J. Fluid Mech. (1974), *vol.* 65, *part* 3, *pp.* 603–624
Printed in Great Britain

Solution of the Boltzmann equation at the upstream and downstream singular points in a shock wave

By J. P. ELLIOTT
Department of Physics, University of Victoria, Victoria, British Columbia
AND D. BAGANOFF
Department of Aeronautics and Astronautics, Stanford University, Stanford, California

(Received 17 October 1973)

A solution of the Boltzmann equation is obtained at the upstream and downstream singular points in a shock wave, for the case of Maxwell molecules. The fluid velocity u, rather than the spatial co-ordinate x, is used as the independent variable, and an equation for $\partial f/\partial u$ at a singular point is obtained from the Boltzmann equation by taking the appropriate limit. This equation is solved by using the methods of Grad and of Wang Chang & Uhlenbeck; and it is observed that the two methods are the same, since they involve not only an equivalent system of moment equations but also the same closure relations. Because many quantities are zero at a singular point, the problem becomes sufficiently simple to allow the solution to be carried out to any desired order. At the supersonic singular point, the solution converges very slowly for strong shock waves; but a simple modification to Grad's method provides a rapidly convergent solution. The solution shows that the Navier–Stokes relations, or the first-order Chapman–Enskog results, do not apply unless the shock-wave Mach number is unity, and that they are grossly in error for strong shock waves. The solution confirms the existence of temperature overshoot in a strong shock wave; shows that the critical Mach number in Grad's solution increases monotonically with the order of the solution; provides a simple explanation as to why Grad's closure relations fail and shows how they can be improved; and provides exact boundary values that can be used to guide future numerical solutions of the Boltzmann equation for shock-wave structure.

1. Introduction

One sometimes encounters problems that prove to be of value more because they are instructive than because they are the occasion of a particular solution. We propose to show that several basic questions in kinetic theory, which are related to the solution of the Boltzmann equation, can be clarified by a study of the problem dealing with the flow in the upstream and downstream wings of a shock wave. These regions are well suited for study, because a perturbation scheme can be employed to solve the Boltzmann equation; many troublesome terms drop out of the analysis, so that a solution can be obtained with a degree of completeness rarely found among other problems; a number of very interesting nonlinear properties of the flow field are retained, even though a perturbation scheme is used; and many of the results are new, and at variance with certain notions developed on the basis of the first-order Chapman–Enskog solution and the corresponding phenomenological laws.

The basic interest in the present problem is founded upon several important facts: the solution can be obtained by using either Grad's (1949) method, or that of Wang Chang & Uhlenbeck (1952); one observes that the two methods involve not only an equivalent system of moment equations, but also the same closure relations; the solution can be carried out to surprisingly high orders and converges at the subsonic singular point, but because of temperature overshoot in strong shock waves it must be carried out to fifth or sixth order; convergence at the supersonic singular point is extremely slow for strong shock waves, but a simple modification provides a rapidly convergent solution.

Many of the steps that lead to the formulation of the problem have been employed by others in related work. The central notion is to consider the fluid velocity u, rather than the spatial variable x, as the independent variable in studying a shock-wave profile. This substitution was used by von Mises (1950) and by Gilbarg & Paolucci (1953), when they showed that a very natural approach in solving the Navier–Stokes equations for shock-wave structure is to solve first for the solution curve in the temperature–velocity (T, u) plane, then use the relation $T = T(u)$ to integrate one of the conservation equations in order to determine the profile in the spatial variable x. In the temperature–velocity plane, the solution curve terminates on the points (T_1, u_1) and (T_2, u_2), as shown in figure 1. The point z_1 is determined by the upstream conditions; and the point z_2 is determined by the Rankine–Hugoniot conditions. They are therefore fixed by the physical problem; but the solution curve connecting the two points is characteristic of the equation, or set of equations, being solved. For the Navier–Stokes equations, von Mises (1950) and Gilbarg & Paolucci (1953) showed that z_1 and z_2 are singular: z_1 is an unstable node, and z_2 is a saddle point. For the Boltzmann equation, the points are again singular; but the character of the two singularities is difficult to establish. As can be seen from figure 1, the singular points are natural points about which to obtain a perturbation solution (i.e. we are interested in the direction of the tangent to the solution curve at either end point, for each dependent variable).

For the shock-wave problem, the flow is steady and one-dimensional and (in terms of the independent variable u) the Boltzmann equation can be written

$$c_x \frac{\partial(\rho f)}{\partial u} = \frac{C(\rho f)}{du/dx}, \tag{1}$$

where $f = f(\mathbf{c}, u)$, $\mathbf{c}$ is the laboratory velocity, ρ is the mass density, and $C(\rho f)$ represents the collision integral. Nordsieck & Hicks (1967) first noticed that (1) is useful for numerical computation; they also first used number density as an independent variable in their numerical work. Hicks, Yen & Reilly (1972) and Yen *et al.* (1974) used (1) to obtain a numerical solution of the Boltzmann equation for shock-wave structure. It is clear that the term on the right-hand side of (1) is indeterminate at z_1 and z_2, since both $C(\rho f)$ and du/dx are zero

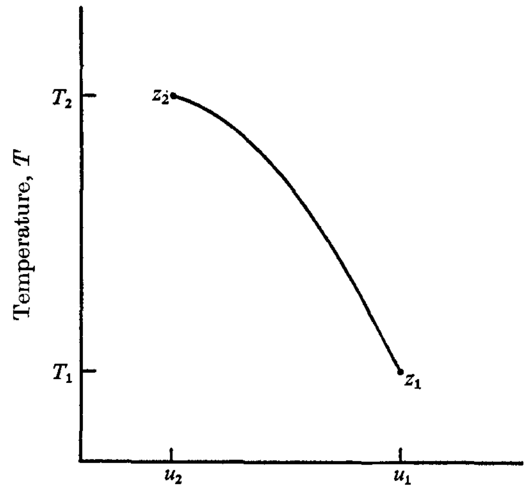

FIGURE 1. Schematic diagram of a typical solution curve in the T, u plane for a shock wave; z_1 and z_2 are the upstream and downstream singular points, respectively.

at those points. Thus an analytic solution near the singular points would also be very useful in guiding future numerical solutions of the Boltzmann equation for shock-wave structure, since it is clear that most numerical error develops near the singular points.

Since we shall be interested in central moments of f, it is convenient to recast (1) in terms of the thermal velocity $\mathbf{C}$. This transformation is given by Chapman & Cowling (1964); and for steady one-dimensional flow it yields

$$(u+C_x)\left[\frac{\partial(\rho f)}{\partial u}-\frac{\partial(\rho f)}{\partial C_x}\right]=\frac{C(\rho f)}{du/dx}, \tag{2}$$

where now $f = f(\mathbf{C}, u)$.

2. Equation of transfer evaluated at a singular point

A standard approach in the solution of the Boltzmann equation is to form the equation of transfer for an arbitrary function ϕ of the thermal velocity (Chapman & Cowling 1964). Since we are interested in the solution near the singular points, the equation of transfer must be evaluated at those points, and this operation yields

$$\left\{\frac{d}{du}[\rho u\langle\phi\rangle+\rho\langle C_x\phi\rangle]+\rho u\left\langle\frac{\partial\phi}{\partial C_x}\right\rangle+\rho\left\langle C_x\frac{\partial\phi}{\partial C_x}\right\rangle\right\}_s=\Delta[\phi]_s, \tag{3}$$

for $s = 1$ or $s = 2$. Here

$$\langle\phi\rangle \equiv \int \phi f \, d\mathbf{C} \tag{4}$$

is a general moment of f, and the operator $\Delta[\phi]_s$ is defined by

$$\Delta[\phi]_s \equiv \lim_{u\to u_s}\left(\frac{\int \phi C(\rho f)\, d\mathbf{C}}{du/dx}\right). \tag{5}$$

The integral in the numerator of (5) has been worked out for only a limited number of ϕ's and for the case of Maxwell molecules (Grad 1949; Ikenberry & Truesdell 1956; Rode & Tanenbaum 1967). To develop a high-order set of moment equations from the equation of transfer, one would have to work out this integral for many additional ϕ's. This is not only a difficult procedure, but also a great waste of effort, since many terms vanish when the limit in (5) is taken.

The wasted effort can be avoided if one uses L'Hospital's rule in taking this limit. Since the xx-component τ of the viscous stress tensor is zero at s, the limit value can be computed as

$$\Delta[\phi]_s = \lim_{u\to u_s}\left(\frac{\tau}{du/dx}\right).\lim_{u\to u_s}\left(\frac{\int \phi \frac{\partial}{\partial u} C(\rho f)\, d\mathbf{C}}{d\tau/du}\right).$$

This seemingly artificial manipulation serves two purposes. (i) It allows the introduction of the important stress ratio $(\tau/\tau^0)_s$, where

$$\tau^0 \equiv \tfrac{4}{3}\mu \frac{du}{dx} \tag{6}$$

is the Navier–Stokes expression for τ while μ is the coefficient of viscosity. (ii) On recognizing

$$\left[\frac{\partial}{\partial u} C(\rho f)\right]_s \propto J\left\{\left[\frac{u}{\rho f^{(0)}} \frac{\partial(\rho f)}{\partial u}\right]_s\right\},$$

where J is the familiar linearized collision operator discussed by e.g. Uhlenbeck & Ford (1963), and where $f^{(0)}$ is the Maxwellian distribution, we can replace the nonlinear operator C by the linear operator J, and write

$$\Delta[\phi]_s = \rho_s \omega_s \int \phi f_s^{(0)} J\left\{\left[\frac{u}{\rho f^{(0)}} \frac{\partial(\rho f)}{\partial u}\right]_s\right\} d\mathbf{C}. \tag{7}$$

The quantity ω_s is defined by

$$\omega_s \equiv \frac{16}{9A_2}(\tau/\tau^0)_s \bigg/ \left(\frac{u}{p}\frac{d\tau}{du}\right)_s, \tag{8}$$

where p is the pressure, and A_2 is the constant defined by Wang Chang & Uhlenbeck (1952, p. 17). (There should be a factor of 2π preceding their integral that defines A_{2k}.) The numerical value of A_2 is 2·7406.† In writing (8), we have restricted ourselves to the case of Maxwell molecules. For the general case ω_s is only slightly more complicated; but then (7) becomes much more difficult to evaluate. With the introduction of (7) we have eliminated terms that vanish at s, and thus avoided much wasted effort; but the remaining terms, nevertheless, require considerable calculation. Although these calculations are straightforward, we shall postpone the discussion of the method by which they can be carried out to § 4, where the required mathematical preparation is found.

The introduction of the equation of transfer (3), together with simplification (7), allows one to construct directly the set of moment equations that contain the

† It is unfortunate that various authors have defined A_2 in slightly different ways. The A_2 defined by Wang Chang & Uhlenbeck (1952) is twice the A_2 defined by Maxwell (1890), and a factor of 2π times the A_2 defined by Chapman & Cowling (1964).

gasdynamic variables. These equations, as we shall see, are important in discovering the scaling rules that give bounded quantities for all shock-wave Mach numbers. In addition, we shall want to refer to this set of equations when we discuss Grad's method of solution. The disadvantage in using (3) to construct a set of moment equations is that the entire reduction must be redone each time a different ϕ is chosen. Since we are interested in eventually constructing a large set, we shall rely upon (3) for physical insight; but we shall seek a more efficient method for actually constructing a large set of moment equations. In the process, the complete similarity between the methods of Grad (1949) and of Wang Chang & Uhlenbeck (1952) will become evident.

3. The Wang Chang equations at a singular point

The key step in the formulation of a more efficient method is to reverse the order of the steps taken in § 2 (i.e. to take the singular point limit of the Boltzmann equation (2) before moments are formed). The limit process can be applied first if we assume from the outset that ρf can be expanded in a Taylor series about each singular point in the form

$$\rho f = \rho_s f_s^{(0)}[1 + \hat{h}_s \Delta u_s + \ldots], \tag{9}$$

where $\Delta u_s \equiv (u - u_s)$. The hat symbol is used to draw attention to the fact that $\hat{h}$ involves a derivative with respect to u, since

$$\left[\frac{\partial(\rho f)}{\partial u}\right]_s = \rho_s f_s^{(0)} \hat{h}_s. \tag{10}$$

As a consequence of (4) we also have

$$\left[\frac{d}{du}\rho \langle\phi\rangle\right]_s = \rho_s \int \phi f_s^{(0)} \hat{h}_s d\mathbf{C}, \tag{11}$$

which relates a general moment of $f_s^{(0)} \hat{h}_s$ to the first derivative of the same moment of f. (Equation (11) yields the relations for the gasdynamic variables when ϕ is replaced by $1, C^2, C_x C^2$, etc.) Substituting (9) into (2), and evaluating the equation at s, we obtain the fundamental equation for $\hat{h}_s$ given by

$$(\tilde{M}_s + V_x)(\tilde{M}_s^{-1} u_s \hat{h}_s + 2V_x) = \omega_s J(u_s \hat{h}_s), \tag{12}$$

where $\tilde{M}_s = u_s(2RT_s)^{-\frac{1}{2}}$ and $\mathbf{V} = \mathbf{C}(2RT_s)^{-\frac{1}{2}}$ is a dimensionless thermal velocity (note the suppression of s on $\mathbf{V}$). For convenience we write (12) in the form

$$\omega_s J(u_s \hat{h}_s) - L(u_s \hat{h}_s) = 2V_x(\tilde{M}_s + V_x); \tag{13}$$

and we note that J and L are linear operators.

It can be seen from (8) that ω_s is inversely proportional to $(d\tau/du)_s$; and it will be seen below that the stress ratio $(\tau/\tau^0)_s$ can be expressed as a linear function of another moment of $f_s^{(0)} \hat{h}_s$. Therefore, (13) is a *nonlinear integral equation* for $\hat{h}_s$. Because of the presence of ω_s, moment equations formed from (13) will generally involve nonlinear algebraic relations among the different moments (more precisely, first derivatives of moments); and this makes it necessary to employ a computer solution in the final analysis. However, the interesting physical aspects of the problem arise because of the nonlinearity; so the need for a computer solution is not viewed as undesirable.

Now, for Maxwell molecules, the eigenfunctions and eigenvalues of the operator J are known (Wang Chang & Uhlenbeck 1952; Waldmann 1958); and the eigenvalues have been exhaustively tabulated by Alterman, Frankowski & Pekeris (1962). The solution of (13) is in principle straightforward, if we follow the method of Wang Chang & Uhlenbeck (1952). Restricting the notation to the case of one-dimensional flow, we first expand $u_s \hat{h}_s$ in terms of the eigenfunctions† of J:

$$u_s \hat{h}_s = \pi^{\frac{3}{4}} \sum_{r,l} \xi_{rl} \psi_{rl}, \tag{14}$$

where the ξ_{rl}'s are coefficients to be determined (note the suppression of s on ξ_{rl}). In fact it can be seen from (11) that the ξ_{rl}'s are simply derivatives of the eigenfunction moments of f, evaluated at s:

$$\xi_{rl} = \pi^{\frac{3}{4}} \left(\frac{u}{\rho} \frac{d}{du} \rho \langle \psi_{rl} \rangle \right)_s. \tag{15}$$

If we now substitute (14) into (13), multiply by $\psi_{r'l'} e^{-V^2}$ and integrate, we obtain the infinite system of equations

$$\sum_{r',l'} [\tilde{M}_s(\omega_s \lambda_{rl} - 1)\, \delta_{rl,r'l'} - M_{rl,r'l'}]\, \xi_{r'l'} = b_{rl}, \tag{16}$$

where
$$M_{rl,r'l'} \equiv \int V_x e^{-V^2} \psi_{rl} \psi_{r'l'}\, d\mathbf{V},$$

$$b_{rl} \equiv 2\pi^{-\frac{3}{4}} \tilde{M}_s \int V_x (\tilde{M}_s + V_x)\, e^{-V^2} \psi_{rl}\, d\mathbf{V},$$

and where λ_{rl} is the eigenvalue corresponding to ψ_{rl}. An explicit formula for $M_{rl,r'l'}$ was worked out by Wang Chang & Uhlenbeck (1952), and their result can be used here. Only four elements of the column vector b_{rl} are non-zero; they are

$$b_{00} = \tilde{M}_s, \quad b_{01} = \sqrt{2}\, \tilde{M}_s^2, \quad b_{10} = -2\tilde{M}_s/\sqrt{6} \quad \text{and} \quad b_{02} = 2\tilde{M}_s/\sqrt{3}.$$

Equation (16) is an infinite set of equations in the eigenfunction moments ξ_{rl}; and it isvirtually identical to Wang Chang & Uhlenbeck's equation (25). The identity includes the method of solution of the truncated set, in that the value of ω_s is determined by the requirement that a certain determinant in (16) vanish. To a given order, this set contains precisely the same information as the set obtained from the equation of transfer (3). The advantage in using (16) is that only the matrix elements $M_{rl,r'l'}$ have to be computed, and this step is trivial. Thus, the set can be easily written down to any order in a purely mechanical fashion, whereas use of (3) requires that each moment equation be worked out individually. However, the disadvantage in using (14) is that the eigenfunction moments themselves cannot be interpreted as physical quantities, and this makes it difficult to anticipate how they should be scaled so that they are bounded for all shock-

† Here we shall deal with the eigenfunctions and eigenvalues defined by Wang Chang & Uhlenbeck (1952). The ψ_{rl} defined by Waldmann (1958) is equal to $\pi^{\frac{3}{4}}$ times the ψ_{lr} of Wang Chang & Uhlenbeck (1952); and his definition of A_2 corresponds to that of Chapman & Cowling (1964).

wave Mach numbers. The transformation relating the ξ_{rl}'s to the gasdynamic variables can be obtained by using (15), and noting from the definition of ψ_{rl} that the $\langle\psi_{rl}\rangle$'s can be expressed as linear combinations of the gasdynamic variables. Before these relations can be exhibited, we must first define the symbols to be used for the higher moments (beyond the gasdynamic variables); this will be done in §4.

4. Mathematical details

In defining symbols for the higher moments, we shall follow Grad's notation in the use of subscripts, but restrict it to the case of one-dimensional flow, with the subscript 1 corresponding to the x direction. We now list the independent moments of order five or less in a one-dimensional flow: the third-order moments are

$$S_1 \equiv \rho\langle C_x C^2\rangle = 2q, \quad S_{111} \equiv \rho\langle C_x^3\rangle; \tag{17}$$

the fourth-order moments are

$$Q \equiv \rho\langle C^4\rangle, \quad Q_{11} \equiv \rho\langle C_x^2 C^2\rangle, \quad Q_{1111} \equiv \rho\langle C_x^4\rangle; \tag{18}$$

and the fifth-order moments are

$$R_1 \equiv \rho\langle C_x C^4\rangle, \quad R_{111} \equiv \rho\langle C_x^3 C^2\rangle, \quad R_{11111} \equiv \rho\langle C_x^5\rangle. \tag{19}$$

Although both S_1 and S_{111} are zero at s, the ratio $(S_{111}/S_1)_s$ is not zero. The importance of the ratio S_{111}/S_1 was first noticed by Baganoff & Nathenson (1970), who reasoned that, in a shock wave, the ratio should lie in the range

$$0 \leqslant S_{111}/S_1 \leqslant 1. \tag{20}$$

Therefore, this ratio is a very useful quantity for determining the point at which a solution becomes physically meaningless and fails. For this reason, we shall want to use it as one of the primary unknowns in the moment equations. This change of variables will be accomplished by means of the substitution

$$\left(\frac{1}{p}\frac{dS_{111}}{du}\right)_s = 2\left(\frac{S_{111}}{S_1}\right)_s\left(\frac{1}{p}\frac{dq}{du}\right)_s, \tag{21}$$

which is obtained by application of L'Hospital's rule. It should also be noted that for Grad's thirteen-moment solution and for the first-order Chapman–Enskog solution the ratio S_{111}/S_1 has the constant value $\frac{3}{5}$.

The foregoing discussion suggests that it may also be useful to consider similar ratios among the fifth-order moments defined by (19), i.e. to write

$$\left(\frac{1}{pu^2}\frac{dR_1}{du}\right)_s = \left(\frac{R_1}{qu^2}\right)_s\left(\frac{1}{p}\frac{dq}{du}\right)_s, \tag{22}$$

$$\left(\frac{1}{pu^2}\frac{dR_{111}}{du}\right)_s = \left(\frac{R_{111}}{R_1}\right)_s\left(\frac{1}{pu^2}\frac{dR_1}{du}\right)_s, \tag{23}$$

$$\left(\frac{1}{pu^2}\frac{dR_{11111}}{du}\right)_s = \left(\frac{R_{11111}}{R_1}\right)_s\left(\frac{1}{pu^2}\frac{dR_1}{du}\right)_s. \tag{24}$$

These three ratios will be of interest in a subsequent discussion of closure relations in §7.

We are now in a position to list several of the transformations defined by (15). In anticipation of what we learn by inspecting the moment equations expressed in terms of the gasdynamic variables, we shall scale the eigenfunction moments ξ_{rl} with M_s such that each combination is bounded. The list is

$$\xi_{00} = -1, \quad \xi_{01} = 0, \tag{25), (26}$$

$$\left.\begin{aligned} M_s^{-2}\xi_{10} &= -\left(\frac{3}{2}\right)^{\frac{1}{2}}\left(M^{-2}\frac{u}{T}\frac{dT}{du}\right)_s, \\ M_s^{-2}\xi_{02} &= -\frac{\sqrt{3}}{2}\left(M^{-2}\frac{u}{p}\frac{d\tau}{du}\right)_s, \end{aligned}\right\} \tag{27}$$

$$\left.\begin{aligned} M_s^{-3}\,\xi_{11} &= -\left(\frac{2}{3}\right)^{\frac{1}{2}}\left(M^{-2}\frac{1}{p}\frac{dq}{du}\right)_s, \\ M_s^{-3}\,\xi_{03} &= \frac{5}{6}\left(M^{-2}\frac{1}{p}\frac{dS_{111}}{du}\right)_s - \left(M^{-2}\frac{1}{p}\frac{dq}{du}\right)_s, \end{aligned}\right\} \tag{28}$$

$$\vdots$$

$$\left.\begin{aligned} M_s^{-5}\xi_{21} &= \frac{1}{\sqrt{42}}\left[-14M_s^{-2}\left(M^{-2}\frac{1}{p}\frac{dq}{du}\right)_s + \frac{5}{6}\left(M^{-2}\frac{1}{pu^2}\frac{dR_1}{du}\right)_s\right], \\ M_s^{-5}\,\xi_{13} &= \frac{1}{\sqrt{18}}\left[\frac{15M_s^{-2}}{2}\left(M^{-2}\frac{1}{p}\frac{dS_{111}}{du}\right)_s - 9M_s^{-2}\left(M^{-2}\frac{1}{p}\frac{dq}{du}\right)_s \right.\\ &\quad \left. -\frac{25}{18}\left(M^{-2}\frac{1}{pu^2}\frac{dR_{111}}{du}\right)_s + \frac{5}{6}\left(M^{-2}\frac{1}{pu^2}\frac{dR_1}{du}\right)_s\right], \\ M_s^{-5}\,\xi_{05} &= \frac{5}{72\sqrt{63}}\left[63\left(M^{-2}\frac{1}{pu^2}\frac{dR_{11111}}{du}\right)_s - 70\left(M^{-2}\frac{1}{pu^2}\frac{dR_{111}}{du}\right)_s \right.\\ &\quad \left. +15\left(M^{-2}\frac{1}{pu^2}\frac{dR_1}{du}\right)_s\right]. \end{aligned}\right\} \tag{29}$$

Since ψ_{rl} is a polynomial of degree $(2r+l)$, we have grouped the ξ_{rl}'s in ascending order and listed them within the group in ascending l. The fifth-order group (29) was also included for later reference. It is of interest to note the rule that $\xi_{rl} \sim M_1^{2r+l}$ upstream as the shock strength increases.

It is appropriate at this point to return to (7), to supply the result alluded to in the discussion following (8). Expanding ϕ in terms of the ψ_{rl}'s by

$$\phi = \pi^{\frac{3}{4}} \sum_{r,l} \beta_{rl}\psi_{rl}, \tag{30}$$

and using (30) together with (10) and (14) in (7), we arrive at the result

$$\Delta[\phi]_s = \rho_s \omega_s \sum_{r,l} \beta_{rl}\lambda_{rl}\xi_{rl}. \tag{31}$$

Since the β_{rl}'s are known, (31), together with the transformations for the ξ_{rl}'s, allows one to express the collision term in the equation of transfer (3) in terms of the gasdynamic variables. Here again we note that the equation of transfer does not provide an efficient route, since the β_{rl}'s must be worked out for each ϕ.

We now exhibit a representative set of moment equations obtained from (3) and the final expression (31) for the collision term. With $\phi = 1$ and $\phi = C^2$, (3) yields, in turn, the familiar continuity and energy equations. (The momentum equation cannot be obtained in this way, as it has been used in the derivation of (3).)

After using the continuity equation, we can write the momentum and energy equations as

$$\left(M^{-2}\frac{u}{T}\frac{dT}{du}\right)_s - \left(M^{-2}\frac{u}{p}\frac{d\tau}{du}\right)_s + \tfrac{5}{3} - M_s^{-2} = 0, \tag{32}$$

and

$$\frac{3}{2}\left(M^{-2}\frac{u}{T}\frac{dT}{du}\right)_s + \left(M^{-2}\frac{1}{p}\frac{dq}{du}\right)_s + M_s^{-2} = 0, \tag{33}$$

respectively. The first non-zero contribution from (31) arises when $\phi = C_x^2$ and (3) yields

$$2\left(\frac{S_{111}}{S_1}\right)_s\left(M^{-2}\frac{1}{p}\frac{dq}{du}\right)_s - \tfrac{5}{3} + 3M_s^{-2} = \frac{4}{3}\left(M^{-2}\frac{\tau}{\tau^0}\right)_s. \tag{34}$$

Here we have introduced the moment ratio $(S_{111}/S_1)_s$ by means of (21). Noting that (34) is an expression for $(\tau/\tau^0)_s$ and on using (8) and (21), we see that ω_s is a rational function of two moments of $f_s^{(0)}\hat{h}_s$; this verifies the statement made following (13) regarding the nonlinearity of (13). With $\phi = C_x C^2$ and $\phi = C_x^3$, equation (3) yields, in turn,

$$2\left(M^{-2}\frac{1}{p}\frac{dq}{du}\right)_s + \left(M^{-2}\frac{1}{pu}\frac{dQ_{11}}{du}\right)_s + 5M_s^{-2} = -\frac{16}{9}\left(M^{-2}\frac{\tau}{\tau^0}\right)_s\left(\frac{q}{\tau u}\right)_s, \tag{35}$$

and

$$\left(M^{-2}\frac{1}{pu}\frac{dQ_{1111}}{du}\right)_s + 2\left(\frac{S_{111}}{S_1}\right)_s\left(M^{-2}\frac{1}{p}\frac{dq}{du}\right)_s + 3M_s^{-2} = -4\left[\left(\frac{S_{111}}{S_1}\right)_s - \frac{1}{3}\right] \times \left(M^{-2}\frac{\tau}{\tau^0}\right)_s\left(\frac{q}{\tau u}\right)_s. \tag{36}$$

In the set (32)–(36), we have preserved the identity of the collision term in (3) by placing contributions from it on the right-hand sides of the equations. In (35) and (36), we have used L'Hospital's rule to introduce the ratio

$$\left(\frac{\tau u}{q}\right)_s = \left(\frac{u}{p}\frac{d\tau}{du}\right)_s \Big/ \left(\frac{1}{p}\frac{dq}{du}\right)_s. \tag{37}$$

The ratios $(S_{111}/S_1)_s$ and $(\tau u/q)_s$ have been introduced for convenience alone; they do not add new unknowns to the system.

The logic used in expressing (32)–(36) in terms of bounded quantities can be illustrated by considering (32) as an example. For $M_1 \gg 1$, the critical situation is at the upstream singular point; and (32) gives

$$\left(\frac{u}{p}\frac{d\tau}{du}\right)_1 - \left(\frac{u}{T}\frac{dT}{du}\right)_1 \sim \tfrac{5}{3}M_1^2.$$

Except for the pathological case where the difference grows like M_1^2, at least one of the two quantities must grow like M_1^2. Therefore, all terms in (32) are expected to be bounded. Similar arguments can be applied to the remaining equations by using condition (20) and identity (37). The motivation for scaling the eigenfunction moments in (27)–(29) as shown is now obvious; and it is easy to see how a purely formal treatment of the system of equations (16) could lead to computational difficulties for large values of M_1.

5. Grad's method of solution

Grad (1949) developed a logically precise method for closing the set of moment equations obtained from (3) at any level of truncation. He expanded the distribution function f in a Hermite-polynomial series of the form

$$f = f^{(0)} \sum_{\nu} \frac{1}{\nu!} a_\nu H_\nu. \tag{38}$$

The orthogonality of the Hermite polynomials implies

$$a_\nu = \langle H_\nu \rangle, \tag{39}$$

so the a_ν's are simply Hermite-polynomial moments of f. To obtain the closure relations at order n, Grad simply sets $a_\nu = 0$ in (39), with $\nu = n+1$. He then automatically obtains an expression for the highest-order monomial moment, which is a tensor of rank $n+1$, in terms of lower-order monomial moments, which are also tensors of appropriate rank. Successive contraction of this expression yields exactly enough information to eliminate from the moment equations all the moments of order $n+1$, which are the extra unknowns. For our problem, the closure relations will be differentiated with respect to u, evaluated at s, and expressed in terms of bounded variables.

Closure at the second-order level is physically unrealistic when one deals with (38), since the heat flux is identically zero in this case. Nevertheless, we shall list the two closure relations

$$\left(M^{-2}\frac{1}{p}\frac{dq}{du}\right)_s = 0, \quad \left(M^{-2}\frac{1}{p}\frac{dS_{111}}{du}\right)_s = 0, \tag{40), (41}$$

as we shall encounter the second-order solution in § 6, outside the context of (38). The third-order closure relations are

$$\left(M^{-2}\frac{1}{pu}\frac{dQ_{11}}{du}\right)_s = 3M_s^{-2}\left[2\left(M^{-2}\frac{u}{T}\frac{dT}{du}\right)_s - M_s^{-2}\right] - \tfrac{21}{5}M_s^{-2}\left(M^{-2}\frac{u}{p}\frac{d\tau}{du}\right)_s \tag{42}$$

and

$$\left(M^{-2}\frac{1}{pu}\frac{dQ_{1111}}{du}\right)_s = \tfrac{9}{5}M_s^{-2}\left[2\left(M^{-2}\frac{u}{T}\frac{dT}{du}\right)_s - M_s^{-2}\right] - \tfrac{18}{5}M_s^{-2}\left(M^{-2}\frac{u}{p}\frac{d\tau}{du}\right)_s, \tag{43}$$

while those of fourth order read

$$\left(M^{-2}\frac{1}{pu^2}\frac{dR_1}{du}\right)_s = \tfrac{84}{5}M_s^{-2}\left(M^{-2}\frac{1}{p}\frac{dq}{du}\right)_s, \tag{44}$$

$$\left(M^{-2}\frac{1}{pu^2}\frac{dR_{111}}{du}\right)_s = \tfrac{9}{5}M_s^{-2}\left[3\left(M^{-2}\frac{1}{p}\frac{dS_{111}}{du}\right)_s + 2\left(M^{-2}\frac{1}{p}\frac{dq}{du}\right)_s\right] \tag{45}$$

and

$$\left(M^{-2}\frac{1}{pu^2}\frac{dR_{11111}}{du}\right)_s = 6M_s^{-2}\left(M^{-2}\frac{1}{p}\frac{dS_{111}}{du}\right)_s. \tag{46}$$

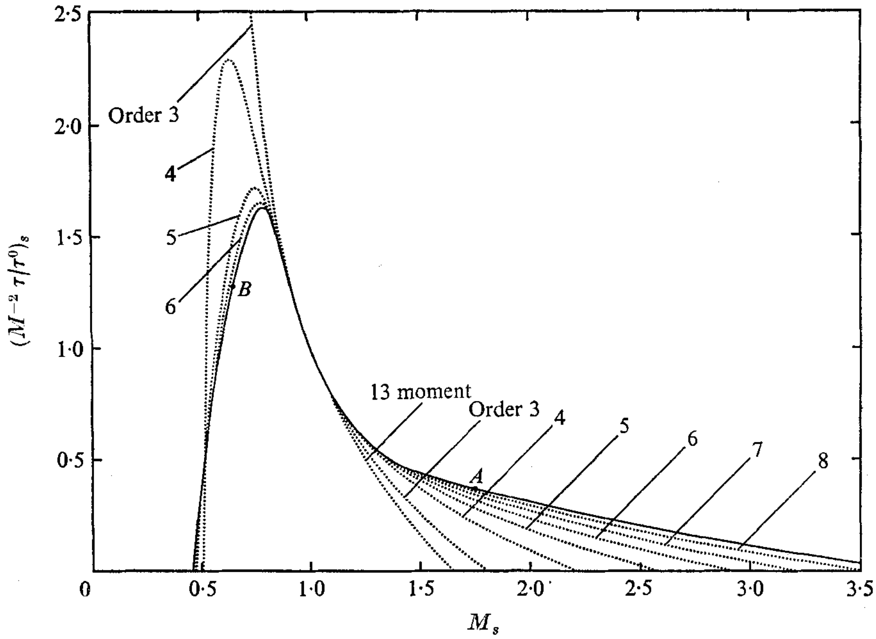

FIGURE 2. Variation of bounded stress ratio $(M^{-2}\tau/\tau^0)_s$ with singular point Mach number M_s in solution based on Grad's closure relations: ——, ninth-order solution; ······, solutions to lower orders (as indicated).

The fifth-order relations were also obtained and used; but they are too lengthy to present here. For completeness, we mention that the closure relations for the thirteen-moment equations are given by

$$\left(\frac{S_{111}}{S_1}\right)_s = \frac{3}{5}, \tag{47}$$

in addition to (42).

Momentarily turning our attention back to the Wang Chang system (16), we observe that, at any order of truncation n, the closure method used by Wang Chang & Uhlenbeck (1952), which consists of setting $\xi_{rl} = 0$ for $2r+l = n+1$, yields exactly the same closure relations as obtained by Grad. This can be seen, for example, by comparing the relations obtained from (29) with Grad's fourth-order set (44)–(46). This correspondence holds true at every order; indeed, it is to be expected, as indicated by Grad (1958). Also, since it is easy to show that (16) consists of linear combinations of the moment equations obtained from (3), we shall henceforth make no distinction between the two methods in discussing the final results, and shall refer simply to Grad's method.

Using the appropriate closure relations, we have solved the nonlinear system of equations on a digital computer for various orders, beginning at the thirteen-moment level. Figure 2 gives the results of the calculation to ninth order for the bounded stress ratio $(M^{-2}\tau/\tau^0)_s$, where the local Mach number M_s is employed as the independent variable. Two points appear on the graph for each shock-wave

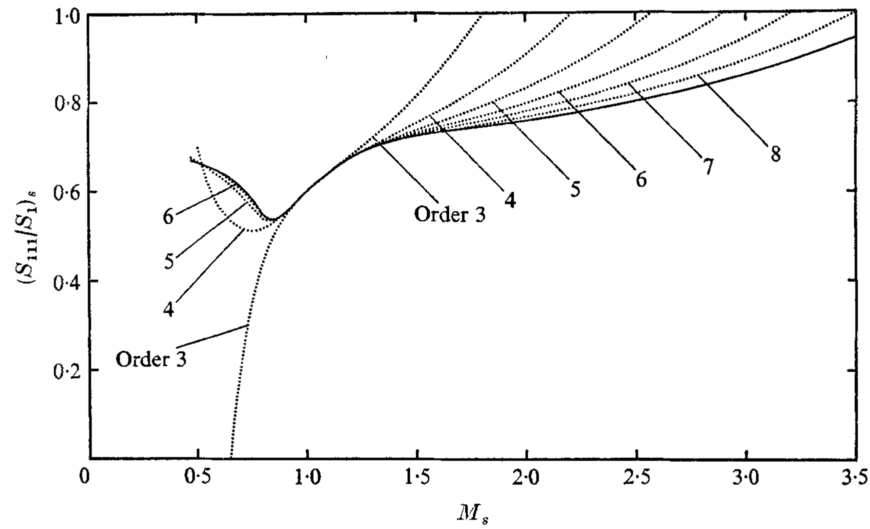

FIGURE 3. Variation of moment ratio $(S_{111}/S_1)_s$ with singular point Mach number M_s in solution based on Grad's closure relations: ——, ninth-order solution; ⋯⋯, solutions to lower orders (as indicated).

Mach number, one corresponding to the upstream singular point ($s = 1$) and the other corresponding to the downstream singular point ($s = 2$). A typical pair for the ninth-order solution is given by the points marked A and B in the figure. The point $M_s = 1$ divides the two branches of each curve. (Several of the solutions are not shown for $M_s < 1$ for aesthetic reasons; the same practice will be followed in subsequent figures for cases where the curves are either too crowded or overlap.) All the calculations were terminated upstream or downstream whenever $(\tau/\tau^0)_s = 0$, because the solutions become physically meaningless beyond these points. That this is so can be seen from two points of view. (i) Since $\tau \leqslant 0$ in a shock wave, we must always have $\tau/\tau^0 \geqslant 0$ in order that u decrease monotonically through the shock wave. (ii) It is clear from (7) that contributions to the moment equations from the collision integral are proportional to $(\tau/\tau^0)_s$. It is therefore inconceivable that $(\tau/\tau^0)_s$ could be zero, unless $(d\tau/du)_s$ were zero as well. Interestingly enough, for strong shock waves, this is exactly what happens *downstream* in the solutions beyond third order, i.e. both $(\tau/\tau^0)_2$ and $(d\tau/du)_2$ undergo sign reversals at exactly the same value of M_2 (e.g. $M_2 \simeq 0{\cdot}5$ in the fourth-order case, and $M_2 \simeq 0{\cdot}47$ in the fifth-order case). For values of M_2 below such values, we still rule out the validity of these solutions on the grounds of our first argument.

The existence of a critical Mach number ($M_1 \simeq 1{\cdot}65$) for the thirteen-moment solution was first noticed by Grad (1952). The failure of the thirteen-moment equations to yield shock structure for $M_1 > 1{\cdot}65$ is due precisely to this situation at the upstream singular point.

Figure 3 presents the corresponding results for the moment ratio $(S_{111}/S_1)_s$. It can be seen that the curves intersect the upper bound at unity [see (20)] at the same values of M_1 for which $(\tau/\tau^0)_1 = 0$ in figure 2. This further substantiates the above allegation that the solution is not valid beyond the point at which $(\tau/\tau^0)_1 = 0$. Downstream, condition (20) is satisfied for all values of M_2 to all orders beyond the third.

Figures 2 and 3 clearly show that the upstream solution converges at a painfully slow rate. Even with the solution to ninth order, the best one can say is that the upstream results are useful only for M_1 considerably less than 2. The present problem is therefore extremely valuable, in that it provides a classic example of a situation in which one cannot significantly improve a solution by adding a few more terms to a series. The problem also shows that the critical Mach number increases monotonically with increasing order. This result contradicts the assertion made by Holway (1964) that a critical Mach number is found, $M_1 = 1{\cdot}851$, above which solutions based on Grad's method do not exist no matter how many terms are retained in (38). Physically, the origin of the slow convergence is obvious. The molecular-beam nature of the upstream flow and the bimodal character of f prohibit one from adequately representing f in a shock wave without retaining an unreasonable number of terms in (38).

6. Rapidly convergent solution

Recognizing that f is a very difficult function to fit, we see that the task could be considerably simplified if we were to use physical knowledge concerning the problem to construct the first term and let the remainder of the series correct the error. (This point of view was expressed by Holway 1965.) If we are successful in picking a suitable function, then the error will be small, in some sense, and the series will converge more rapidly than Grad's. Thus, we would obtain more rapid convergence if our choice were good; if not, the error term would also be difficult to fit, and the series would converge as slowly as before. Therefore, there is no guarantee of success, but at least it is worth a try.

Since the Mott-Smith distribution has received considerable study, and has been found generally to be a fairly good approximation to the actual case, we shall use it as our first term; we write

$$f = f_{MS} + f_E, \tag{48}$$

where the error term f_E will be represented by the Hermite-polynomial series (38). This approach allows us to use exactly the same steps used by Grad, except that our closure relations will be different, because we use (38) to represent f_E instead of f.

If we define $\langle\phi\rangle_{MS}$ and $\langle\phi\rangle_E$ in accordance with (4) and the respective distribution functions f_{MS} and f_E, we see from (48) that

$$\langle\phi\rangle - \langle\phi\rangle_{MS} = \langle\phi\rangle_E. \tag{49}$$

Therefore, to obtain the closure relations based on (48), we merely have to replace every derivative $d\zeta/du$ in (40)–(46) by the difference $(d\zeta/du) - (d\zeta_{MS}/du)$, where $\zeta = T, \boldsymbol{\tau}, q, S_{111}$, etc. This is to be done on both sides of the equations. To carry

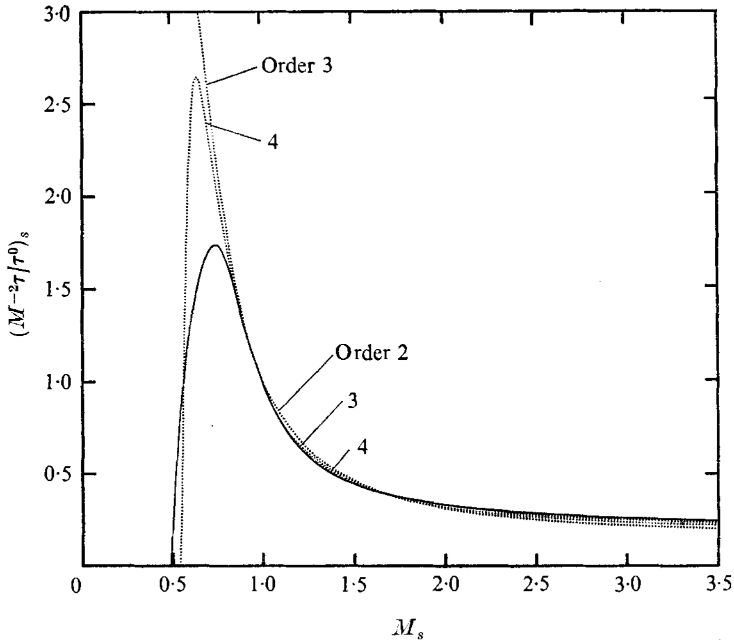

FIGURE 4. Variation of bounded stress ratio $(M^{-2}\ \tau/\tau^0)_s$ with singular point Mach number M_s in present solution: ——, fifth-order solution; ······, solutions to lower orders (as indicated).

out this procedure, the expressions for the various $d\zeta_{MS}/du$ must be worked out. A list of some of the lower-order results follows:

$$\left(M^{-2}\frac{u}{T}\frac{dT_{MS}}{du}\right)_s = \frac{10}{9}\left(2-\frac{u_1+u_2}{u_s}\right)+M_s^{-2}-\tfrac{5}{3}, \tag{50}$$

$$\left(M^{-2}\frac{u}{p}\frac{d\tau_{MS}}{du}\right)_s = \frac{10}{9}\left(2-\frac{u_1+u_2}{u_s}\right), \tag{51}$$

$$\left(M^{-2}\frac{1}{p}\frac{dq_{MS}}{du}\right)_s = \frac{5}{3}\left(2-\frac{u_1+u_2}{u_s}\right), \tag{52}$$

$$\left(M^{-2}\frac{1}{p}\frac{d(S_{111})_{MS}}{du}\right)_s = \frac{2}{3}\left(2-\frac{u_1+u_2}{u_s}\right)\left(5-\frac{u_1+u_2}{u_s}\right). \tag{53}$$

Since $\langle 1\rangle_{MS} = 1$ and $\langle C_x\rangle_{MS} = 0$, the series for f_E actually commences with the term involving H_2. In other words, the error term does not contribute either to the normalization of f, or to the fluid velocity u. (The fluid velocity is a free parameter in the Mott-Smith distribution function.)

Using the new closure relations together with the moment equations up to fifth order, one obtains the results shown in figures 4 and 5. The solution was termined at fifth order, because the new closure relations become quite complicated as the order increases. We see that the solution satisfies the conditions $(\tau/\tau^0)_1 \geqslant 0$ and $0 \leqslant (S_{111}/S_1)_s \leqslant 1$ for all orders and for all shock-wave Mach numbers. Downstream $(\tau/\tau^0)_2 = 0$ for $M_2 \simeq 0{\cdot}55$ in the fourth-order solution and

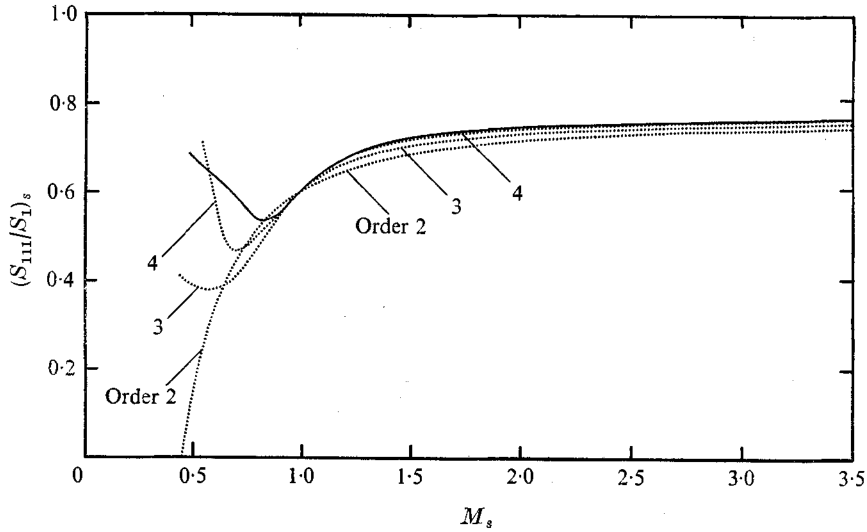

FIGURE 5. Variation of moment ratio $(S_{111}/S_1)_s$ with singular point Mach number M_s in present solution: ——, fifth-order solution; ⋯⋯, solutions to lower orders (as indicated).

for $M_2 \simeq 0{\cdot}49$ in the fifth-order solution. As was the case previously, $(d\tau/du)_2$ also reverses sign at these values of M_2. In fact, downstream, there is very little to choose between the present fourth- and fifth-order solutions and those based on Grad's closure relations. Upstream, the present solution exhibits dramatic improvement over the previous solution; although convergence cannot be proved with the data at hand, the consistency of the results at various orders leads one to believe that the exact solution is within reach.

The moment ratio S_{111}/S_1 was discussed within the context of the Mott-Smith solution by Nathenson & Baganoff (1973), who showed that, in the interior of a shock wave, good agreement exists between the Mott-Smith solution and the numerical solution of Hicks *et al.* (1972). Since the Mott-Smith solution corresponds to the second-order solution in figure 5, one can view this agreement as tending to support the present results, at least upstream. A direct comparison with the present work cannot be made because singular point values are presented in figure 5, whereas the numerical calculations of Hicks *et al.* (1972) are limited to the interior of a shock wave.

We conclude from figures 4 and 5 that the present upstream solution to fifth order has converged to the point where it adequately represents the upstream flow. Since Grad's ninth-order downstream solution has essentially converged, we shall use it to represent the downstream flow. Therefore, we shall use this combination of results in all subsequent figures, and shall refer to it simply as the composite solution.

7. Results and discussion

Figures 6 and 7 present summary plots of several quantities that reveal important conclusions about the physical flow near the singular points. The crossing of the axis by the three curves at point A in figure 6 is an artifact of

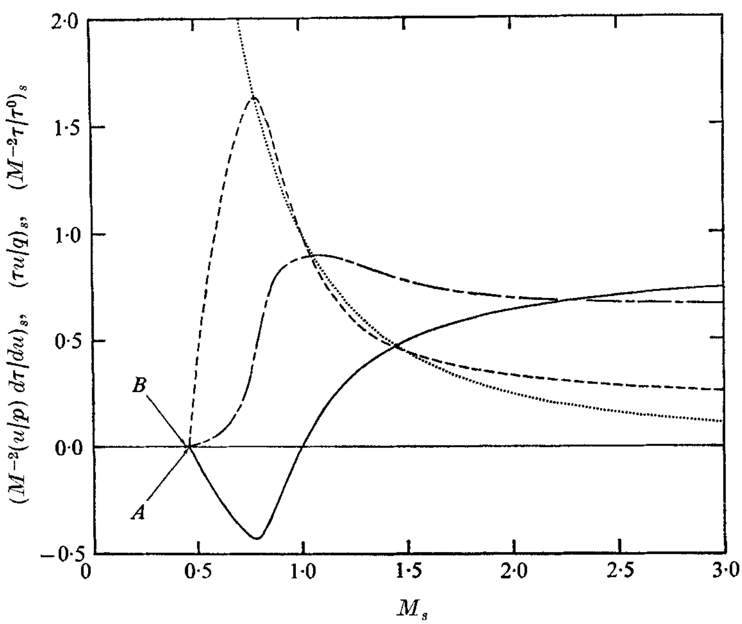

FIGURE 6. Variation of three stress-related quantities with singular point Mach number M_s in composite solution: ——, $(M^{-2}(u/p)\,d\tau/du)_s$; — — —, $(\tau u/q)_s$; - - - -, $(M^{-2}\tau/\tau^0)_s$; ·····, $(M^{-2}\tau/\tau^0)_s$ for Navier–Stokes relation.

the solution. We have observed that the position of the crossing varies as the order of the solution is increased (see figure 2); and it is clear from this trend that it approaches the limiting point $M_2 = 1/\sqrt{5}$ as the order of the solution becomes infinite. Therefore, our discussion will be based on the conclusion that all three of the quantities shown are zero at $M_2 = 1/\sqrt{5}$ (point B). For the quantities shown, this conclusion is somewhat unexpected. For example, the figure shows that the function $\tau = \tau(u)$ has a zero slope at the downstream singular point for $M_1 = \infty$. The Navier–Stokes solution, by contrast, yields a non-zero slope for the same conditions. However, both solutions predict

$$\left(\frac{u}{p}\frac{d\tau}{du}\right)_1 \sim M_1^2 \quad \text{for} \quad M_1 \gg 1.$$

The ratio $\tau u/q$ is of interest, as discussed by Nathenson & Baganoff (1973), because it has the constant value $\frac{2}{3}$ for the Mott-Smith distribution; it takes on the value $\frac{8}{9}$ in a very weak shock wave, as confirmed by figure 6; and it takes on the constant value unity if one assumes total enthalpy is conserved in a shock wave. The fact that $(\tau u/q)_2$ is zero at B shows that the heat-flux solution curve $q = q(u)$ does *not* have a zero slope at the downstream singular point, for $M_1 = \infty$ [see (37)].

The stress ratio τ/τ^0 is the most interesting quantity in figure 6. It is evident that a large difference exists between the Navier–Stokes relation $\tau = \tau^0$ (the dotted line) and the result obtained from the solution of the Boltzmann equation. Approximate agreement exists only for $M_1 \lesssim 1{\cdot}5$. We find from the figure that, for a strong shock wave, $\tau \sim M_1^2 \tau^0$ at the upstream singular point, while $\tau \ll \tau^0$ at the downstream singular point. This is in complete contrast to the Navier–Stokes prediction, and is contrary to the usual assumption made by many in formulating boundary conditions at either end of a shock wave. This result teaches us that the Chapman–Enskog procedure does not apply in the wings of a shock wave, regardless of how far upstream or downstream the point is chosen and how small the perturbation becomes. The basic reason for this is that, on setting $f = f^{(0)} + \Delta f$ in the Chapman–Enskog procedure, one assumes that the dominant term on the left-hand side of the Boltzmann equation comes from the spatial and temporal variation of $f^{(0)}$ and the term containing Δf is ignored. In this problem we see that just the opposite is true [see (12)]; the full contribution comes from Δf and none comes from $f^{(0)}$. This is the basic and sole reason for the difference; it has nothing to do with the size of the perturbation. We feel that this is one of the important points the present problem has clarified. Therefore, one should no longer allude to physical arguments and use $\tau = \tau^0$ as a limiting condition in a shock wave, as has been done in the past. Examples of where this assumption has been used can be found in Liepmann *et al.* (1962) and Hicks & Yen (1967), among others. Narasimha (1968) was one of the first to notice the error, when he analysed the case of a very weak shock wave and arrived at the conclusion that the Navier–Stokes relations are violated throughout the flow.

Once the derivative with respect to velocity of each of the variables is calculated at the singular points, one can determine the spatial variation of the same variable in the wings of the shock wave in the following manner. For a particular shock Mach number, we can use figure 6 to read the constants

$$\alpha_s \equiv (M^{-2}\tau/\tau^0)_s \quad \text{and} \quad \beta_s \equiv \left(M^{-2}\frac{u}{p}\frac{d\tau}{du}\right)_s.$$

Now, in the immediate vicinity of a singular point in the τ, u plane, the above two relations allow us to write

$$\tau = (M^2\alpha)_s \tau^0 \quad \text{and} \quad \tau = (M^2\beta p/u)_s (u-u_s),$$

where we limit $|u-u_s|/u_s$ to some small value ϵ. Using definition (6) for τ^0, we then obtain the differential equation

$$\frac{du}{(u-u_s)} = \frac{dx}{l_s} \quad \text{with} \quad l_s \equiv \tfrac{3}{4} A_2 \left(\frac{\mu u \omega}{p}\right)_s, \tag{54), (55}$$

where definition (8) for ω_s was used. Equation (54) shows that the velocity profile in the wings of a shock wave is an exponential function with a length scale $|l_s|$.

A physical interpretation of l_s can be given by writing (55) in terms of the mean free path length λ_s. Using the expression for viscosity in terms of λ_s, we introduce the characteristic length ratio

$$\tilde{l}_s \equiv \frac{|l_s|}{\lambda_s} = \frac{1}{4}\left(\frac{30}{\pi}\right)^{\frac{1}{2}} A_2 M_s |\omega_s|. \tag{56}$$

Figure 6 and equation (8) show that $|\omega_s|$ becomes infinite as $M_s \to 1$. Therefore, the characteristic ratio $\tilde{l}_s$ becomes infinite as the shock wave becomes a sound

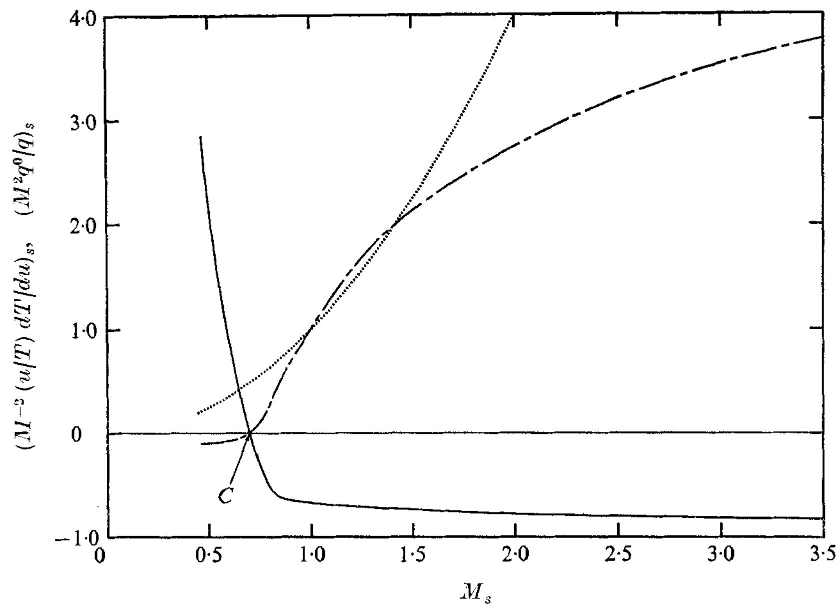

FIGURE 7. Variation of bounded temperature derivative $(M^{-2}(u/T)\,dT/du)_s$ and bounded heat-flux ratio $(M^2q^0/q)_s$ with singular point Mach number M_s in composite solution: ——, $(M^{-2}(u/T)\,dT/du)_s$; — — —, $(M^2q^0/q)_s$; ·····, $(M^2q^0/q)_s$ for Fourier relation.

wave, as we know it should. Equation (56) also allows one to interpret $|\omega_s|$ as a non-dimensional length scale; and this is extremely interesting in view of the prominent role played by ω_s in (7) and (16). In fact, the similarity between (16) and Wang Chang & Uhlenbeck's equation (25) extends even further than mentioned above. In our problem, $|\omega_s|$ scales the wings of the shock wave, while in their problem the corresponding variable, $\mathscr{R}(\sigma_0)$, determines the wavelength of the sound wave.

Since μ is proportional to T for Maxwell molecules, (55) yields the length-scale ratio

$$|l_2/l_1| = (u_2/u_1)^2|\omega_2/\omega_1|. \tag{57}$$

The calculated results summarized in figure 6 show that the value of $|\omega_2/\omega_1|$ approaches 20 (approximately) as M_1 becomes large. Therefore, the ratio lies in the range

$$1 \leqslant |l_2/l_1| \lesssim \tfrac{5}{4};$$

and one concludes that the shock-wave profile is essentially symmetric with respect to the wings. This conclusion is consistent with the profiles observed in recent experimental work (Schmidt 1969), and obtained from a direct-simulation Monte Carlo method for the solution of the Boltzmann equation (Bird 1970).

In contrast to figure 6, the crossing of the axis by the two curves at point C in figure 7 is not an artifact of the solution; it is a real effect, and it develops at a shock Mach number of $M_1 \simeq 1{\cdot}55$, which corresponds to a relatively weak shock wave. The figure shows that, for all shock waves of strength $M_1 > 1{\cdot}55$, the derivative $(dT/du)_2$ is positive. Therefore, in the T, u plane (see figure 1), there are points in the flow where the temperature is greater than the Rankine–Hugoniot value T_2 (i.e. a temperature overshoot exists in the shock wave). We feel the present solution gives a definitive proof that a temperature overshoot exists in strong shock waves; but we cannot determine whether the overshoot encompasses a large portion of the profile, or whether it is a phenomenon that is restricted to the immediate vicinity of the downstream singular point (see figure 1). The total evidence may point to the latter, because figure 7 shows that the value of the slope (dT/du_2) is quite significant, while Monte Carlo calculations by Hicks & Yen (1969) and by Bird (1970) show essentially no evidence of overshoot over most of the *interior* of a shock wave (their work covers a variety of molecular models).

The existence of a temperature overshoot explains why convergence at the subsonic end of the shock wave is so unexpectedly difficult for both the Grad solution and our modified solution. The answer, of course, lies in the fact that neither representation for f (i.e. neither (38) nor (48)) can generate, in just a few terms, the degree of asymmetry needed to represent temperature overshoot. We now understand that use of (48) allowed accelerated convergence at the supersonic side, because the bimodal distribution function of Mott-Smith is a good representation for the molecular-beam-like nature of the upstream flow. However, a further modification to the first guess for f in (48) would be needed to accommodate temperature overshoot and thus accelerate convergence at the subsonic side.

The second quantity in figure 7 is shown in a form inverted with respect to our normal manner of listing bounded variables. The reason this was done is that the Fourier heat flux,

$$q^0 \equiv -k(dT/dx),$$

changes sign with the onset of temperature overshoot, and the inverted form gives the simplest curve. The relation used to compute the heat-flux ratio is

$$(M^{-2}q/q^0)_s = -\frac{16}{27}\left(\frac{q}{\tau u}\right)_s (\tau/\tau^0)_s \Big/ \left(\frac{u}{T}\frac{dT}{du}\right)_s. \tag{58}$$

Here again in figure 7, we see a wide departure from the Navier–Stokes relation $q = q^0$, except for the points near $M_s = 1$. For a strong shock wave, the figure shows that $q \sim M_1^2 q^0$ at the supersonic singular point (which implies that dT/dx approaches zero faster than q), and $q \simeq -2q^0$ at the subsonic singular point. Here, there is a complete breakdown in the association between q and q^0: the Fourier expression q^0 loses its physical significance. Viscous stress τ and heat flux q are physical quantities for all degrees of kinetic non-equilibrium; but this is not necessarily the case for the so-called kinetic temperature T. This is why figures 6 and 7 show that τ and q have physically correct signs and understandable functional forms, while it is only T that behaves in a rather peculiar manner.

The improvement achieved by our representation (48) over Grad's representation (38) indicates that our closure relations are superior to his, since the moment equations used are identical. It is also true that our closure relations are more complicated than his, and this is unfortunate in the following sense: one of the most intriguing aspects of this work is the opportunity it affords one to examine

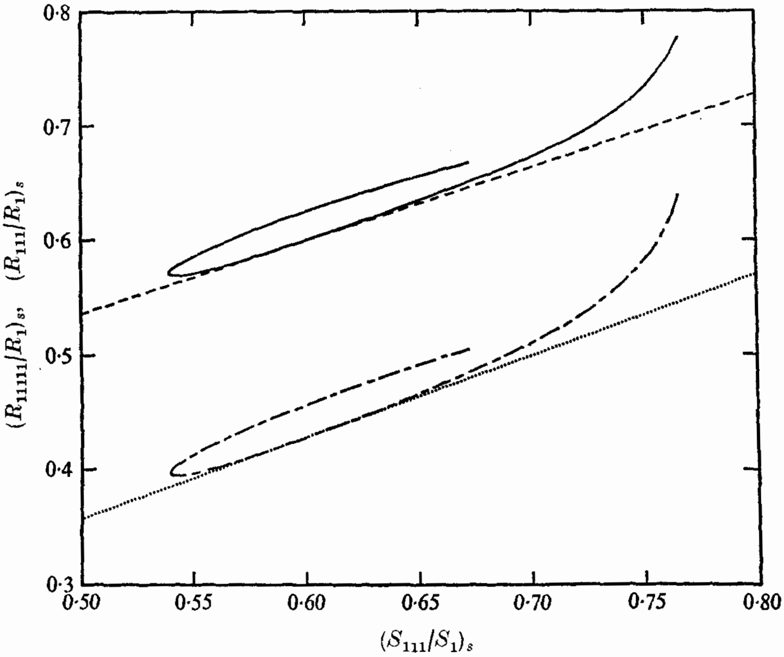

FIGURE 8. Variation of moment ratios $(R_{111}/R_1)_s$ and $(R_{11111}/R_1)_s$ with moment ratio $(S_{111}/S_1)_s$: ——, $(R_{111}/R_1)_s$ from composite solution; – – – –, $(R_{111}/R_1)_s$ from Grad's fourth-order closure relations; — — —, $(R_{11111}/R_1)_s$ from composite solution; ······, $(R_{11111}/R_1)_s$ from Grad's fourth-order closure relations.

a very specific problem, yet learn enough to be able to draw more general conclusions. Specifically, one would like to develop constitutive relations for several of the higher moments of f, and in essence, this is exactly the sort of information that one obtains from the closure relations.

Since Grad's closure relations are simpler than ours, it is worthwhile to see if there is anything useful that can be salvaged from them. Taking the fourth-order relations as a case in point, we again list (44)–(46), with (45) and (46) re-written by means of (21) and (44):

$$\left(M^{-2}\frac{1}{pu^2}\frac{dR_1}{du}\right)_s = \frac{84}{5}M_s^{-2}\left(M^{-2}\frac{1}{p}\frac{dq}{du}\right)_s, \tag{59}$$

$$\left(M^{-2}\frac{1}{pu^2}\frac{dR_{111}}{du}\right)_s = \frac{3}{14}\left[3\left(\frac{S_{111}}{S_1}\right)_s + 1\right]\left(M^{-2}\frac{1}{pu^2}\frac{dR_1}{du}\right)_s, \tag{60}$$

$$\left(M^{-2}\frac{1}{pu^2}\frac{dR_{11111}}{du}\right)_s = \frac{5}{7}\left(\frac{S_{111}}{S_1}\right)_s\left(M^{-2}\frac{1}{pu^2}\frac{dR_1}{du}\right)_s. \tag{61}$$

Comparison of these with (22)–(24) shows that Grad's fourth-order closure relations are equivalent to the set

$$\left(\frac{R_1}{qu^2}\right)_s = \frac{84}{5M_s^2}, \quad \left(\frac{R_{111}}{R_1}\right)_s = \frac{3}{14}\left[3\left(\frac{S_{111}}{S_1}\right)_s + 1\right], \quad \left(\frac{R_{11111}}{R_1}\right)_s = \frac{5}{7}\left(\frac{S_{111}}{S_1}\right)_s.$$

(62), (63), (64)

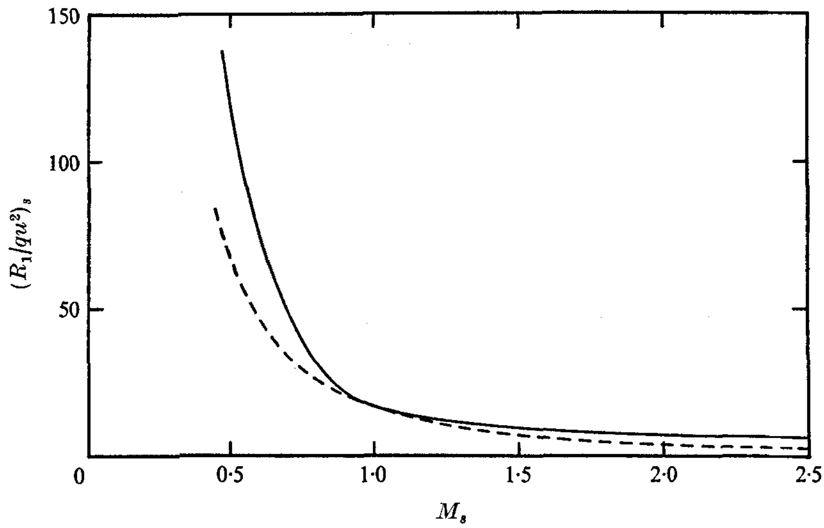

FIGURE 9. Variation of ratio $(R_1/qu^2)_s$ with singular point Mach number M_s: ——, composite solution; – – – –, Grad's fourth-order closure relations.

In figure 8 we show $(R_{111}/R_1)_s$ and $(R_{11111}/R_1)_s$ as functions of $(S_{111}/S_1)_s$, as defined by (63) and (64). For comparison, we also display the values obtained from the composite solution. The agreement is seen to be surprisingly good, which indicates that the major problem with Grad's fourth-order closure relations lies with (62).

In view of this conclusion, we compare in figure 9 the moment ratio $(R_1/qu^2)_s$ from Grad's fourth-order closure relation (62) with the value obtained from the composite solution. The difference as seen is trivial, yet of the utmost importance. Grad's upstream value approaches zero for $M_1 \gg 1$, whereas the more correct value is 4·07. The existence of a critical Mach number at every order in Grad's solution can be shown to arise from the vanishing upstream of such a moment ratio in Grad's closure relations. Figure 9 shows that it would be a trivial step to modify the functional form of Grad's closure relation (62) to produce a fourth-order set that would yield a solution uniformly valid in shock-wave Mach number. Once this were done, the obvious next step would be to introduce the same modification into Grad's fourth-order closure relations before they were evaluated at the singular point s. This would allow the complete computation of shock-wave structure. However, in order that the steps be physically meaningful, rather than just a mathematical exercise, it would be necessary to ensure that the modification left (62) invariant to a Galilean transformation. This possibility of formulating closure relations beyond the Navier–Stokes level is extremely exciting, and has provided much of the justification and direction for the present work.

One of the authors (JPE) would like to acknowledge support from the National Research Council of Canada, grant A6006, and from the University of Victoria, in the form of a Faculty Research Grant.

REFERENCES

ALTERMAN, Z., FRANKOWSKI, K. & PEKERIS, C. L. 1962 *Astrophys. J. Suppl. Ser.* **7**, 291.

BAGANOFF, D. & NATHENSON, M. 1970 *Phys. Fluids*, **13**, 596.

BIRD, G. A. 1970 *Phys. Fluids*, **13**, 1172.

CHAPMAN, S. & COWLING, T. G. 1964 *The Mathematical Theory of Non-Uniform Gases.* Cambridge University Press.

GILBARG, D. & PAOLUCCI, D. 1953 *J. Rat. Mech. Anal.* **2**, 617.

GRAD, H. 1949 *Commun. Pure Appl. Math.* **2**, 331.

GRAD, H. 1952 *Commun. Pure Appl. Math.* **5**, 257.

GRAD, H. 1958 *Handbuch der Physik*, **12**, 205.

HICKS, B. L. & YEN, S. M. 1967 *Phys. Fluids*, **10**, 458.

HICKS, B. L. & YEN, S. M. 1969 *Proc. 6th Int. Symp. on Rarefied Gas Dynamics*, vol. 1, p. 313.

HICKS, B. L., YEN, S. M. & REILLY, B. J. 1972 *J. Fluid Mech.* **53**, 85.

HOLWAY, L. H. 1964 *Phys. Fluids*, **7**, 911.

HOLWAY, L. H. 1965 *Proc. 4th Int. Symp. on Rarefied Gas Dynamics*, vol. 1, p. 193.

IKENBERRY, E. & TRUESDELL, C. 1956 *J. Rat. Mech. Anal.* **5**, 1.

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

MAXWELL, J. C. 1890 *The Scientific Papers of James Clerk Maxwell*, vol. 2, p. 26. Cambridge University Press.

MISES, R. VON 1950 *J. Aero. Sci.* **17**, 551.

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

NATHENSON, M. & BAGANOFF, D. 1973 *Phys. Fluids*, **16**, 2110.

NORDSIECK, A. & HICKS, B. L. 1967 *Proc. 5th Int. Symp. on Rarefied Gas Dynamics*, vol. 1, p. 695.

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

SCHMIDT, B. 1969 *J. Fluid Mech.* **39**, 361.

UHLENBECK, G. E. & FORD, G. W. 1963 *Lectures in Statistical Mechanics.* American Mathematical Society.

WALDMANN, L. 1958 *Handbuch der Physik*, **12**, 295.

WANG CHANG, C. S. & UHLENBECK, G. E. 1952 *Engng Res. Inst. Rep., University of Michigan*, M 999.

YEN, S. M., WALTERS, W. P., NG, W. & FLOOD, J. R. 1974 *Proc. 8th Int. Symp. on Rarefied Gas Dynamics*, p. 134.