$

The second is to minimize the total error $\bar{E}$; the function $\nu(x)$ that does this can be obtained as a solution of the Euler equation associated with the variational problem $\delta\bar{E}=0$. Using the boundary conditions on ν, the governing equation is easily found to be

$$\nu' = (Z/X)^{\frac{1}{2}}\,\nu(1-\nu). \tag{2.9}$$

In either case the solution for ν is the well-known hyperbolic tangent,

$$\nu(x) = \tfrac{1}{2}\{1+\tanh(2x/\delta)\}, \tag{2.10}$$

where

$$\delta \equiv \frac{n_2-n_1}{(dn/dx)_{\max}} = 1/\nu'_{\max} \tag{2.11}$$

is the usual maximum density-slope shock thickness. Using subscripts L and T to denote values obtained by minimizing local and total error respectively, we find from (2.8) and (2.9)

$$\delta_L = 4(X/Y), \quad \delta_T = 4(X/Z)^{\frac{1}{2}}, \tag{2.12a}$$

$$\delta_L^2 - \delta_T^2 = 16(X/Y^2Z)(XZ-Y^2). \tag{2.12b}$$

Now the discriminant $XZ-Y^2$ of the error quadratic (2.6) is proportional to the minimum value of $\bar{E}$ and hence is a measure of the 'distance' between the approximate and exact solutions. From (2.12b), we therefore see that the closeness of δ_L to δ_T is a good indication of the accuracy of either solution (at least as long as the factor X/Y^2Z remains nonzero).

3. The error coefficients

Among the three quantities X, Y, and Z appearing in (2.6) X is easily found as it involves standard integrals commonly encountered in kinetic theory. We may write

$$X = \sum_{i,j}(-)^{i+j}X_{ij}, \quad (i,j = 1,2) \tag{3.1a}$$

where

$$\begin{aligned} X_{ij} &\equiv \int v_x^2 F_i(\mathbf{v})\,F_j(\mathbf{v})\,D\mathbf{v} \\ &= \tfrac{1}{2}n_i n_j(\beta_i\beta_j/\pi)^{\frac{3}{2}}(\beta_i+\beta_j)^{-\frac{7}{2}} \\ &\quad\times\{\beta_i+\beta_j+2(\beta_i u_i+\beta_j u_j)^2\}\exp\{-\beta_i\beta_j(\mathbf{u}_i-\mathbf{u}_j)^2/(\beta_i+\beta_j)\}. \end{aligned} \tag{3.1b}$$

In the following sections, we consider the coefficients Y and Z.

3.1. *Evaluation of* Y

From (2.7), it is seen that Y represents a moment of the collision integrals, and so can be looked upon as a rather complicated effective cross-section of the molecule. By a well known lemma about such moments (e.g. Chapman & Cowling 1960, § 3.5) we have relations of the type

$$\int H(\mathbf{v})\,\mathscr{J}(f_i,f_j)\,D\mathbf{v} = \int [H(\mathbf{v}')-H(\mathbf{v})]f_i(\mathbf{v})f_j(\mathbf{w})\,gb\,db\,d\epsilon\,D\mathbf{w}\,D\mathbf{v}, \tag{3.2}$$

where the notation is the same as in I and $H(\mathbf{v})$ is any function of the velocity vector $\mathbf{v}$. Using (3.2) in (2.7), Y can be written as

$$Y = \Sigma\,(-)^i n_i n_j n_k(\beta_i\beta_j\beta_k/\pi^3)^{\frac{3}{2}}\,(Y'_{ijk}-Y_{ijk}), \tag{3.3}$$

where the summation is over all $(i,j,k) = (1,2)$,

$$Y_{ijk} = \int v_x \exp\{-\beta_i(\mathbf{v}-\mathbf{u}_i)^2-\beta_j(\mathbf{v}-\mathbf{u}_j)^2-\beta_k(\mathbf{w}-\mathbf{u}_k)^2\}\,gb\,db\,d\epsilon\,D\mathbf{v}\,D\mathbf{w}, \tag{3.4a}$$

$$Y'_{ijk} = \int v'_x \exp\{-\beta_i(\mathbf{v}'-\mathbf{u}_i)^2-\beta_j(\mathbf{v}-\mathbf{u}_j)^2-\beta_k(\mathbf{w}-\mathbf{u}_k)^2\}\,gb\,db\,d\epsilon\,D\mathbf{v}\,D\mathbf{w}. \tag{3.4b}$$

From the symmetry in (3.4a), and from the vanishing of the collision integrals $\mathscr{J}(F_i,F_j)$ in (3.2) when $i=j$, we have†

$$Y_{ijk} = Y_{jik}, \quad Y'_{ijj} = Y_{ijj}.$$

Therefore only four integrals of the type (3.4) contribute to Y.

All these integrals can be evaluated analytically; the procedure is rather laborious, but the main idea is to use $\mathbf{g}$ as one of the two independent velocity variables, choose the other one so that the exponentials in (3.4) take on a simple

† We are *not* using the summation convention in this paper.

form, and integrate with respect to the new variables instead of $\mathbf{v}$ and $\mathbf{w}$. A particularly convenient way of achieving this is to use a set of transformations employed by Suchy (1963) in a study of certain cross-section integrals. The new variables are defined by the relations

$$\left.\begin{aligned} \mathbf{V} &= \tfrac{1}{2}\bar{\beta}^{\frac{1}{2}}(\mathbf{v}-\mathbf{u}_{ij}+\mathbf{w}-\mathbf{u}_k)+\tfrac{1}{2}\bar{\beta}^{-\frac{1}{2}}(\beta_i+\beta_j-\beta_k)(\mathbf{g}-\mathbf{u}_{ij}+\mathbf{u}_k), \\ \mathbf{G} &= \{(\beta_i+\beta_j)\beta_k/\bar{\beta}\}^{\frac{1}{2}}\mathbf{g}, \quad \mathbf{U} = \{(\beta_i+\beta_j)\beta_k/\bar{\beta}\}^{\frac{1}{2}}(\mathbf{u}_{ij}-\mathbf{u}_k), \end{aligned}\right\} \tag{3.5}$$

where $\bar{\beta} \equiv \beta_i+\beta_j+\beta_k, \quad (\beta_i+\beta_j)\mathbf{u}_{ij} \equiv \beta_i\mathbf{u}_i+\beta_j\mathbf{u}_j.$

The set $(\mathbf{V}, \mathbf{G})$ is linearly related to the set $(\mathbf{v}, \mathbf{w})$, so either member of each set is easily found in terms of the other set. In particular, the volume elements transform as

$$D\mathbf{v}D\mathbf{w} = \{(\beta_i+\beta_j)/\beta_k\}^{-\frac{3}{2}}D\mathbf{V}D\mathbf{G} \tag{3.6}$$

and the exponentials take the simple form shown in (3.8) below. Substituting from (3.5) and (3.6) into (3.4*a*) and completing the trivial integrations in b and ϵ we can write

$$Y_{ijk} = \frac{\pi\sigma^2}{\beta_k^{\frac{3}{2}}(\beta_i+\beta_j)^2}\exp\left[-\frac{\beta_i\beta_j(\mathbf{u}_i-\mathbf{u}_j)^2}{\beta_i+\beta_j}\right] \times[\bar{\beta}^{\frac{1}{2}}\bar{u}_x I_1(\mathbf{U})+\{(\beta_i+\beta_j)/\beta_k\}^{-\frac{1}{2}}I_2(\mathbf{U})], \tag{3.7}$$

where $\bar{\beta}\bar{\mathbf{u}} \equiv \beta_i\mathbf{u}_i+\beta_j\mathbf{u}_j+\beta_k\mathbf{u}_k,$

subscript x denotes the component on an axis along v_x, and I_1 and I_2 are integrals defined by

$$I_1(\mathbf{U}) \equiv \int G\exp\{-V^2-(\mathbf{G}-\mathbf{U})^2\}D\mathbf{V}D\mathbf{G}, \tag{3.8a}$$

$$I_1(\mathbf{U}) \equiv \int GG_x\exp\{-V^2-(\mathbf{G}-\mathbf{U})^2\}D\mathbf{V}D\mathbf{G}. \tag{3.8b}$$

These integrals can be evaluated in closed form in terms of certain confluent hypergeometric functions as shown in appendix A, so that the Y_{ijk} can be easily computed from (3.7).

Now consider the integrals Y'_{ijk}. We first write the velocity $\mathbf{v}'$ after collision as $\mathbf{v}+\mathbf{s}$, obtaining

$$\mathbf{s} = \mathbf{v}'-\mathbf{v} = \tfrac{1}{2}(\mathbf{g}'-\mathbf{g}), \quad s^2 = g^2\cos^2\psi \tag{3.9}$$

from the dynamics of a collision. In (3.9) ψ is the angle defining the apse-line (see figure 1 of I). Substituting from (3.9) into (3.4*b*), and transforming from $\mathbf{v}, \mathbf{w}$ to $\mathbf{V}, \mathbf{G}$ as before using (3.5), we obtain

$$\begin{aligned} Y'_{ijk} = \frac{\bar{\beta}^{\frac{1}{2}}}{\beta_k^{\frac{3}{2}}(\beta_i+\beta_j)^2}&\exp\left[-\frac{\beta_i\beta_j}{\beta_i+\beta_j}(\mathbf{u}_i-\mathbf{u}_j)^2\right] \\ &\times\int(\bar{u}_x+s_x+\bar{\beta}^{-\frac{1}{2}}V_x+\{\bar{\beta}(\beta_i+\beta_j)/\beta_k\}^{\frac{1}{2}}G_x) \\ &\times\exp[-V^2-(\mathbf{G}-\mathbf{U})^2-\beta_i s^2-2\beta_i\mathbf{s}.(\bar{\mathbf{u}}-\mathbf{u}_i+\bar{\beta}^{-\frac{1}{2}}\mathbf{V} \\ &+\{\bar{\beta}(\beta_i+\beta_j)/\beta_k\}^{-\frac{1}{2}}\mathbf{G})]\,Gb\,db\,d\epsilon D\mathbf{G}D\mathbf{V}. \end{aligned} \tag{3.10}$$

It is clear that the integration with respect to $\mathbf{V}$ can again be performed as before. We find it convenient to express the result in terms of the angles θ, θ' made by the vectors $\mathbf{g}, \mathbf{g}'$ respectively with the axis along v_x. From the geometry of the encounter, it is easily shown that the two angles are actually related to each other:

$$\cos\theta' = -\cos\theta\cos 2\psi + \sin\theta\sin 2\psi\sin\epsilon. \tag{3.11a}$$

Also, from (3.9)

$$s_x = \tfrac{1}{2}g(\cos\theta' - \cos\theta), \tag{3.11b}$$

recalling that conservation of energy in an encounter between two molecules requires that $g = g'$.

Using (3.11), the result of integrating (3.10) in $\mathbf{V}$ is

$$\begin{aligned} Y'_{ijk} = {} & \frac{\pi^{\frac{3}{2}}\bar{\beta}^{\frac{1}{2}}}{\beta_k^{\frac{3}{2}}(\beta_i+\beta_j)^2}\exp\left[-\frac{\beta_i\beta_j(\mathbf{u}_i-\mathbf{u}_j)^2+\bar{\beta}\beta_k(\bar{\mathbf{u}}-\mathbf{u}_k)^2}{\beta_i+\beta_j}\right] \\ & \times[\bar{u}_x + \{\bar{\beta}(\beta_i+\beta_j)/\beta_k\}^{-\frac{1}{2}}G\cos\theta + \tfrac{1}{2}(\beta_j+\beta_k)\{\bar{\beta}\beta_k(\beta_i+\beta_j)\}^{-\frac{1}{2}} \\ & \times G(\cos\theta'-\cos\theta)]\exp[-G^2(1+\alpha_1\cos^2\psi) \\ & + G(\alpha_2\cos\theta+\alpha_3\cos\theta')]\,Gb\,db\,d\epsilon\,D\mathbf{G}, \end{aligned} \tag{3.12}$$

where

$$\left.\begin{aligned} &\alpha_1 = \beta_i(\beta_j-\beta_k)/\bar{\beta}, \quad \alpha_2 = \{\beta_k(\beta_i+\beta_j)/\bar{\beta}\}^{-\frac{1}{2}}\{2(\bar{\mathbf{u}}-\mathbf{u}_k)\beta_k+\beta_i(\bar{\mathbf{u}}-\mathbf{u}_i)\}_x, \\ &\alpha_3 = \{\beta_k(\beta_i+\beta_j)/\bar{\beta}\}^{-\frac{1}{2}}\beta_i(\mathbf{u}_i-\bar{\mathbf{u}})_x. \end{aligned}\right\} \tag{3.13}$$

Finally, we replace b by $\sigma\sin\psi$ for rigid spheres, and $D\mathbf{G}$ by the appropriate form in a spherical co-ordinate system in which G is the radius and θ the polar angle. Integration with respect to the azimuthal angle merely yields a factor 2π. Equation (3.12) then takes the form

$$\begin{aligned} Y'_{ijk} = {} & \frac{\pi^{\frac{5}{2}}\sigma^2\bar{\beta}^{\frac{1}{2}}}{\beta_k^{\frac{3}{2}}(\beta_i+\beta_j)^2}\exp\left[-\frac{\beta_i\beta_j(\mathbf{u}_i-\mathbf{u}_j)^2+\bar{\beta}\beta_k(\bar{\mathbf{u}}-\mathbf{u}_k)^2}{\beta_i+\beta_j}\right] \\ & \times[\bar{u}I_{000} + \{[\bar{\beta}(\beta_i+\beta_j)/\beta_k]^{-\frac{1}{2}}-1\}I_{110} + \tfrac{1}{2}\{\bar{\beta}\beta_k(\beta_i+\beta_j)\}^{-\frac{1}{2}}(\beta_j+\beta_k)I_{101}], \end{aligned} \tag{3.14}$$

where

$$\begin{aligned} I_{lmn} = {} & \int_0^{2\pi}d\epsilon\int_0^{\frac{1}{2}\pi}d\psi\int_0^{\pi}d\theta\int_0^{\infty}dG\exp[-G^2(1+\alpha_1\cos^2\psi) \\ & + G(\alpha_2\cos\theta+\alpha_3\cos\theta')]\,G^l\cos^m\theta\cos^n\theta'. \end{aligned} \tag{3.15}$$

It is actually enough to evaluate I_{000}, because the other two integrals in (3.14) follow from the relations

$$I_{110} = \frac{\partial}{\partial\alpha_2}I_{000}, \quad I_{101} = \frac{\partial}{\partial\alpha_3}I_{000}. \tag{3.16}$$

It is shown in appendix A that I_{000} can also be evaluated in closed form in terms of confluent hypergeometric functions.

Thus using the programme mentioned in I for computing these functions, the the coefficient Y can be evaluated from (3.3), (3.7) and (3.14).

3.2. *Evaluation of Z*

The computation of the terms $\mathscr{J}_{ij}$ in the integral (2.7) defining Z has already been described in I; to obtain Z itself, it appears necessary to resort to numerical integration. The problem can be simplified to some extent by exploiting the symmetry of the integrand about the v_x-axis to write the volume element $D\mathbf{v}$

as $2\pi v_n dv_n dv_x$, where v_n is the velocity component normal to the v_x-axis. The range of integration thus becomes the half-plane $-\infty < v_x < +\infty$, $0 \leqslant v_n < \infty$. Even so, constructing an effective numerical scheme for integration turned out to be far from simple. After extensive trials with various well-known schemes, it was eventually found that the quadrature procedure suggested by Romberg (see e.g. Bauer *et al.* 1962) was both successful and efficient. The details of the programme finally written will be described elsewhere, but as it was crucial to the success of the final calculations, it may be worthwhile to mention some of its salient features here.

First, for some fixed value of v_x the range in v_n was divided into certain sections whose length depended on β. The integral was then evaluated over each section carrying out successively finer sub-divisions of the section as dictated by the Romberg procedure till the convergence was satisfactory. The number of sections was determined by the requirement that the contribution from the last section be a prescribed small fraction of an estimate of the total integral (this estimate being improved if necessary as the computation progressed). After the integration with respect to v_n was complete at the assumed v_x, a similar procedure was employed for integration with respect to v_x.

Typically about 35 sec were required on a CDC-3600 to evaluate the double integral to three significant figures.

4. Results

Knowing the coefficients X, Y and Z the shock thickness is easily obtained from (2.12). We first consider the limiting case of infinite Mach number, for which the results are particularly simple and interesting. In the minimum total error method, we recover the value for shock thickness found by Oberai (1967) and postulated by Sakurai (1957).

The value of δ_L, the thickness from the minimum local error solution, can be written down analytically (at any Mach number) since both X and Y are known in closed form. By a rather lengthy but quite straightforward analysis of the expressions derived for these coefficients in § 3, we can also obtain their asymptotic behaviour as $M_1 \rightarrow \infty$. It is found that

$$X \approx X_{11} = \tfrac{1}{2} n_1^2 \beta_1^{\frac{1}{2}} \gamma M_1^2 (2\pi)^{-\frac{3}{2}} [1 + O(M_1^{-2})] \tag{4.1}$$

from (3.1), and

$$\begin{aligned} Y &\approx n_1^2 n_2 (\beta_1^2 \beta_2/\pi^3)^{\frac{3}{2}} Y_{112} [1 + O(M_1^{-2})] \\ &= \frac{1}{2} \frac{n_1^3 \beta_1^{\frac{1}{2}}}{n_2 l} \frac{\gamma M_1^2}{\pi^2 (\gamma - 1)^{\frac{1}{2}}} \exp\left(-\frac{1}{\gamma - 1}\right) \Phi\left(2, \tfrac{3}{2}, \frac{1}{\gamma - 1}\right) \end{aligned} \tag{4.2}$$

from (3.3), (3.7) and (3.14). Substituting in (2.12*a*), we obtain δ_L at $M_1 = \infty$. For $\gamma = \frac{5}{3}$, the result is

$$\delta_L / l = 8(3/\pi)^{-\frac{1}{2}} e^{\frac{3}{2}} / \Phi(2, \tfrac{3}{2}, \tfrac{3}{2}) = 5{\cdot}691999 \tag{4.3}$$

which is exactly the same as the limiting value for δ_T.

At finite Mach numbers, the solutions have to be found partly by computation, as already described. Table 1 is a summary of the results obtained, which are displayed along with those of some other well-known approximate methods. It may be worth recalling that the shock thickness in this table is quoted in terms of the hot side mean free path, anticipating an argument that will be spelled out in § 5. Of course conversion to the cold side mean free path as the scaling length is easily effected for rigid spheres, using the density ratio across the shock.

M_1	Minimum local error	Minimum total error	$H = v_x^2$	$H = v_x^3$	$H = F_1 - F_2$	Navier–Stokes
1·2	0·0463	0·05	0·0460	0·0409	0·0555	—
1·4	0·0750	—	0·0629	0·0569	0·0863	—
1·5	—	0·0883	—	—	—	0·1003
2·0	0·1173	0·1200	0·1047	0·1064	—	0·1428
2·2	0·1246	0·1267	—	—	0·1264	—
2·5	0·1316	—	0·1123	0·1226	0·1317	—
3·0	—	0·1420	0·1152	0·1322	0·1379	0·1811
4·0	0·1503	0·1515	—	—	0·1470	—
5·0	0·1563	0·1573	0·1172	0·1475	—	0·2058
6·0	0·1604	0·1613	—	—	0·1586	—
7·0	0·1643	0·1641	—	—	—	—
8·0	0·1657	0·1662	—	—	0·1647	—
9·0	0·1673	0·1678	—	—	—	—
10·0	0·1685	0·1684	0·1172	0·1545	0·1681	0·2174
15·0	—	0·1723	—	—	—	
20·0	—	0·1736	—	—	—	—
30·0	—	0·1747	—	—	0·1747	—
∞	0·1757	0·1757	0·1172	0·1569	0·1757	—

TABLE 1. Values of l/δ as computed by various methods. In the figures quoted for the minimum total error method, there is an uncertainty of a few units in the last place.

There are several interesting features in the data of table 1 which call for comment. First of all, not only is $\delta_L = \delta_T$ in the limit $M_1 \to \infty$, but the difference $(\delta_L - \delta_T)$ is always small; it is less than 2 % for $M_1 > 2$. From the remark already made in § 2 about the relation between this difference and the accuracy of the solutions, we must now conclude that these minimum error solutions must be very close to the exact values. (Actual values of the residual error itself will be given in § 6.) Secondly, accepting these values as providing a suitable standard of comparison for other approximate solutions, we note that the most popular method, which uses v_x^2 as the moment function, is also the least satisfactory (of the three methods with which comparison is offered in table 1). At $M_1 = \infty$, it yields a value which is about a third in error. The v_x^3-moment results are much better at higher Mach numbers, but rather poorer at lower ones. (The entries in the table for these two methods are taken from Mott-Smith (1951).)

We have also given in table 1 results obtained with $F_1 - F_2$ as the moment function. This choice is equivalent to an application of the restricted variational technique of Rosen (1954). As the numerical results presented by Rosen do not go beyond a Mach number of 4·0, we made independent calculations which incidentally revealed slight errors in Rosen's computations. (Thus at $M_1 = 1{\cdot}2$, his results are too high by about 4 %.) The calculations at high Mach numbers brought to light the remarkable fact that the $(F_1 - F_2)$ moment solutions are always very good approximations, and at $M_1 = \infty$ are identical with the minimum error solution. The last statement is relatively easily confirmed by an asymptotic analysis of Rosen's results, which also yields (4.3) in the limit $M_1 \to \infty$.

Finally, for the sake of completeness, we have included in the table Navier–Stokes values for the shock-thickness at a few Mach numbers (taken from some unpublished computations by Chahine & Narasimha). Making the reasonable assumption that the Navier–Stokes theory is valid near $M_1 = 1{\cdot}5$, it is interesting to note how close the present minimum error solutions are even at these low Mach numbers.†

5. Discussion

It remains to consider the significance of our results for a real gas, whose molecules can rarely be represented as hard spheres.

It is well-known, from both continuum and gas-kinetic theories of shock structure, that the ratio δ/Λ_1, i.e. the shock-thickness expressed in terms of the Maxwell mean free path on the cold side, is very sensitive to the intermolecular potential (or, equivalently, to the viscosity-temperature law for the gas) at high Mach numbers. (The limiting values at $M_1 = \infty$ go all the way from a finite value to infinity.) From time to time, it has been suggested that the choice of a more appropriate length scale will suppress this sensitivity. For example, Liepmann *et al.* (1962) have shown that the use of the Maxwell mean free path Λ_* at the sonic point inside the shock is particularly appropriate for the Navier–Stokes solutions; Muckenfuss (1962) has proposed the value (say Λ_0) at the point where $\nu = \frac{1}{2}$, from a study of Mott-Smith type solutions. The disadvantage with these scales is that Λ has to be known at an interior point of the shock where the state of the gas (in a real shock) cannot be determined with certainty, because experiments do not provide complete information and the theories are not exact.

We propose here that the use of Λ_2 (the Maxwell mean free path on the hot side of the shock) as a scaling length has many advantages. (For a rigid sphere gas $\Lambda_2 = l$.) For weak shocks the mean free path is of the same order everywhere in the shock, and so one choice is nearly as good as another. Therefore, the merit of the proposal must be judged largely by its usefulness for strong shocks. Now as $M_1 \to \infty$, it is easily shown that δ/Λ_2 always tends to finite non-zero values in both continuum and kinetic theories. In fact, this is a simple consequence of the success of the other scales mentioned earlier. Consider first the kinetic theories. Muckenfuss (1962) has shown that as $M_1 \to \infty$, $\delta/\Lambda_1 = O(M_1^{2\omega-1})$, where ω is the index in the viscosity law $\mu \sim T^{\omega}$. But as

$$\Lambda \sim \mu(T)/nT^{\frac{1}{2}} \tag{5.1}$$

we see that $\Lambda_1/\Lambda_2 = O(M_1^{1-2\omega})$, and hence $\delta/\Lambda_2 = O(1)$ for all ω.

† We note here that the Monte-Carlo calculations of Bird (1967) give, at $M_1 = 10{\cdot}0$, the value $l/\delta = 0{\cdot}078 \pm 0{\cdot}004$, which is considerably lower than the present values as well as the other figures quoted in table 1. The reasons for this rather large discrepancy may partly lie in the sampling procedures adopted by Bird.

These order-of-magnitude statements are quite general, and do not depend on the particular choice of moment function that Muckenfuss actually made in evaluating the ν of (2.4). The crux of the matter is simply that where the density slope is maximum (i.e. at $\nu = \frac{1}{2}$ for the solution (2.10)), the temperature $T_0 = O(T_2)$. What is even more interesting is that T_0 is very nearly *equal* to T_2: working out the relation between T and ν for the bimodal ansatz (2.4), we get

$$\frac{T}{T_1} = \frac{1-\nu}{1+\nu(n_{21}-1)} + \frac{\nu n_{21} T_{21}}{1+\nu(n_{21}-1)} + \tfrac{1}{3}\gamma M_1^2 \left\{\frac{n_{21}-1}{1+\nu(n_{21}-1)}\right\}^2 \frac{\nu(1-\nu)}{n_{21}} \tag{5.2}$$

where $$n_{21} \equiv n_2/n_1, \quad T_{21} \equiv T_2/T_1.$$

Putting $\nu = \frac{1}{2}$ and taking the limit $M_1 \to \infty$, we can show from (5.2) that

$$\frac{T_0}{T_2} \approx \frac{(\gamma+1)(3\gamma+1)}{6\gamma^2};$$

for $\gamma = \frac{5}{3}$, T_0/T_2 is $\frac{24}{25}$.

Now if we define an effective diameter for a molecule which is a centre of force by equating its Maxwell mean free path with that for a rigid sphere gas, we will of course find that this diameter depends in general on the temperature. But then the closeness of T_0 to T_2 noted above leads to the interesting conclusion that near and beyond $\nu = \frac{1}{2}$, the temperature changes so little that the molecules do indeed behave very nearly like rigid spheres, with a diameter corresponding to their effective cross-section at the temperature on the hot side. This strongly suggests that Λ_2 is the appropriate length scale for the density profile.

Although we are not here directly concerned with Navier–Stokes solutions, it may not be out-of-place to point out that these also show that $\delta/\Lambda_2 = O(1)$ as $M_1 \to \infty$, irrespective of ω. Indeed this has been recognized by Lighthill (1956), who gives interesting bounds for the Navier–Stokes shock thickness in terms of essentially the same length scale as our Λ_2. It also follows from the result of Liepmann *et al.* (1962) mentioned above, for $T_* = O(T_2)$ and hence $\Lambda_* = O(\Lambda_2)$. These statements are particularly easy to verify for a gas with a Prandtl number of $\frac{3}{4}$, for which the stagnation enthalpy is constant across the shock and the temperature is easily calculated from the velocity. We find then that

$$T_* \approx T_2(\gamma+1)/2\gamma$$

as $M_1 \to \infty$, and for $\gamma = \frac{5}{3}$ the factor is 0·8: again T_* is quite close to T_2.

The choice of Λ_2 as the scaling length has the advantage that there is no uncertainty about the state of the gas where it is to be evaluated. Finally, we may mention that work on the BGK model (Ananthasayanam & Narasimha 1968) has also demonstrated the superiority of Λ_2 as the scale for shock thickness.

Following these arguments, we make a comparison, in figure 2, of the present calculations with the measurements made in argon by Russell (1965), Camac (1965) and Linzer & Hornig (1963). The experimental data are invariably given in terms of Λ_1, and have been reduced to Λ_2 assuming $\omega = 0{\cdot}816$, which is the commonly accepted value for argon. However, there is some uncertainty regarding ω, and if we insist on a viscosity law of the type $\mu \sim T^\omega$, one should probably take ω as a weak function of the temperature. The point, however, is that even if ω were somewhat different, the theoretical predictions in figure 2 would not be materially altered; see for example the small range in which the v_x^2-moment results lie even for different values of ω, showing definitely that the v_x^2-moment calculations do not agree with experiment. On the other hand, there is excellent agreement between the measurements and the minimum error solutions found here.

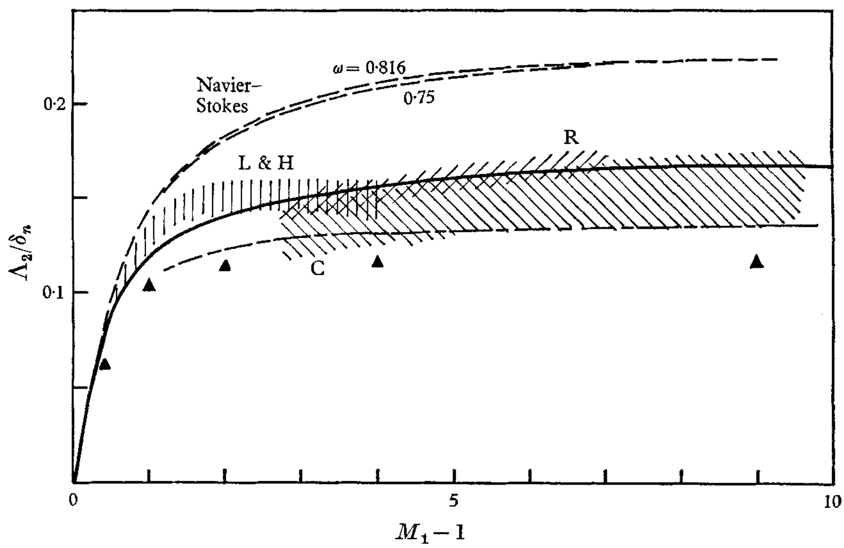

FIGURE 2. Maximum density-slope shock thickness in argon; – —— –, v_x^2, moment values for $\omega = 0.816$; ▲, same for $\omega = 0.5$; ———, minimum total error solution. Hatched areas represent experimental data; L & H, Linzer & Hornig (1963); C, Camac (1965); R, Russell (1965).

6. Conclusions

Although the closeness of the results obtained by the two minimum error methods indicates that their accuracy is high, the fact that the results tend to coincide as $M_1 \to \infty$ does not imply that we have an exact solution. The reason is that the error E of the solutions does not tend to zero. As all three coefficients X, Y and Z in (2.6) have been obtained by us, detailed results for $E(\nu)$ also become available, but it is enough to consider the minimum value of E at $\nu = \frac{1}{2}$. Calling this $E_{\min}$, we obtain from (2.6), (2.8) and (2.12*a*)

$$E_{\min} = X\Lambda_1^2(\delta_T^{-2} - \delta_L^{-2}).$$

As $M_1 \to \infty$ we have $\delta_T \to \delta_L$, but from (4.1) $X \to \infty$ like M_1^2, with the result that $E_{\min}$ remains non-zero and finite. Figure 3 shows computed values of $E_{\min}$ as a function of M_1.

It follows that the value of shock thickness that Sakurai postulated is not the exact value, and *a fortiori* that the bimodal distribution is not an exact (uniformly valid) solution of the Boltzmann equation. It does represent a 'solution' in what was called the inner limit in I, i.e. near the supersonic peak in velocity space. But this is not enough for obtaining the moments accurately, as the outer limit makes contributions of the same order. It is shown in appendix B, by an asymptotic analysis of e, that the Mott-Smith ansatz is indeed not a solution of the Boltzmann equation in the outer limit even when $M_1 \to \infty$.

It must, however, be emphasised that in spite of this, the present work shows that the bimodal ansatz can lead to quite accurate estimates of the shock thickness, provided the proper criteria are employed to determine the free parameter. It will be generally agreed that minimum error methods are the most rational

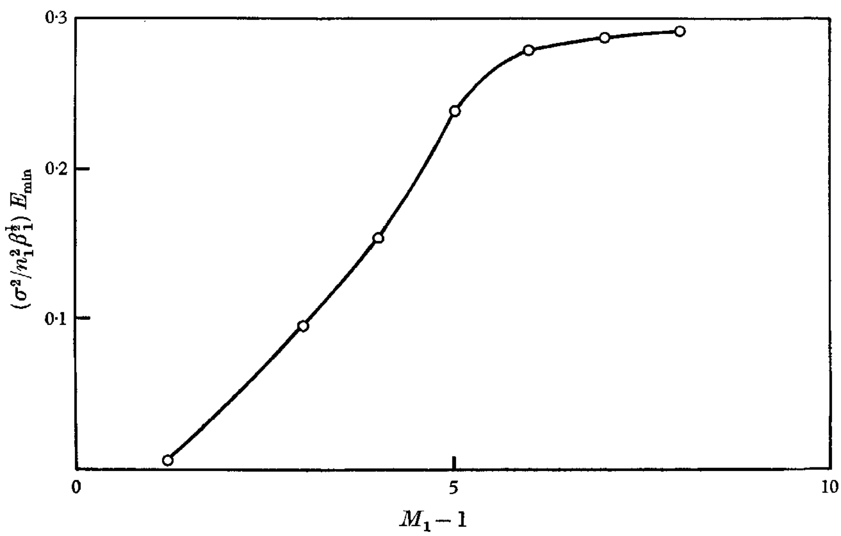

FIGURE 3. Non-dimensional minimum error at $\nu = \frac{1}{2}$. The curve is drawn through the values obtained from the computations, denoted by open circles.

when feasible, and hence the minimum 'local' error criterion, possessing the further advantage of simplicity, invites widespread use. Among the moment methods, the power functions v_x^n yield rather divergent results and are generally unsatisfactory. But $F_1 - F_2$ appears to be a very good choice, and the reason for its success is almost certainly that it weights properly those regions in velocity space that contribute appreciably to the number density, as discussed in some detail by Ananthasayanam & Narasimha (1968) for solutions of the BGK model equation.

From the data presented in figure 2, we may conclude that the Navier–Stokes equations are satisfactory up to $M_1 \lesssim 2$, and beyond this the shock thickness is nearly a constant multiple of the downstream Maxwell mean free path, decreasing to an asymptotic value of about $5{\cdot}7\,\Lambda_2$ at large Mach numbers. Incidentally as all available evidence (both theoretical and experimental) indicates that Λ_2 is the most appropriate scaling length for the density-slope shock thickness, we would like to suggest here that, in future, experimental results should if possible be quoted in terms of Λ_2. Although the properties of the gas at the high temperatures usually encountered on the hot side of the shock may not be known as well as one might desire, it may be possible to obtain Λ_2 as a part of the experiment itself; for example, in beam-attenuation experiments, data on the attenuation on the hot side might provide a direct measure of Λ_2.

Most of the computations reported here were made at the Tata Institute of Fundamental Research, Bombay. We thank Mr H. S. Mukunda for his timely help in running a part of the programme on the computer. S.M.D. is grateful to the University Grants Commission for the award of a fellowship during the course of this work.

Appendix A

We evaluate here certain integrals encountered in § 3. First consider $I_1(\mathbf{U})$, $I_2(\mathbf{U})$, defined by (3.8).

The integration with respect to **V** yields a factor $\pi^{\frac{3}{2}}$. For the integration in **G**, choose spherical polar co-ordinates (G, θ, ϕ) with **U** as axis. The exponential in (3.8) then contains a term $\mathbf{G}.\mathbf{U} = GU\cos\theta$, and we use the expansion in spherical harmonics

$$\exp(-2GU\cos\theta) = \sum_{n=0}^{\infty}(2n+1)\,P_n(\cos\theta)\,i_n(2GU) \tag{A 1}$$

as in I. Termwise integration in θ is easily carried out remembering that

$$\int_0^{\pi} P_n(\cos\theta)\sin\theta\,d\theta = 2 \quad \text{if} \quad n = 0$$
$$= 0 \quad \text{if} \quad n \neq 0;$$

and integration in ϕ gives a factor of 2π. We are therefore left with

$$I_1(\mathbf{U}) = 4\pi^{\frac{5}{2}}\,e^{-U^2}\int_0^{\infty} G^3\,e^{-G^2} i_0(2GU)\,dG. \tag{A 2}$$

Using (2.13) of I, this becomes

$$I_1(\mathbf{U}) = 2\pi^{\frac{5}{2}}\,e^{-U^2}\,\Phi(2, \tfrac{3}{2}, U^2). \tag{A 3}$$

$I_2(\mathbf{U})$ can be evaluated using exactly similar methods

$$I_2(\mathbf{U}) = \tfrac{8}{3}\pi^{\frac{5}{2}}\,e^{-U^2}\,U\Phi(3, \tfrac{5}{2}, U^2). \tag{A 4}$$

Next we study the integrals I_{lmn}, defined by (3.15). As pointed out in the text, it is enough to evaluate

$$I_{000} = \int_0^{2\pi} d\epsilon \int_0^{\pi} d\theta \int_0^{\infty} dG \int_0^{\frac{1}{2}\pi} d\psi \exp[-G^2(1+\alpha_1\cos\psi) + G(\alpha_2\cos\theta + \alpha_3\cos\theta')]. \tag{A 5}$$

Substituting here for $\cos\theta'$ from (3.11*a*), the integrations in ϵ and θ are easily performed (e.g. Watson 1944, p. 51), giving

$$\int_0^{2\pi} d\epsilon \int_0^{\pi} d\theta \exp[G(\alpha_2\cos\theta + \alpha_3\cos\theta')] = 4\pi i_0\{G(\alpha_2^2 + \alpha_3^2 - 2\alpha_2\alpha_3\cos 2\psi)^{\frac{1}{2}}\}.$$

Putting this result into (A 5), we see that the integration in G can again be performed using (2.13) of I so that (A 5) becomes

$$I_{000} = 2\pi \int_0^{\frac{1}{2}\pi} \frac{\sin 2\psi\,d\psi}{1+\alpha_1\cos^2\psi}\,\Phi\left(2, \tfrac{3}{2}, \frac{\alpha_2^2 + \alpha_3^2 - 2\alpha_2\alpha_3\cos 2\psi}{1+\alpha_1\cos^2\psi}\right).$$

If we write the argument of Φ here as t, the above integral is found to transform to

$$I_{000} = \frac{8\pi}{\alpha_2\alpha_3 + 4\alpha_1(\alpha_2+\alpha_3)^2}\int_{t_1}^{t_2} \Phi(2, \tfrac{3}{2}, t)\,dt, \tag{A 6}$$

where $t_1 = \tfrac{1}{4}(\alpha_2-\alpha_3)^2/(1+\alpha_1), \quad t_2 = \tfrac{1}{4}(\alpha_2+\alpha_3)^2.$

Integrating (A 6) by using the series expansion for Φ we obtain the final result

$$I_{000} = \frac{4\pi}{\alpha_2\alpha_3 + 4\alpha_1(\alpha_2+\alpha_3)^2}[\Phi\{1, \tfrac{1}{2}, \tfrac{1}{4}(\alpha_2+\alpha_3)^2\} - \Phi\{1, \tfrac{1}{2}, \tfrac{1}{4}(\alpha_2-\alpha_3)^2/(1+\alpha_1)\}]. \tag{A 7}$$

Appendix B

We make here a brief analysis of the inner and outer limit of the error function e, defined by (2.5a). The two limiting processes, as well as the corresponding variables in velocity space, have already been described in I.

In the inner limit $v_x \approx u_1$, and hence the first term in (2.5a) is $-u_1 F_1 \nu'$ to the lowest order as $M_1 \to \infty$. By an examination of the result given in I, we see that the lowest order contribution to $\mathscr{J}$ in the inner limit is due to $F_1\mathscr{L}[F_2(\mathbf{u}_1)]$, where the loss operator on F_2 is evaluated at $\mathbf{v} = \mathbf{u}_1$. It follows that e is zero in the inner limit if

$$\frac{\nu'}{\nu(1-\nu)} = \frac{\mathscr{L}[F_2(\mathbf{u}_1)]}{u_1}. \tag{B 1}$$

This is essentially Sakurai's result. As F_1 becomes a delta function in the limit $M_1 \to \infty$, we can look upon the result as being obtained by a balance of delta functions on either side of the Boltzmann equation.

If (B 1) is worked out using the results of I for $\mathscr{L}(F_2)$ we find that the corresponding shock thickness is the same as that given by (4.3).

To see that (2.4) does not provide an exact solution of the Boltzmann equation uniformly in velocity space, it is enough to consider the behaviour of the outer limit of e near the origin in velocity space. The first term in (2.5a) is now asymptotically $v_x F_2(0)\,\nu'$, and is linear in v_x. But from the analysis in I of the outer limit of the $\mathscr{J}_{ij}$, it can be easily shown that for $v_x \to 0$ the collision term does not tend to zero like v_x. Hence e cannot vanish for all velocities.

REFERENCES

ANANTHASAYANAM, M. R. & NARASIMHA, R. 1968 To appear in *Acta Mechanica*.

BAUER, F. L., RUTISHAUER, H. & STIEFEL, E. 1962 *Proc. Symp. Appl. Math.* **15**, 199.

BIRD, G. A. 1967 *J. Fluid Mech.* **30**, 479.

CAMAC, M. 1965 *Proceedings of the 4th International Symposium on Rarefied Gas Dynamics*. Toronto, **1**, 240.

CHAHINE, M. T. & NARASIMHA, R. 1965 *Proceedings of the 4th International Symposium on Rarefied Gas Dynamics*. Toronto, **1**, 140.

CHAPMAN, S. & COWLING, T. G. 1960 *Mathematical Theory of Nonuniform Gases*. Cambridge University Press.

DESHPANDE, S. M. & NARASIMHA, R. 1969 *J. Fluid Mech.* **36**, 545.

GUSTAFSON, W. A. 1960 *Phys. Fluids*, **3**, 732.

LIEPMANN, H. W., NARASIMHA, R. & CHAHINE, M. T. 1962 *Phys. Fluids*, **5**, 1313.

LIGHTHILL, M. J. 1956 *Surveys in Mechanics*. Cambridge University Press.

LINZER, M. & HORNIG, D. F. 1963 *Phys. Fluids*, **6**, 1661.

MOTT-SMITH, H. M. 1951 *Phys. Rev.* **82**, 885.

MUCKENFUSS, C. 1962 *Phys. Fluids*, **5**, 1325.

NARASIMHA, R. 1966 *Phys. Fluids*, **9**, 2524.

NARASIMHA, R. 1968 *J. Fluid Mech.* **34**, 1.

NORDSIECK, A. & HICKS, B. L. 1967 *Proceedings of the 5th International Symposium on Rarefied Gas Dynamics*. Oxford, **1**, 695.

OBERAI, M. M. 1967 *J. de Mec.* **6**, 317.

RODE, D. L. & TANENBAUM, B. S. 1967 *Phys. Fluids*, **10**, 1352.

ROSEN, P. 1954 *J. Chem. Phys.* **22**, 1045.

RUSSELL, D. A. 1965 *Proceedings of the 4th International Symposium on Rarefied Gas Dynamics*. Toronto, **1**, 265.

SAKURAI, A. 1957 *J. Fluid Mech.* **3**, 255.

SUCHY, K. 1963 *Proceedings of the 3rd International Symposium on Rarefied Gas Dynamics*. Paris, **1**, 181.

WATSON, G. N. 1944 *Theory of Bessel Functions*. Cambridge University Press.