SOLUTION OF THE BOLTZMANN EQUATION AT THE SINGULAR POINTS IN A SHOCK WAVE BY THE METHOD OF RATIONAL TRUNCATION AND COORDINATE STRAINING

by

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ABSTRACT

A solution of the Boltzmann equation at the upstream and downstream singular points in a shock wave, for the case of Maxwell molecules, is obtained by application of the method of rational truncation and coordinate straining. The method is based of the idea that a rational procedure for truncating and closing any system of moment equations must be developed from an orthonormal expansion for the distribution function, and that the convergence of the expansion can be accelerated if the coordinates in velocity space are scaled in accordance with the nature of the distribution function. The use of an orthonormal expansion for the distribution function is shown to yield significant improvement over the method of Grad, but the further step of coordinate straining is necessary to provide a rapidly convergent solution. The solution shows that the Navier-Stokes and Fourier relations (i.e., first-order Chapman-Enskog results) are approximately valid only for weak shock waves; confirms the existence of temperature overshoot in strong shock waves; and provides exact boundary values that can be used to guide numerical solutions of the Boltzmann equation for shock-wave structure.

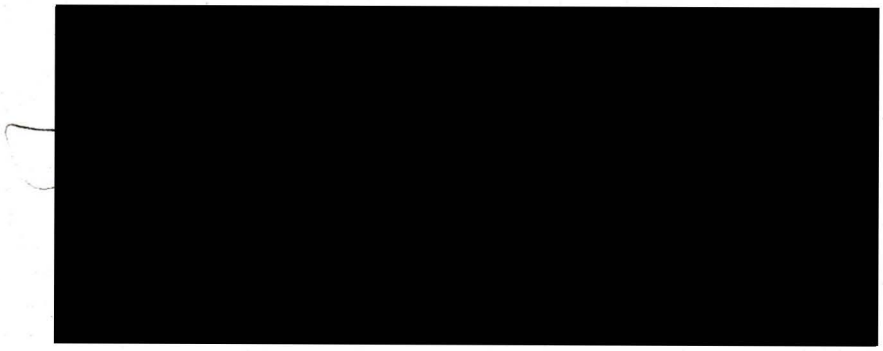

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

CHAPTER 1

INTRODUCTION

In the kinetic theory of gases, the fundamental problem is to obtain solutions of the Boltzmann equation for various situations of physical interest. This equation is a nonlinear integro-differential equation that describes the rate of change, with respect to position and time, of the distribution function of the gas molecules, where $f(t,\vec{x},\vec{c})d\vec{x}d\vec{c}$ is the probability that a molecule has position $\vec{x}$ and velocity $\vec{c}$ at time t. For situations without external forces, the Boltzmann equation can be written

$$\frac{\partial(\rho f)}{\partial t} + \sum_{i=1}^{3} c_i \frac{\partial(\rho f)}{\partial x_i} = \mathcal{C}(\rho f) \quad , \tag{1.1}$$

where ρ is the mass density and $\mathcal{C}(\rho f)$ represents the collision integral. Solution of the Boltzmann equation for f determines the macroscopic behavior of the flow since all the gasdynamic variables are just moments of f.

Due to the nonlinear nature of the collision integral, exact solutions of the Boltzmann equation are available for only a few problems. In particular, for a gas in equilibrium, solution of the Boltzmann equation yields the familiar Maxwellian velocity distribution $f^{(o)}=\pi^{-3/2}\exp(-V^2)$. Here we have used the nondimensional thermal velocity $\vec{V}=(2RT)^{\frac{1}{2}}\vec{C}$. For situations involving small disturbances from equilibrium, a linearized form of the Boltzmann equation can be used, while in more general situations, the nonlinearity must be treated more indirectly.

Of some interest is the Chapman-Enskog procedure in which f is written as the power series

$$f = f^{(o)}(1+\varepsilon\phi_1+\varepsilon^2\phi_2+\ldots)$$

where the parameter ε has the physical interpretation of being proportional to the ratio of a characteristic time between collisions (the relaxation time) to a characteristic flow time. In the

Chapman-Enskog solution of the Boltzmann equation, terms of first order in ε are retained and this expansion leads to the familiar Navier-Stokes equations of macroscopic gas dynamics. Retention of second-order terms in ε leads to the Burnett equations. It is interesting to note that, in the problem of shock-wave structure, the Navier-Stokes equations give a valid solution for all shock-wave Mach numbers (although for strong shock waves the distribution function assumes a highly improbable form), while the Burnett equations are applicable only for $M_1 \lesssim 2.1$ (Sherman and Talbot 1960).

An indirect method for solving the Boltzmann equation was proposed by Maxwell (1879). For any set of linearly independent functions of the molecular velocity, one can multiply the Boltzmann equation by these functions and integrate over velocity to obtain an infinite system of *moment equations*. Of particular interest are sets of polynomials, since only polynomial moments of the collision integral can be computed directly. It is implicitly assumed in this process that f decays sufficiently rapidly as $V \to \infty$ in order that polynomial moments exist. Also, it is a characteristic of the Boltzmann equation that truncating the infinite system of moment equations at any point always yields a system containing a greater number of unknowns (moments) than equations. Although the system of moment equations is exact, at this point a particular representation for the distribution function must be specified. The approximate representation for f will then give *closure relations* among the moments in order to form a determinate system of equations.

The representation for f that is often chosen is

$$f = f^{(o)}(1+\Phi) \tag{1.2}$$

where $f^{(o)}$ is the local Maxwellian (local in the sense that it varies throughout the flow because of its temperature dependence). Expanding Φ in terms of a set of functions which are orthonormal with respect to $f^{(o)}$ then gives

$$f = f^{(o)} \sum_{i=1}^{\infty} \zeta_i \psi_i \tag{1.3}$$

where, for example, the ψ_i's are normalized three-dimensional Hermite polynomials in the case of Grad's method (Grad 1949). Although a general three-dimensional flow involves multiple subscripts, an appropriate ordering of the subscripts is assumed and replaced with a single subscript to simplify the discussion.

For certain physical problems (in particular, the strong shock wave), mathematical difficulties arise from the expansion (1.3). Using (1.3) and the orthonormal properties of the ψ_i's, we obtain Bessel's inequality in the form

$$\langle f, f^{(o)-1} f \rangle \geq \sum_{i=1}^{n} \zeta_i^2 \tag{1.4}$$

where we have used the notation

$$\langle f, \chi \rangle \equiv \int f \chi d\vec{V} \quad .$$

Holway (1964) has shown that near the upstream end of a strong shock wave $f^{(o)}$ decreases much faster than f^2 as $V \to \infty$, thus $\langle f, f^{(o)-1} f \rangle$ is not bounded and the series (1.3) does not converge. For Grad's procedure of obtaining closure relations, in which the series is truncated by setting all the ζ_i's beyond a certain point equal to zero, we see that this truncation is inconsistent with Bessel's inequality, at least for one flow.

This conflict between the desire to use the representation (1.3) for f because of its subsequent mathematical convenience and the lack of convergence of the expansion (1.3) led to the development, by Baganoff and Elliott (1975), of the *method of rational truncation and coordinate straining* for closing a system of moment equations. Since the object of the present work is to apply this method to the problem of shock-wave structure, the theory of the aformentioned paper will be outlined here to provide the necessary background for subsequent discussion.

In order to develop a systematic method of closing any set of moment equations, an orthonormal representation for the distribution function of the form

$$f = f^{(o)} + \sum_{j=1}^{\infty} a_j \phi_j \tag{1.5}$$

is chosen because the set of coefficients in a truncated orthonormal expansion is the best approximation in the sense of least squares; here, the ϕ_j's are some suitable orthonormal set. With this representation, Bessel's inequality becomes

$$\langle \Delta f, \Delta f \rangle \geq \sum_{j=1}^{k} a_j^2 \tag{1.6}$$

and thus guarantees convergence of (1.5) (in the mean-square sense) since $\Delta f \equiv f - f^{(o)}$ must be square-integrable in any physical problem (the terms $f^2, ff^{(o)}$, and $f^{(o)\,2}$ must yield finite values when integrated over all $\vec{V}$). Using the representation (1.5) for f, a system of moment equations in the a_j's could be formed. Representing this system by

$$\mathcal{M}_i(a_1, a_2, \ldots) = 0 \quad , \qquad i=1,2,\ldots \tag{1.7}$$

and truncating after K equations, we see that the process of closing the system by setting

$$a_n = 0 \quad , \qquad n>K \tag{1.8}$$

is a rational approximation as shown by Bessel's inequality (1.6). Unfortunately, the system (1.7) will not in general contain the conservation equations, which must be satisfied at every level of truncation. However, the rational truncation procedure (1.8) can still be applied even if the system of moment equations (1.7) is not used. For example, if the system of moment equations

$$\tilde{\mathcal{M}}_i(\zeta_1, \zeta_2, \ldots) = 0 \quad , \qquad i=1,2,\ldots \tag{1.9}$$

is chosen, where the ζ_i's are the moments appearing in (1.3), then the rational truncation procedure (1.8) can be applied to the system (1.9) since the two sets of moments are related by a linear transformation

$$\zeta_i = \sum_{j=1}^{\infty} T_{ij} a_j \quad , \qquad i=1,2,\ldots \quad . \tag{1.10}$$

Upon substitution of the closure relations (1.8), the transformation (1.10) can be solved to obtain closure relations in the ζ_i variables. This process is more easily seen if (1.10) is written in matrix form

$$\begin{bmatrix} \zeta^0 \\ \zeta^* \end{bmatrix} = \begin{bmatrix} T_A & T_C \\ T_B & T_D \end{bmatrix} \begin{bmatrix} a^0 \\ a^* \end{bmatrix} \tag{1.11}$$

where T_A is a K by K submatrix of (T_{ij}) and the vectors ζ^0 and a^0 are of length K. With this notation, the closure relations (1.8) become

$$a^* = 0 \tag{1.12}$$

and, on substitution into (1.11), the following approximate matrix relations result:

$$\zeta^0 = T_A a^0 \quad ,$$

$$\zeta^* = T_B a^0 \quad .$$

From these it follows that

$$\zeta^* = T_B T_A^{-1} \zeta^0 \quad . \tag{1.13}$$

Thus, for the system of moment equations (1.9), the necessary closure relations are given by (1.13) where these relations are a direct consequence of the rational truncation of (1.5).

Since the form of the representation (1.5) for f allows a choice for the scale of the ϕ_j's that differs from the scale of the local Maxwellian, we see that a clever choice of this scale may improve the efficiency with which the series (1.5) represents f. In other words, the ϕ_j's can be assigned to have, as their arguments, new dimensionless velocity components W_i which can be related to the original velocity components V_i in a manner dictated by the particular problem.

In summarizing the method of rational truncation and coordinate straining, it should be noted that the important step is the use of an expansion for f in terms of an orthonormal set ϕ_j so that the truncation procedure will yield rational closure relations. The further idea of coordinate straining serves to accelerate the convergence of the representation for f and thus may be valuable for achieving a physically realistic solution at a low level of truncation.

We now proceed to describe the application of this method to the problem of shock-wave structure, and specifically to the singular-point analysis as formulated by Elliott and Baganoff (1974), the details of which are reviewed in Chapter 2. In Chapter 3, we restrict the present general discussion of the method of rational truncation and coordinate straining to the case of one-dimensional flow, and introduce the

machinery necessary for numerical solution of the singular-point problem; this constitutes the bulk of the present effort. Results of the calculations are displayed and discussed in Chapter 4, while Chapter 5 contains brief suggestions for further development of the general method.

CHAPTER 2

THE PROBLEM OF SHOCK-WAVE STRUCTURE

A steady, normal shock wave in a perfect, monatomic gas is a simple non-equilibrium situation in which the mean properties of the gas vary greatly over distances of the order of a mean free path. Because of the degree of non-equilibrium involved, the problem of shock-wave structure provides an excellent test for any method of closing the system of moment equations. Also, the shock wave has the desirable feature that the region of non-uniformity is bounded on either side by a gas in equilibrium, as opposed to solid walls, and thus the problem is not complicated by the details of gas-solid interactions on a molecular scale.

In order to demonstrate the effectiveness of the method of rational truncation and coordinate straining in closing a system of moment equations, it is sufficient to study the flow in the upstream and downstream wings of a shock wave, because it is in these regions that conventional methods fail (Elliott and Baganoff 1974). Restricting our attention to these regions greatly reduces the complexity of the problem, since many terms drop out of the analysis; the nonlinear features of the flow are nonetheless retained.

In studying shock-wave structure, it will be convenient to adopt an approach employed by others, such as Gilbarg and Paolucci (1953), and consider the fluid velocity u, rather than the spatial coordinate x as the independent variable. With this substitution, the solution curve for a dependent variable such as temperature is terminated at each end by a singular point. The upstream, or supersonic singular point is fixed by the upstream flow conditions; and the downstream singular point is determined by the Rankine-Hugoniot equations, which relate the flow conditions on either side of a shock wave. It is at these singular points that we wish to determine the direction of the tangent to the solution curve, for each dependent variable.

Rather than present a detailed development of the system of moment equations to be used, it will be convenient to simply outline the procedure in order to preserve continuity of the present discussion regarding the application of the method of rational truncation and coordinate straining to the shock-wave problem. For a more complete development, the reader is referred to Elliott and Baganoff (1974).

For a steady, normal shock wave, the Boltzmann equation (1.1) can be written (using u as the independent variable) in the form

$$c_x \frac{\partial(\rho f)}{\partial u} = \frac{\mathcal{C}(\rho f)}{du/dx} \quad . \tag{2.1}$$

A more useful form of (2.1) can be obtained by transforming from the laboratory velocity $\vec{c}$ to the thermal velocity $\vec{C} \equiv (\vec{c} - \vec{u})$. As shown by Chapman and Cowling (1964), this transformation gives

$$(u+C_x)\left[\frac{\partial(\rho f)}{\partial u} - \frac{\partial(\rho f)}{\partial C_x}\right] = \frac{\mathcal{C}(\rho f)}{du/dx} \tag{2.2}$$

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

For the purpose of the singular-point analysis, we wish to take the singular-point limit of (2.2). Although the left-hand side presents no difficulty, the right-hand side is indeterminate at a singular point, so L'Hospital's rule must be employed. Details of this manipulation are given in Elliott and Baganoff (1974); the final result is

$$(\tilde{M}_s + V_x)(\tilde{M}_s^{-1} h_s + 2V_x) = \omega_s J(h_s) \quad , \tag{2.3}$$

for $s=1$ (upstream) or $s=2$ (downstream). Here

$$h_s \equiv \left[\frac{u}{\rho f^{(\omega)}} \frac{\partial(\rho f)}{\partial u}\right]_s \quad , \tag{2.4}$$

$\tilde{M}_s \equiv u_s (2RT_s)^{-\frac{1}{2}}$, $\vec{V} \equiv \vec{C}(2RT_s)^{-\frac{1}{2}}$ (note the suppression of s), and J is the familiar linearized collision operator (Cercignani 1969). The quantity ω_s is related to certain moments of h_s (the explicit relationship will be given in Chapter 3). Therefore (2.3) is a nonlinear integral equation for h_s, and direct solution is impossible. We shall proceed instead by the moment method, as discussed in Chapter 1.

By restricting the discussion to the case of Maxwell molecules[1],

[1]Maxwell molecules are defined as having an intermolecular force which is inversely proportional to the fifth power of the separation between molecules.

we can follow the method of Wang Chang and Uhlenbeck (1952) and, in analogy to (1.3), formally write

$$h_s = \pi^{3/4} \sum_{r,l} \xi_{rl} \psi_{rl} \quad , \tag{2.5}$$

where the ψ_{rl}'s are eigenfunctions of J as defined by Wang Chang and Uhlenbeck (1952) and the coefficients ξ_{rl} are eigenfunction-moment derivatives, to be determined. A partial list of the eigenfunctions is displayed in Table 1. Substituting (2.5) into the fundamental equation (2.3) for h_s, multiplying by $\psi_{r'l'} \exp(-V^2)$ and integrating, we obtain the infinite system of moment equations

$$\sum_{r'l'} \left[\tilde{M}_s (\omega_s \lambda_{rl} - 1) \delta_{rl,r'l'} - M_{rl,r'l'} \right] \xi_{r'l'} = b_{rl} \quad , \tag{2.6}$$

where

$$M_{rl,r'l'} \equiv \int V_x \exp(-V^2) \psi_{rl} \psi_{r'l'} d\vec{V} \quad ,$$

$$b_{rl} \equiv 2\pi^{-3/4} \tilde{M}_s \int V_x (M_s + V_x) \exp(-V^2) \psi_{rl} d\vec{V} \quad ,$$

and where λ_{rl} is the eigenvalue corresponding to ψ_{rl}. It should be stressed that although (2.5) was used as a formal convenience in obtaining (2.6), the validity of (2.6) does not depend upon the convergence of (2.5). In fact, (2.6) is an exact system of algebraic equations in the ξ_{rl}'s. However, we recall from the discussion above that (2.6) is nonlinear because of the presence of ω_s; and thus solution by computer is required.

Before proceeding to the mathematical details concerning the solution of the moment equations (2.6), a comment regarding the small-perturbation assumption implicit in (2.3) is appropriate. Although it may seem that this assumption would imply convergence of (2.5), this is not necessarily true, since even near a singular point where $|\Delta f|$ is small, we may still have $|\Delta f / f^{(\infty)}| \to \infty$ as $V \to \infty$. Thus the same difficulties can arise with (2.5) as with (1.3).

TABLE 1. First nine of the eigenfunctions of the linearized collision operator for Maxwell molecules and ordering of r and l with respect to a single subscript, i.

i	r	l	degree $(2r+l)$	ψ_i
1	0	0	0	$\pi^{-3/4}$
2	0	1	1	$(2)^{\frac{1}{2}}\pi^{-3/4}V_x$
3	1	0	2	$(2/3)^{\frac{1}{2}}\pi^{-3/4}(3/2-V^2)$
4	0	2		$(3)^{-\frac{1}{2}}\pi^{-3/4}(3V_x{}^2-V^2)$
5	1	1	3	$2(5)^{-\frac{1}{2}}\pi^{-3/4}V_x(5/2-V^2)$
6	0	3		$(2/15)^{\frac{1}{2}}\pi^{-3/4}(5V_x{}^3-3V^2V_x)$
7	2	0	4	$(2/15)^{\frac{1}{2}}\pi^{-3/4}(15/4-5V^2+V^4)$
8	1	2		$(2/21)^{\frac{1}{2}}\pi^{-3/4}(3V_x{}^2-V^2)(7/2-V^2)$
9	0	4		$\frac{1}{2}(105)^{-\frac{1}{2}}\pi^{-3/4}(35V_x{}^4-30V_x{}^2V^2+3V^4)$

CHAPTER 3

MATHEMATICAL DETAILS

Before discussing the development of closure relations (1.13) appropriate for closing the system of moment equations (2.6), we should point out that equation (1.10) is slightly more complicated than it appears. The formal procedure for obtaining this transformation is to multiply (1.5) by ψ_i and integrate over $\vec{V}$ (noting that $\zeta_i = \langle \psi_i, f \rangle$). The result of this operation is

$$\zeta_i - \langle \psi_i, f^{(0)} \rangle = \sum_{j=1}^{\infty} \langle \psi_i, \phi_j \rangle a_j \quad , \tag{3.1}$$

where we have returned to the single subscript notation for simplicity. Since the left-hand side of (3.1) yields zero when $i=1$, and ζ_i when $i>1$, we must remember to replace ζ_1 by zero in all relations explicitly involving ζ_1 in order that we may use the simple notation of (1.13).

In view of the fact that convergence of (1.5) is guaranteed by Bessel's inequality, and since coordinate straining can be employed to accelerate convergence, it is desirable to make the selection of the ϕ_j's on the basis of mathematical convenience. To this end, we note that the combination $\left[f^{(0)}\right]^{\frac{1}{2}}\psi_j$ forms an orthonormal set and thus we make the selection

$$\phi_j(\vec{W}) = \exp(-W^2/2)\psi_j(\vec{W}) \quad , \tag{3.2}$$

where the eigenfunctions $\psi_j(\vec{W})$ for a one-dimensional flow are given by

$$\psi_{r\ell}(\vec{W}) = \left[\frac{r!\,(\ell+\frac{1}{2})}{\pi\,(\ell+\frac{1}{2}+r)!}\right]^{\frac{1}{2}} W^{\ell} P_{\ell}(\cos\theta) L_r^{(\ell+\frac{1}{2})}(W^2) \tag{3.3}$$

and are polynomials of degree $2r+\ell$. In (3.3), $W_x = W\cos\theta$, P_ℓ is the Legendre polynomial, and

$$L_r^{(\ell+\frac{1}{2})}(W^2) = \sum_{k=0}^{r} (-1)^k W^{2k} \frac{(\ell+\frac{1}{2}+r)!}{j!\,(r-j)!\,(\ell+\frac{1}{2}+j)!}$$

is the Laguerre polynomial. When using the single subscript notation, it is assumed that the $\psi_{r\ell}$'s are ordered in groups of increasing $2r+\ell$ and, within each group, in order of decreasing r. This particular

ordering of r and l with respect to a single subscript or index is displayed in Table 1 and will be used throughout the present work.

As a direct consequence of (3.1) and (3.2), the matrix elements can be written explicitly as

$$T_{ij} = \int \psi_i(\vec{V}) \psi_j(\vec{W}) \exp(-W^2/2) d\vec{V} \tag{3.4}$$

Here we relate $\vec{W}$ to $\vec{V}$ by a linear transformation

$$W_i = \sum_{j=1}^{3} P_{ij} V_j \quad , \qquad i=1,2,3 \quad , \tag{3.5}$$

where the elements of the transformation matrix will be parameters chosen to characterize the flow. In writing (3.5) we have restricted ourselves to linear coordinate straining since anything more complicated would be difficult to handle algebraically.

Since the distribution function for a one-dimensional flow is axially symmetric in velocity space, a realistic form for the coordinate straining (3.5) is

$$W_x = \alpha V_x \quad , \qquad W_\perp = \beta V_\perp \tag{3.6}$$

where the subscripts x and $\perp$ refer to the axial and transverse directions in velocity space, respectively, and where α and β are to be specified. For convenience in subsequent discussion we rewrite (3.6) as

$$V_x = \lambda W_x \quad , \qquad V_\perp = \mu W_\perp \tag{3.7}$$

where we have defined $\lambda \equiv \alpha^{-1}$ and $\mu \equiv \beta^{-1}$. Under the straining (3.7), the expression (3.4) for T_{ij} becomes

$$T_{ij} = \lambda \mu^2 \int \psi_i(\lambda W_x, \mu W_\perp) \psi_j(\vec{W}) \exp(-W^2/2) d\vec{W} \quad . \tag{3.8}$$

Although the elements of the transformation matrix (T_{ij}) could be computed directly from (3.8), it would not be a practical approach for high-order computer solution of (2.6) due to the large number of elements which are needed for the closure relations (1.13). A more efficient approach can be realized by defining a vector having elements

$$e_k(\vec{W}) = W^{2r_k} W_x^{l_k} \quad , \qquad k=1,2,\ldots \tag{3.9}$$

where r_k and l_k have the values defined in Table 1. With the definition

(3.9), the eigenfunctions can be expressed in the form

$$\psi_i(\vec{V}) = \sum_{k=1}^{i} \alpha_{ik} e_k(\vec{V}) \tag{3.10}$$

where the matrix of coefficients (α_{ik}) is lower-triangular. Due to the linearity of the straining (3.7), the vector $\vec{e}(\vec{V})$ is related to $\vec{e}(\vec{W})$ by the linear transformation

$$e_k(\vec{V}) = \sum_{m=1}^{N(k)} \omega_{km} e_m(\vec{W}) \quad , \qquad N(k) \equiv k + r_k \quad , \tag{3.11}$$

where it can be seen from the relation

$$V^2 = \mu^2 W^2 + (\lambda^2 - \mu^2) W_x^2$$

that the only non-zero elements in row k of the matrix (ω_{km}) involve the factor λ^{l_k} multiplied by combinations of powers of μ^2 and $(\lambda^2-\mu^2)$. Combining (3.10) and (3.11), we can write

$$\psi_i(\vec{V}) = \sum_{k=1}^{i} \sum_{m=1}^{N(k)} \alpha_{ik} \omega_{km} e_m(\vec{W}) \quad ,$$

and subsequently

$$T_{ij} = \lambda\mu^2 \sum_{k=1}^{i} \sum_{m=1}^{N(k)} \sum_{n=1}^{j} \alpha_{ik} \omega_{km} \alpha_{jn} \int e_m(\vec{W}) e_n(\vec{W}) \exp(-W^2/2) d\vec{W} \ . \tag{3.12}$$

With the further definition

$$\pi_{mn} \equiv \int e_m(\vec{W}) e_n(\vec{W}) \exp(-W^2/2) d\vec{W} \quad ,$$

the transformation matrix (T_{ij}) assumes the form of a product of four matrices, specifically,

$$T_{ij} = \lambda\mu^2 \sum_{k=1}^{i} \sum_{m=1}^{N(k)} \sum_{n=1}^{j} \alpha_{ik} \omega_{km} \pi_{mn} \alpha^{T}_{nj} \quad , \tag{3.13}$$

where we have used the fact that π_{mn} is symmetric, and where the matrix $(\alpha^{T}_{nj}) = (\alpha_{jn})$. Equation (3.13) is not yet suitable for computer evaluation of the matrix elements T_{ij}, since the elements ω_{km} are polynomials in λ and μ. However, by defining a vector $\vec{s}$ with elements

$$s_n = \mu^{2r_n} \lambda^{l_n} \tag{3.14}$$

in direct analogy with (3.9), the matrix elements ω_{km} can be expressed in the form

$$\omega_{km} = \sum_{p=1}^{m} \phi_{kmp} s_p \quad .$$

From this, it follows that

$$T_{ij} = \lambda\mu^2 \sum_{p=1}^{N(i)} \gamma_{ijp} s_p \quad , \tag{3.15}$$

where the matrix elements

$$\gamma_{ijp} \equiv \sum_{k=1}^{p} \sum_{m=1}^{N(k)} \sum_{n=1}^{j} \alpha_{ik} \phi_{kmp} \pi_{mn} \alpha^{T}_{nj} \tag{3.16}$$

are simply constants. Appendix A contains the FORTRAN computer program used to evaluate the matrix elements γ_{ijp}. Knowing these, it is a simple matter to evaluate the transformation matrix elements T_{ij}, using (3.15), for any particular choice of the straining parameters λ and μ.

We now turn our attention to the way in which the closure relations (1.13) are applied to a truncated set of the moment equations (2.6). Figure 1 shows the location of all non-zero elements of the (symmetric) matrix of coefficients in (2.6). The "d" entries represent the diagonal elements $\tilde{M}_s(\omega_s \lambda_{rl} - 1)$ and the "m" entries represent the elements $-M_{rl,r'l'}$. Truncation of the system at a certain order n is accomplished by eliminating all equations for which $2r+l>n$. The structure of the matrix in figure 1 shows that the truncated system is not closed since the n^{th} order equations contain ξ_{rl}'s of order $n+1$ (having, as their coefficients, elements of the submatrix C). However, using the closure relations (1.13), we can write

$$C\xi^{(n+1)} = CT_B T_A^{-1} \xi^0$$

where $\xi^{(n+1)}$ is a vector of the ξ_{rl}'s of order $n+1$. Thus closure of the truncated system is accomplished by deleting C and adding the matrix $CT_B T_A^{-1}$ to the remaining matrix of coefficients for the n^{th} order equations of the truncated system, as shown in figure 2. This is in contrast to the closure based on Grad's method, in which the ξ_{rl}'s of order $n+1$ are simply set to zero (rather than being related to the lower-order ξ_{rl}'s).

From the normalization of f and the definition of the thermal velocity, it follows that $\xi_{00}=-1$ and $\xi_{01}=0$, so the equation for $r=l=0$

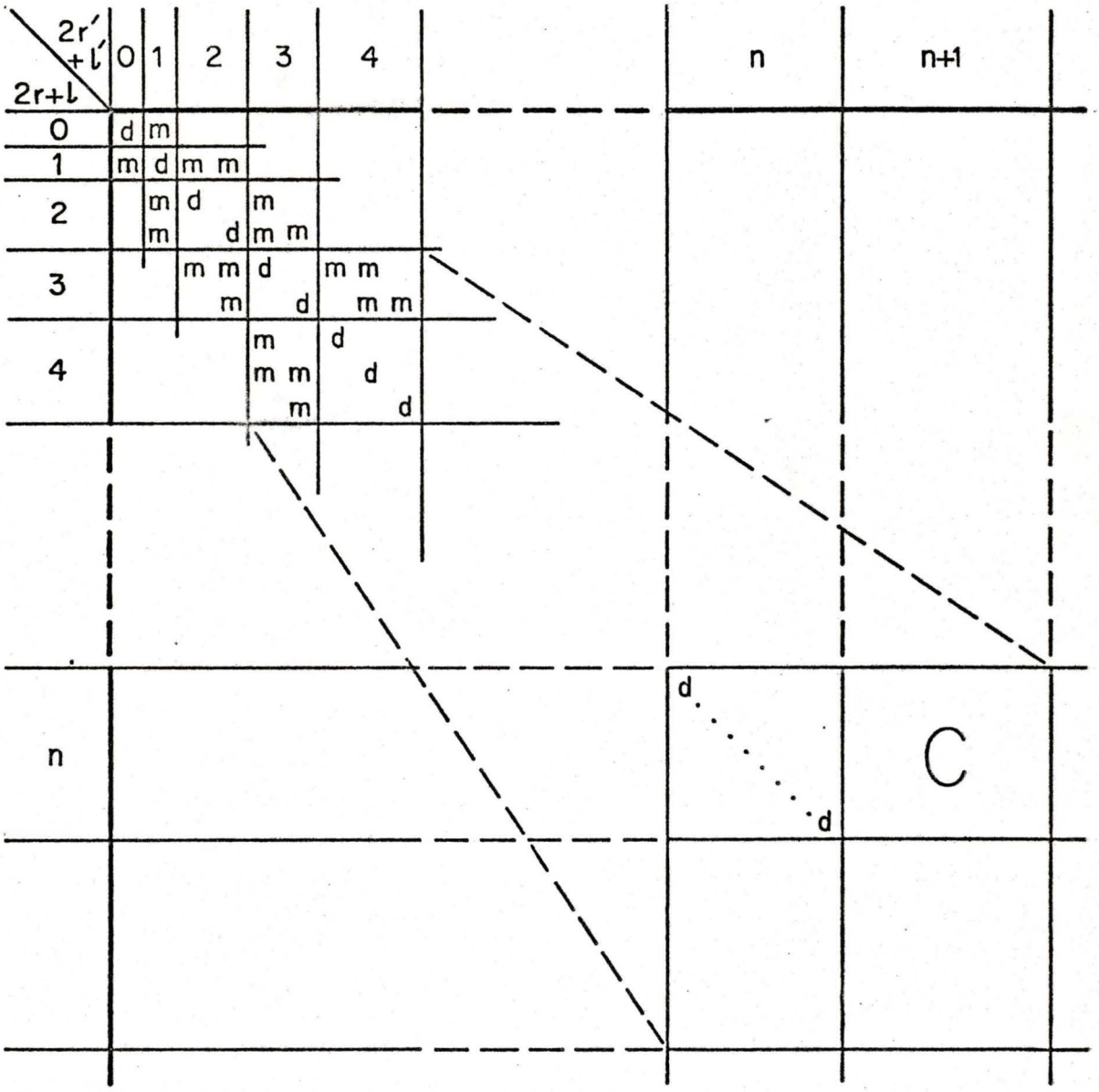
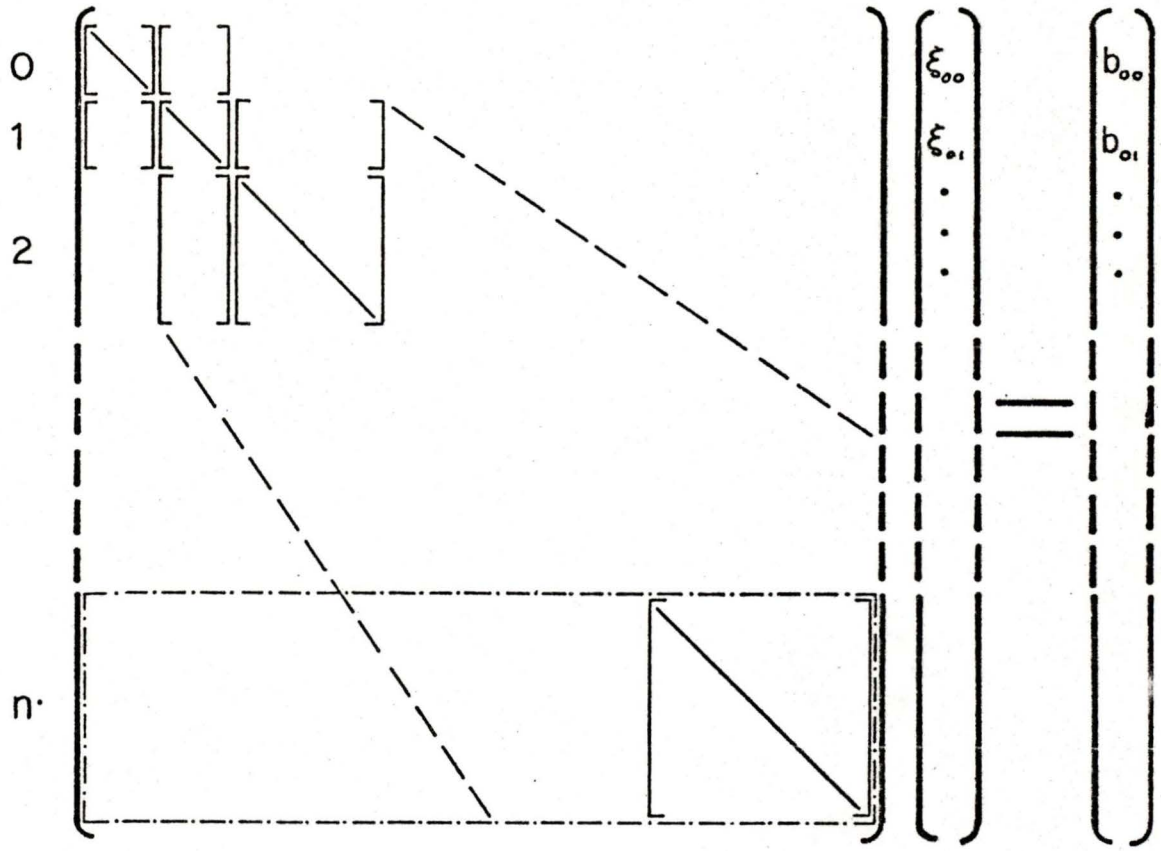


FIGURE 1. Location of the nonzero elements in the matrix of coefficients for the system of moment equations (2.6).



Legend:


represents the diagonal submatrices of figure 1.


represents the off-diagonal submatrices of figure 1.


shows the location of the closure matrix $CT_B T_A^{-1}$.

FIGURE 2. The system of moment equations (2.6) after truncation and closure.

is identically satisfied and can be discarded from the system.[2] Thus, after closure at any order, there is always one less ξ_{rl} than the number of equations, N-1, to be satisfied. The extra unknown is ω_s and it completes the system.

The solution of the system can be accomplished by isolating the second equation of the system,

$$(2)^{-\frac{1}{2}}+(3)^{-\frac{1}{2}}\xi_{10}-(2/3)^{\frac{1}{2}}\xi_{02}-b_{01} = 0 \quad . \tag{3.17}$$

The left-hand side of (3.17) can be regarded as a function, $\delta(\xi_{10},\xi_{02},M_s)$, and solution of the system can be achieved by using a Newton-Raphson iteration process for finding the value of ω_s that gives the optimum solution vector for the remaining set of N-2 equations in N-2 ξ_{rl}'s, i.e., the solution vector which minimizes $|\delta(\xi_{10},\xi_{02},M_s)|$.

From a practical point of view, the nature of $\delta(\xi_{10},\xi_{02},M_s)$ makes it difficult to use an iterative technique for finding its roots. This problem arises because $\delta(\xi_{10},\xi_{02},M_s)$ is implicitly a ratio of two polynomials of degree N-2 in ω_s where, for example, N-2=10 for truncation of the system at order 5, and N-2=34 for truncation at order 10. This functional dependence gives rise to computational problems such as roots of δ that lie immediately adjacent to asymptotes.

A more practical approach can be achieved by not removing equation (3.17) from the system, and noting that the determinant of the augmented matrix for the over-determined set of equations in the ξ_{rl}'s must vanish in order that there exist a non-trivial solution. The technique, therefore, is to use the Newton-Raphson iterative procedure to find the value of ω_s for which this determinant vanishes and then solve the system of N-2 equations in the N-2 unknown ξ_{rl}'s for this value of ω_s. When the ξ_{rl}'s are known, the quantities of physical interest can be determined from

$$\xi_{rl} = \pi^{3/4}\left[\frac{u}{\rho}\frac{d}{du}\rho\langle\psi_{rl},f\rangle\right]_s \quad .[3]$$

[2]Here we have made use of the results $\lambda_{00}=0$ and $b_{00}=\tilde{M}_s$.

[3]Several of these transformations are listed by Elliott and Baganoff (1974).

The FORTRAN program used to solve the system of moment equations for any order of truncation up to eleven is presented in Appendix B.

Before displaying the results obtained, we note that the quantity ω_s is defined by

$$\omega_s \equiv \frac{16}{9A_2}(\tau/\tau^0)_s \Big/ \left[\frac{u}{p}\frac{d\tau}{du}\right]_s \quad ,$$

where p is the pressure, A_2=2·7406... is the constant defined by Wang Chang and Uhlenbeck (1952), and

$$\tau^0 \equiv \frac{4}{3}\eta\frac{du}{dx}$$

is the Navier-Stokes expression for the axial component τ of the viscous stress tensor. Here η is the coefficient of viscosity. The stress ratio $(\tau/\tau^0)_s$ will be very useful for displaying and interpreting the results.

CHAPTER 4

RESULTS AND DISCUSSION

Following the practice of Elliott and Baganoff (1974) we shall restrict ourselves to discussion of moment ratios which have been scaled with M_s such that they are bounded. We shall be particularly interested in the variation of the bounded ratio $(M^{-2}\tau/\tau^0)_s$ with the singular-point Mach number M_s. Since $\tau \leq 0$ in a shock wave, this ratio must be non-negative in order that u decrease monotonically through the shock wave; thus, it provides a convenient way for determining the existence of a critical Mach number at which a solution becomes physically meaningless.

The variation of $(M^{-2}\tau/\tau^0)_s$ with M_s for solution of the moment equations based on Grad's closure relations is displayed in figure 3. The thirteen-moment level of approximation corresponds to retention of the first five equations of the system (2.6), as opposed to six equations for the third-order solution. For a given order of solution, two points appear for each shock-wave Mach number (i.e., upstream singular-point Mach number): one corresponding to the upstream singular point (s=1), and the other corresponding to the downstream singular point (s=2). The point M_s=1 separates the upstream and downstream branches of each curve. A typical pair of upstream and downstream points for the ninth-order solution is given by the points A and B, respectively. Several of the solutions are not shown downstream to avoid crowding and overlapping. Figure 3 shows that the downstream solutions based on Grad's closure relations have essentially converged by ninth order. On the other hand, the upstream solutions converge extremely slowly and all orders exhibit a critical Mach number. Although these critical Mach numbers increase monotonically with the order of solution, even the ninth-order results are valid only for M_1 significantly less than two. Since only thirteen-moment calculations are practical over the interior of a shock wave, it is clear that computation of a shock-wave profile based on Grad's closure relations is not justified, except for the case of a weak shock wave.

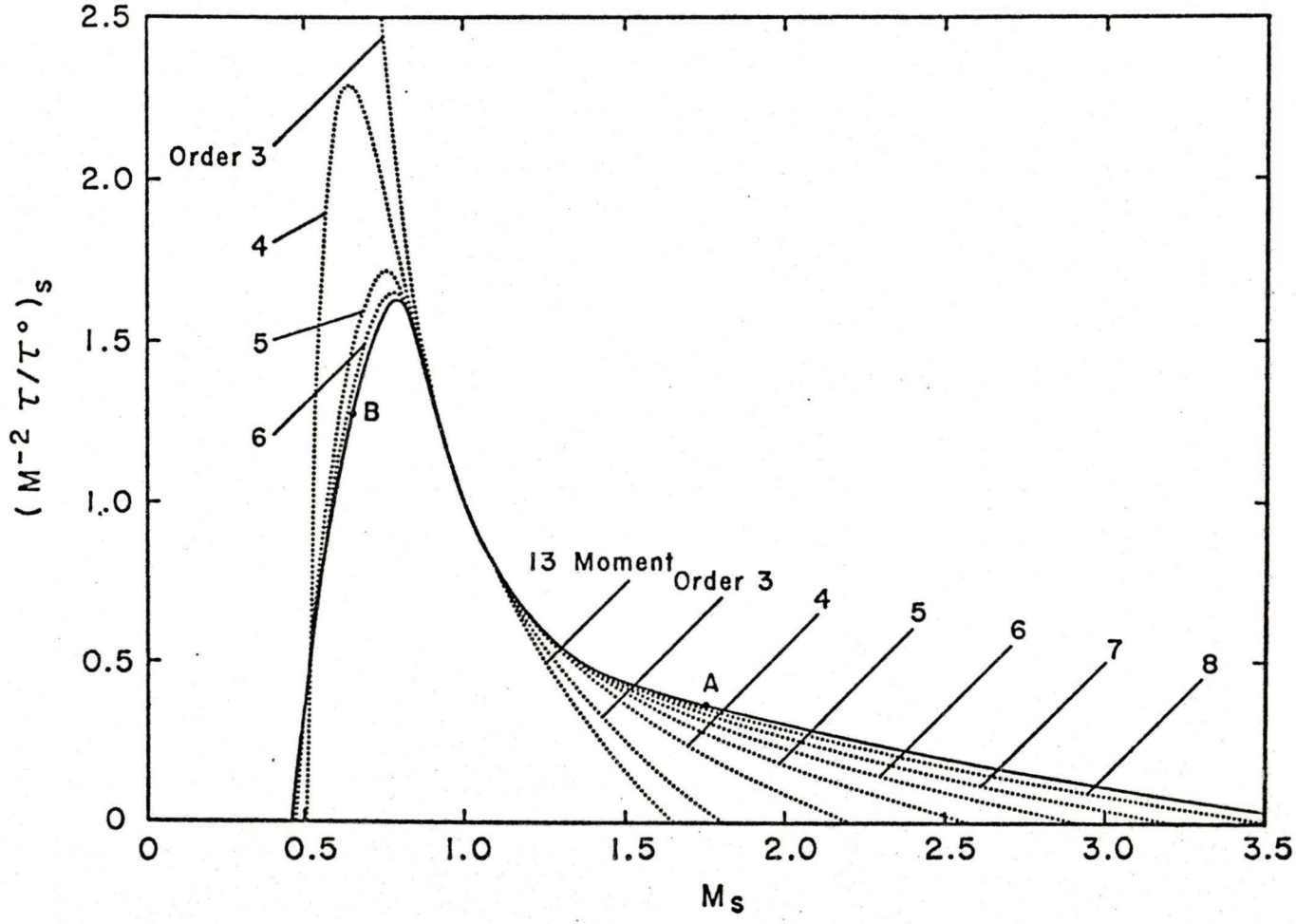


FIGURE 3. Bounded stress ratio $(M^{-2}\tau/\tau^{0})_{s}$ as function of singular-point Mach number in solution based on Grad's closure relations: ———, ninth-order solution; ·····, solutions to lower orders (as indicated).

To exhibit the improvement achieved by the rational truncation procedure over Grad's method, we consider the choice

$$\lambda = \mu = 1$$

for the straining parameters since this selection corresponds to the case of no coordinate straining. The results obtained using the closure relations (1.13) for the case of no straining are shown in figure 4, where the bounded ratio $(M^{-2}\tau/\tau^0)_s$ is again displayed versus M_s. The solutions were terminated at thirteenth order for computational reasons; and a number of orders are not shown for aesthetic purposes. Downstream, the results are virtually identical to those based on Grad's closure relations, while upstream, the results show significant improvement. All orders still exhibit critical upstream Mach numbers, but for each order, the value of the critical Mach number has increased significantly over that in Grad's method. The fifth-order solution in figure 4 displays a peculiarity which arises in the present approach, but not in Grad's method, namely that certain orders of approximation have a range of M_1 below the critical value over which no solution exists. This problem occurs primarily in the sixth and seventh order solutions for various choices of the straining parameters. Although the cause of this problem is not understood, it does not portend any great difficulty, since the situation corrects itself at higher order. As expected, we conclude from figure 4 that the solution based on an orthonormal expansion for the distribution function is an improvement over Grad's results, but the convergence upstream is still not sufficiently rapid. We now turn to coordinate straining in search of further improvement.

We recall from the discussion in Chapter 1 that, near the upstream singular point, the outer regions of f may decay more slowly than the local Maxwellian $f^{(0)} \sim \exp(-C^2/2RT)$; the representation for f must therefore be able to simulate this behavior. To see how this can be done, we consider the case of isotropic straining ($\lambda=\mu$), for which the argument of the exponential in (3.2) becomes

$$\frac{W^2}{2} = \frac{V^2}{2\lambda^2} = \frac{C^2}{2R(2\lambda^2 T)} \quad .$$

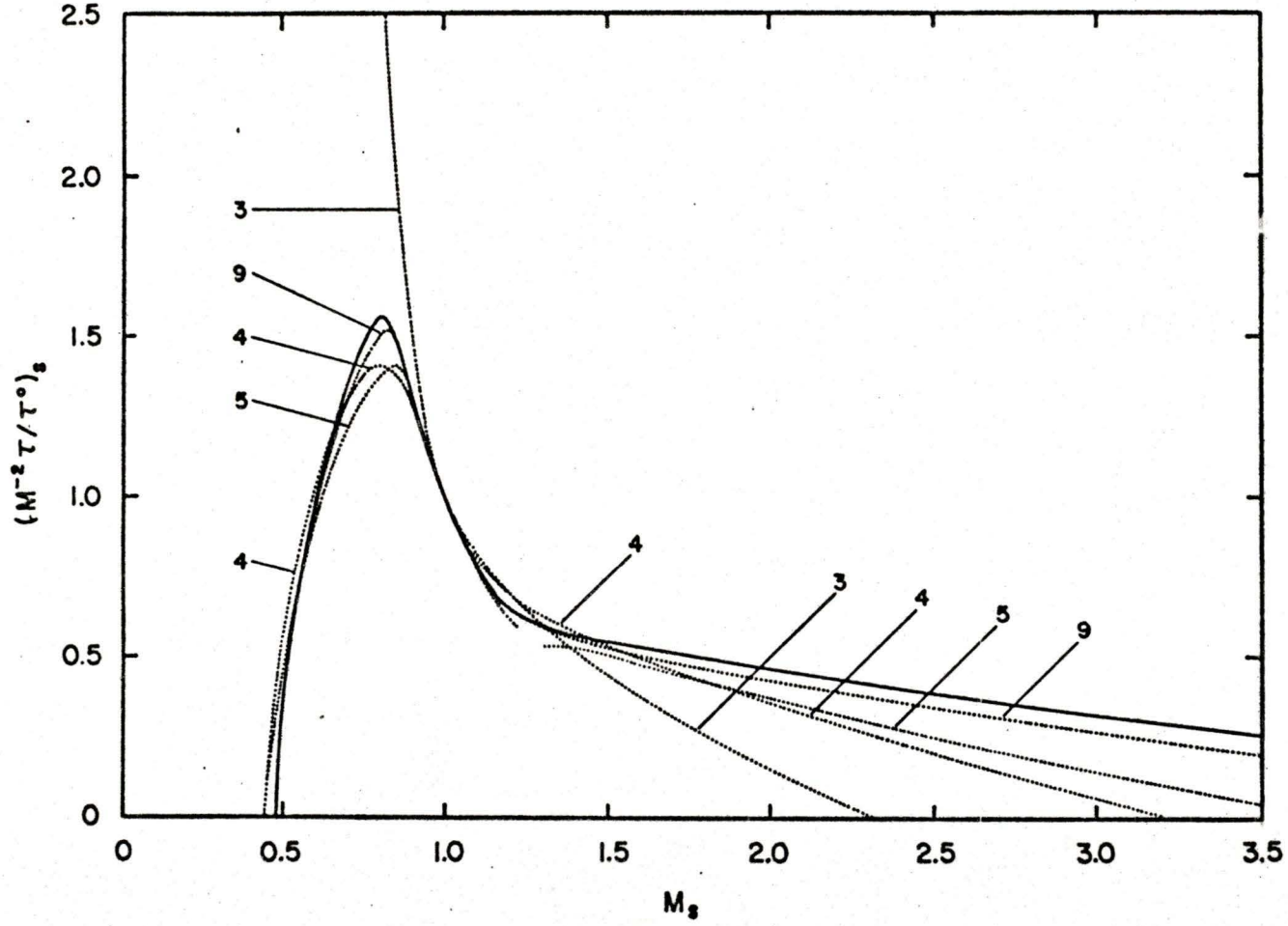


FIGURE 4. Bounded stress ratio $(M^{-2}\tau/\tau^0)_s$ as function of singular-point Mach number M_s in solution with $\lambda=\mu=1$: ———, thirteenth-order solution; ·····, solutions to lower order (as indicated).

The wings of f thus decay in this case like a Maxwellian at temperature

$$\hat{T} = 2\lambda^2 T \quad . \tag{4.1}$$

Equation (4.1) shows that in the case of no strain (λ=1) considered above, the orthonormal expansion doubles the effective temperature in wings of f; however, figure 4 indicates that a further increase in $\hat{T}$ is necessary for $M_1 \gg 1$. Noticing that the Rankine-Hugoniot temperature ratio across a shock wave (for a perfect gas) is given by

$$T_2/T_1 = (M_1^2+3)(5M_1^2-1)/16M_1^2$$

and that $T_2/T_1 \sim M_1^2$ for $M_1 \gg 1$, we propose that $\hat{T}$ be identified with a temperature $T^\dagger$, where

$$T^\dagger/T = (M^2+3)(5M^2-1)/16M^2$$

is the hypothetical Rankine-Hugoniot temperature ratio corresponding to *local* flow conditions. The corresponding selection for λ (or μ) is given by

$$\lambda = \mu = 2^{-\frac{1}{2}}(T^\dagger/T)^{\frac{1}{2}} \quad , \tag{4.2}$$

from equation (4.1). At the upstream singular point, this choice of straining effectively raises the characteristic temperature in the outer regions of f to the temperature at the downstream singular point. Since $T^\dagger \to T$ as $M \to 1$, Grad's results are automatically recovered in the limit of a weak shock wave, as indeed they should be. At the downstream singular point no straining is really necessary, and this particular straining may even be undesirable, since $\hat{T}/T < 1$ for $M_s < 1$. However, no serious problems are anticipated since convergence at the downstream singular point is generally quite rapid.

The results obtained using the straining (4.2) are displayed in figure 5. The same orders are shown here as were presented in figure 4 except that, downstream, the fourth-order solution is omitted for aesthetic reasons. Downstream the results are comparible to the previous results and comparison with the results based on Grad's closure relations shows that the present straining is not detrimental. In fact, the downstream thirteenth-order solutions are identical in the two cases. Upstream, the present solution exhibits dramatic improvement over both

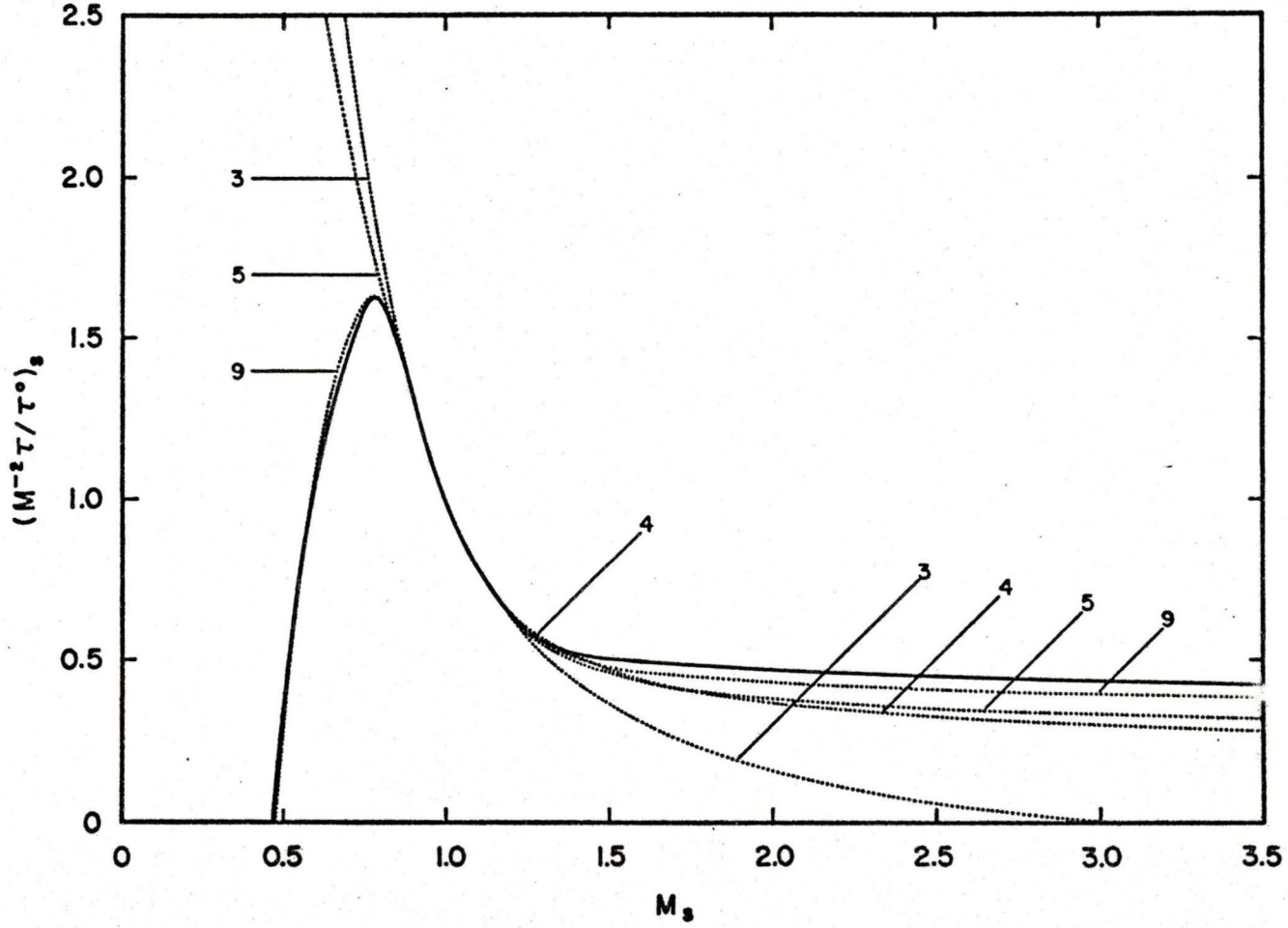


FIGURE 5. Bounded stress ratio $(M^{-2}\tau/\tau^0)_s$ as function of singular-point Mach number M_s in solution with $\lambda=\mu=(2)^{-\frac{1}{2}}(T^\dagger/T)^{\frac{1}{2}}$: ———, thirteenth-order solution; ·····, solutions to lower orders (as indicated).

previous solutions; and, for all practical purposes, the solution has converged by thirteenth order. The fact that the present solution is uniformly valid in the shock-wave Mach number and is correct in the weak-shock limit is a consequence of the coordinate straining (4.2), and thus demonstrates the importance of the role played by coordinate straining.

Although convergence has still not occurred at a sufficiently low order for accurate computation of a shock-wave profile in the case of a strong shock wave, the present thirteenth-order solution is essentially exact and is thus valuable for drawing conclusions about the physical flow near the singular points. On the basis of this thirteenth-order solution, figure 6 presents summary plots of several quantities from which interesting observations can be made. The curve for the bounded stress ratio $(M^{-2}\tau/\tau^0)_s$ in figure 6 shows that the Navier-Stokes relation $\tau=\tau^0$ has approximate validity only for $M_s\simeq 1$. For strong shock waves it is grossly incorrect since the figure shows that $\tau\sim M_1{}^2\tau^0$ at the upstream singular point, while $\tau<<\tau^0$ at the downstream singular point. Also shown in figure 6 is the bounded heat-flux ratio $(M^2q^0/q)_s$ where

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

is the Fourier relation for the heat flux q. Comparison between the result obtained from the solution of the Boltzmann equation and the Fourier relation $q=q^0$ shows that the Fourier heat-flux relation is also approximately valid only for weak shock waves. For strong shock waves, we see that $q\sim M_1{}^2q^0$ at the supersonic singular point, and $q\simeq -2q^0$ at the subsonic singular point. The remaining quantity in figure 6 is the bounded temperature derivative, $[M^{-2}(u/T)dT/du]_s$. The crossing of the axis by both this quantity and the heat-flux ratio at $M_2\simeq 0.700$ (which corresponds to a shock Mach number of $M_1\simeq 1.55$) is indicative of an interesting physical phenomenon, namely that, for all shock waves for which $M_1\gtrsim 1.55$, the derivative $(dT/du)_2$ is positive. This implies that a temperature overshoot exists on the subsonic side of a shock wave (i.e., there is a region in the flow where T is greater than the Rankine-Hugoniot value T_2). The existence of temperature overshoot can also be

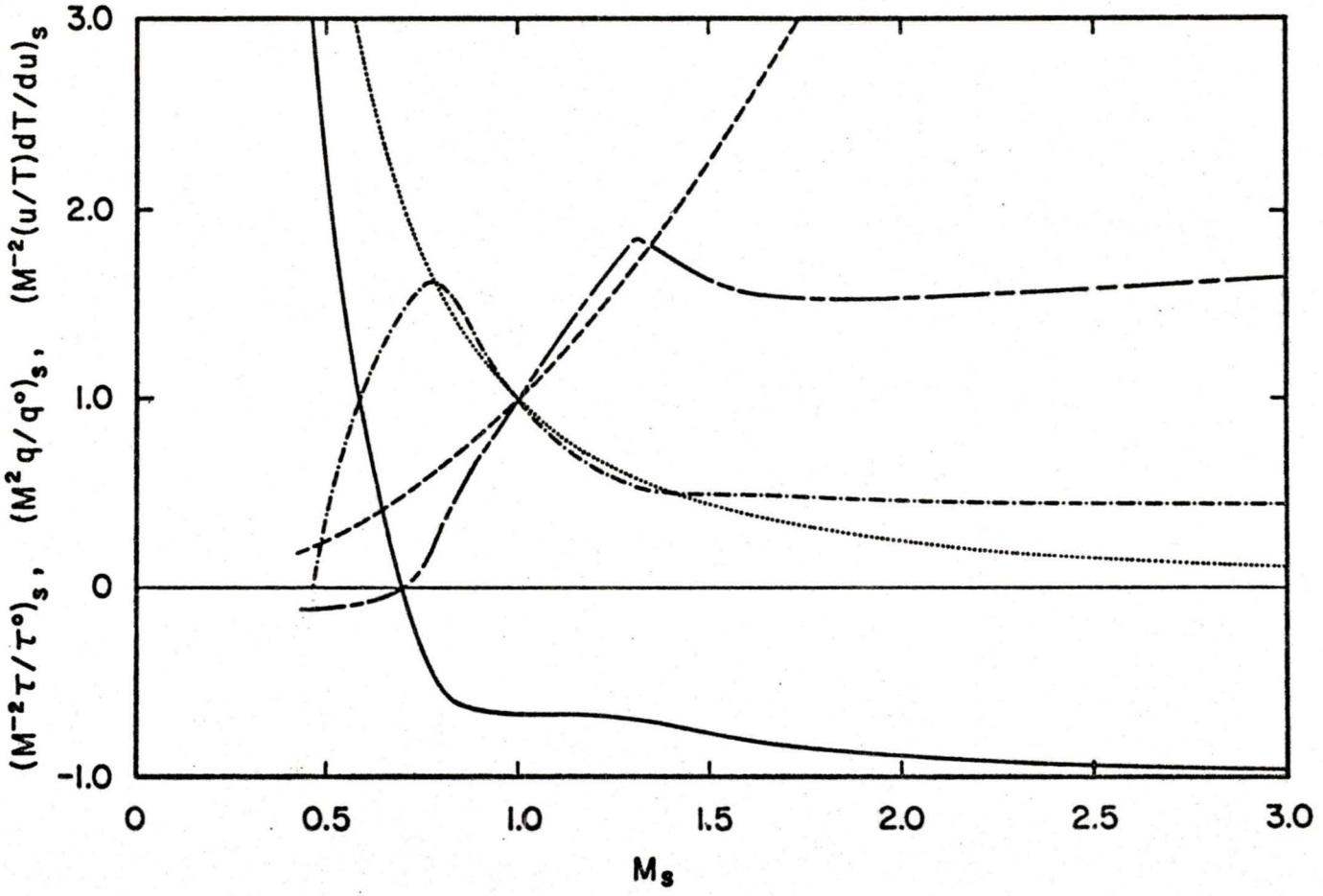


FIGURE 6. Bounded stress ratio $(M^{-2}\tau/\tau^0)_s$, heat-flux ratio $(M^2q^0/q)_s$, and temperature derivative $(M^{-2}(u/T)dT/du)_s$ as functions of singular-point Mach number M_s in thirteenth-order solution with $\lambda=\mu=(2)^{-\frac{1}{2}}(T^\dagger/T)^{\frac{1}{2}}$: ———, $(M^{-2}(u/T)dT/du)_s$; – – – –, $(M^{-2}\tau/\tau^0)_s$; ·····, $(M^{-2}\tau/\tau^0)_s$ for Navier-Stokes relation; —— – ——, $(M^2q^0/q)_s$; – – – –, $(M^2q^0/q)_s$ for Fourier relation.

concluded from the downstream results based on Grad's closure relations, and from the work of Elliott and Baganoff (1974).

CHAPTER 5

CONCLUDING REMARKS

Application of the method of rational truncation and coordinate straining to the singular point analysis in a shock wave gives results which are uniformly valid at the upstream singular point and therefore superior to anything previously available. The use of an orthonormal expansion for the distribution function leads to rational closure relations; however, the additional procedure of coordinate straining is important in that it allows rapid convergence of the expansion, upstream, by introducing a reference temperature sufficiently high that the expansion produces a reasonable model of the outer regions of f.

The solution based on this "temperature straining" shows that the Navier-Stokes and Fourier relations (i.e., first-order Chapman-Enskog results) are not valid at the singular points in all but the weakest shock waves and confirms the existence of temperature overshoot in a strong shock wave. The thirteenth-order solution is exact for all practical purposes and thus provides accurate boundary values which would be useful for guiding numerical solutions of the Boltzmann equation for shock-wave structure, since most numerical error develops near the singular points.

We recall that our selection (3.2) for the set of orthonormal functions was based on mathematical convenience. From a physical point of view, this selection was particularly appropriate since the ϕ_j's resemble the eigenstates of the quantized harmonic oscillator and therefore cannot easily represent the functional form of Δf with just a few terms of the series. A logical extension of the present work would be to improve the selection of the orthonormal set in an effort to achieve a nearly-exact solution at the thirteen-moment level for the purpose of computing shock-wave profiles.

The application of coordinate straining in the present work was shown to be quite valuable. However, analysis of the nature of the outer regions of f would contribute greatly to improvement upon this

work by allowing selection of the straining parameters to be made on a much more rigorous basis. In particular, a better understanding of the relationship between the nature of f and the appropriate choice of straining would be valuable when applying the method of rational truncation and coordinate straining to other flow problems.

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APPENDIX A

FORTRAN PROGRAM FOR COMPUTING THE MATRIX ELEMENTS γ_{iln}

This program computes the matrix elements γ_{iln} defined by (3.16). Sufficient elements are computed to allow closure of the system (2.6) for truncation as high as order 11. The matrix elements needed for the twelfth and thirteenth order solutions were obtained using a streamlined version of this program restricted to the case of isotropic straining only.

A general outline of the program is included at the top of the listing and more specific information is appropriately distributed throughout the listing. It should be noted that the Sonine polynomial $S_{l+\frac{1}{2}}^{(r)}$ which appears in the program is simply the Laguerre polynomial $L_r^{(l+\frac{1}{2})}$.

```
C
C
C THIS PROGRAM CALCULATES THE MATRIX ELEMENTS
C
C      GAMMA(I,L,N)=ALPHA(I,J)*PHI(J,K,N)*PI(K,M)*ALPHA(L,M)
C
C WHERE, HERE, THE ELEMENTS OF GAMMA(I,L,N) FOR EACH PAIR OF I AND L ARE
C STORED TEMPORARILY IN THE VECTOR G(N) AND PUT ON TAPE FOR USE IN THE
C "SHOCK-WAVE PROGRAM".
C
C THE FOLLOWING NOTATION IS USED:
C
C      A(I,J)=ALPHA(I,J)
C
C      P(I,J)=PI(I,J)
C
C      B1,,,,,B7 ARE 3-DIMENSIONAL ARRAYS CONTAINING THE BLOCKS OF NON-
C      ZERO ELEMENTS OF PHI(J,K,N)
C
C      S(M,N,I) ARE THE COEFFICIENTS OF THE SONINE POLYNOMIAL WITH
C      SUBSCRIPT L+1/2=N-1+1/2 AND SUPERSCRIPT R=M-1
C
C      WP(N,K) ARE THE COEFFICIENTS OF THE LEGENDRE POLYNOMIAL OF ORDER
C      L=N-1
C
C THE MAJORITY OF COMPUTATIONS IN THIS PROGRAM ARE DONE USING INTEGER
C ARITHMETIC, EXCEPT FOR THE FINAL MATRIX MULTIPLICATION. THIS WAS
C ACCOMPLISHED BY OMITTING THE NORMALIZATIONFACTOR FROM THE ROWS OF
C A(I,J) AND BY INTRODUCING VECTORS OF "DIVIDING FACTORS" (I.E., LOWEST
C COMMON DENOMINATORS) FROM THE LEGENDRE AND SONINE POLYNOMIALS. THESE
C FACTORS ARE REPLACED IN THE FOLLOW-UP PROGRAM WHEN THE TRUNCATED
C SYSTEM OF MOMENT EQUATIONS IS CLOSED.
C
      IMPLICIT INTEGER(A-Z)
      REAL*8 A(49,49),B1(1,1,1),B2(2,2,2),B3(3,3,3),B4(4,4,4),
     &B5(5,5,5),B6(6,6,6),B7(7,7,7),G(28),P(49,49),R1,R2,S(7,13,7),
     &WP(13,7),R3,ZERO(28)
      DIMENSION DFS(7),DF(49),BSIZE(49),BI(49),EF(28),PW(49),
     &PWX(49),EO(49)
      COMMON/AREA1/ A,WP,DF
      COMMON/AREA2/  P,PW,PWX,EO,IMAX
      COMMON/AREA3/ S,DFS
      DATA B1,B2,B3,B4,B5,B6,B7/1.DO,783*0.D0/
C
      ORDER=12
      IMAX=49
      LMAX=42
      NMAX=28
C     INPUT COEFFICIENTS OF LEGENDRE POLYNOMIALS
      DO 2 N=1,13
      READ(5,1) (WP(N,K),K=1,7)
    1 FORMAT(4D20.9)
    2 CONTINUE
C     INPUT ELEMENTS OF TOP PLANES OF BLOCK MATRICES B2,,,,,B7
      READ(5,3) ((B2(1,K,N),N=1,2),K=1,2)
      READ(5,3) ((B3(1,K,N),N=1,3),K=1,3)
      READ(5,3) ((B4(1,K,N),N=1,4),K=1,4)
      READ(5,3) ((B5(1,K,N),N=1,5),K=1,5)
      READ(5,3) ((B6(1,K,N),N=1,6),K=1,6)
      READ(5,3) ((B7(1,K,N),N=1,7),K=1,7)
    3 FORMAT(5D16.4)
C
      B2(2,2,2)=B1(1,1,1)
```

```
      DO 35 J=1,6
      DO 30 K=1,6
      DO 25 N=1,6
      IF(N.GT.2 .OR. K.GT.2 .OR. J.GT.2) GOTO 5
      B3(J+1,K+1,N+1)=B2(J,K,N)
    5 IF(N.GT.3 .OR. K.GT.3 .OR. J.GT.3) GOTO 10
      B4(J+1,K+1,N+1)=B3(J,K,N)
   10 IF(N.GT.4 .OR. K.GT.4 .OR. J.GT.4) GOTO 15
      B5(J+1,K+1,N+1)=B4(J,K,N)
   15 IF(N.GT.5 .OR. K.GT.5 .OR. J.GT.5) GOTO 20
      B6(J+1,K+1,N+1)=B5(J,K,N)
   20 B7(J+1,K+1,N+1)=B6(J,K,N)
   25 CONTINUE
   30 CONTINUE
   35 CONTINUE
C
C     IN BF(N), STORE THE VALUE OF THE BLOCK FILE INDEX (I.E., THIRD
C     SUBSCRIPT OF THE APPROPRIATE BLOCK MATRIX) CORRESPONDING TO THE
C     FILE INDEX N OF GAMMA(I,L,N)
      BS=1
      BN=1
      DO 45 N=1,NMAX
      BF(N)=BN
      IF(BN.EQ.BS) GOTO 40
      BN=BN+1
      GOTO 45
   40 BN=1
      BS=BS+1
   45 CONTINUE
C
C     STORE THE BLOCK ROW INDICES IN BI(I); STORE THE BLOCK SIZES IN
C     BSIZE(I); STORE THE POWER TO WHICH THE VELOCITY W IS RAISED (I.E.,
C     2*"R") IN PW(I) AND THE POWER TO WHICH ITS X COMPONENT IS RAISED
C     (I.E., "L") IN PWX(I) APPROPRIATE TO THE I'TH COMPONENT OF THE
C     VECTOR E; LET EO(I) BE 0 IF THE ORDER "2R+L" OF THE I'TH ROW IS
C     EVEN AND 1 IF IT IS ODD
      BS=1
      BN=1
      BCNTR=1
      NW=0
      NWX=0
      DO 60 I=1,IMAX
      PW(I)=NW
      PWX(I)=NWX
      EO(I)=BCNTR-1
      BI(I)=BN
      BSIZE(I)=BS
      IF(BN.EQ.BS) GOTO 50
      BN=BN+1
      NW=NW-2
      NWX=NWX+2
      GOTO 60
   50 BN=1
      IF(BCNTR.EQ.2) GOTO 55
      BCNTR=2
      NW=2*(BS-1)
      NWX=1
      GOTO 60
   55 BCNTR=1
      NW=2*BS
      NWX=0
      BS=BS+1
   60 CONTINUE
```

```
C
      REWIND 4
      CALL SCPCCO(ORDER)
      CALL CALCA
      CALL CALCP
      DO 70 IJ=1,28
   70 ZERO(IJ)=0.D0
      WRITE(6,80)
   80 FORMAT('1')
      DO 450 I=1,IMAX
      EOI=EO(I)
      ZI=BSIZE(I)
      ZIP=(ZI+1)*ZI/2
      KEND=I+ZI-BI(I)
      DO 400 L=1,LMAX
C     SKIP COMPUTATION OF MATRIX ELEMENTS WHICH ARE IDENTICALLY ZERO DUE
C     TO THE EVEN-ODD CHARACTER OF THE EIGENFUNCTIONS
      IF(EOI+EO(L).NE.1) GOTO 95
      WRITE(4) ZERO
      WRITE(6,90)I,L
   90 FORMAT('0','GAMMA(',I2,',',I2,',N)'/(' ','      (EVEN-ODD)'))
      GOTO 400
   95 DO 350 N=1,NMAX
      B3=0.D0
      IF(N.GT.ZIP) GO TO 330
      BEN=BE(N)
      DO 300 M=1,L
C     SKIP ELEMENTS OF MATRIX PRODUCT A(I,J)*PHI(J,K,N)*P(K,M) WHICH ARE
C     IDENTICALLY ZERO
      IF(EOI+EO(M).EQ.1) GOTO 300
      B2=0.D0
      DO 250 K=1,KEND
C     SKIP MATRIX MULTIPLICATION INVOLVING ELEMENTS OF P(K,M) WHICH ARE
C     IDENTICALLY ZERO
      IF(EO(K)+EO(M).EQ.1) GOTO 250
      BIK=BI(K)
      Z=BSIZE(K)
      X=(Z-1)*Z/2
      IF(N.LT.X+BEN) GOTO 250
      IF(N.GT.X+Z) GOTO 250
      B1=0.D0
      Y=K-BIK+1
      GOTO(100,110,120,130,140,150,160),Z
  100 DO 105 J=Y,K
      B1=A(I,J)*B1(BI(J),BIK,BEN) + B1
  105 CONTINUE
      GOTO 200
  110 DO 115 J=Y,K
      B1=A(I,J)*B2(BI(J),BIK,BEN) + B1
  115 CONTINUE
      GOTO 200
  120 DO 125 J=Y,K
      B1=A(I,J)*B3(BI(J),BIK,BEN) + B1
  125 CONTINUE
      GOTO 200
  130 DO 135 J=Y,K
      B1=A(I,J)*B4(BI(J),BIK,BEN) + B1
  135 CONTINUE
      GOTO 200
  140 DO 145 J=Y,K
      B1=A(I,J)*B5(BI(J),BIK,BEN) + B1
  145 CONTINUE
      GOTO 200
```

```
  150 DO 155 J=Y,K
      R1=A(I,J)*B6(EI(J),EIK,BFN) + R1
  155 CONTINUE
      GOTO 200
  160 DO 165 J=Y,K
      R1=A(I,J)*B7(EI(J),EIK,BFN) + R1
  165 CONTINUE
  200 R2=R1*P(K,M)+R2
  250 CONTINUE
      R3=R2*A(L,M)+R3
  300 CONTINUE
  330 G(N)=R3
  350 CONTINUE
      WRITE(4) G
      WRITE(6,360)I,L
      WRITE(6,370)(G(N),N=1,ZIP)
  360 FORMAT('0','GAMMA(',I2,',',I2,',N)')
  370 FORMAT(' ',5F20.2)
  400 CONTINUE
  450 CONTINUE
      ENDFILE 4
      REWIND 4
      WRITE(6,500)
  500 FORMAT('1')
      STOP
      END
C
C
C COMPUTE "N FACTORIAL"
      INTEGER FUNCTION FAC(N)
      FAC=1
      IF(N.EQ.0) GO TO 10
      DO 5 I=1,N
      FAC=FAC*I
    5 CONTINUE
   10 RETURN
      END
C
C
C COMPUTE "N DOUBLE FACTORIAL"
      DOUBLE PRECISION FUNCTION DFAC(N)
      DFAC=1.
      DO 5 I=1,N,2
    5 DFAC=DFAC*I
      RETURN
      END
C
C
C COMPUTE SONINE POLYNOMIAL COEFFICIENTS
      SUBROUTINE SONCOE(ORDER)
      IMPLICIT INTEGER(A-Z)
      REAL*8 S(7,13,7),DFLOAT
      DIMENSION DFS(7)
      COMMON/AREA3/ S,DFS
      MMAX=7
      NMAX=ORDER+1
      DO 20 M=1,MMAX
      R=M-1
      DO 15 N=1,NMAX
      L=N-1
      DO 10 I=1,MMAX
      J=I-1
      S(M,N,I)=0.
```

```
      IF(N.GT.NMAX-2*(M-1)) GO TO 10
      IF(I.GT.M) GO TO 10
C     COMPUTE N1 AND D1 SUCH THAT N1/D1=(L+1/2+R) FACTORIAL / (L+1/2+J)
C     FACTORIAL
      N1=1
      D1=1
      K=L
    4 IF((R+K).LT.(L+J+1)) GO TO 8
      N1=N1*(2*(K+R)+1)
      D1=D1*2
      K=K-1
      GO TO 4
    8 DENOM=D1*FAC(J)*FAC(R-J)
      IF(J.EQ.0) DFS(M)=DENOM
      S(M,N,I)=DFLOAT((-1)**J*N1*(DFS(M)/DENOM))
   10 CONTINUE
   15 CONTINUE
   20 CONTINUE
      RETURN
      END
C
C
C COMPUTE MATRIX ELEMENTS A(I,J)
      SUBROUTINE CALCA
      IMPLICIT INTEGER(B-R,T-V,X-Z)
      REAL*8 WP(13,7),S(7,13,7),A(49,49)
      DIMENSION IMAT(7,13),DEP(13),DFS(7),DF(49)
      COMMON/AREA1/ A,WP,DF
      COMMON/AREA3/S,DFS
      ORDER=12
      DO 4 J=1,49
      DO 2 I=1,49
      A(I,J)=0.
    2 CONTINUE
    4 CONTINUE
      DO 20 N=1,13
      DEP(N)=0
      DO 10 K=1,7
      DEP(N)=DEP(N)+WP(N,K)
   10 CONTINUE
   20 CONTINUE
      ICNTR=0
      MMAX=1
      N=1
      M=1
      IMAT(M,N)=1
   30 I=IMAT(M,N)
      DF(I)=DEP(N)*DFS(M)
      DO 50 K=1,7
      IF (N-2*K+1.LT.0) GO TO 50
      DO 40 J=1,M
      A(I,IMAT(K+J-1,N-2*K+2))=S(M,N,J)*WP(N,K)
   40 CONTINUE
   50 CONTINUE
      IF (M.EQ.1) GO TO 80
      M=M-1
      N=N+2
      IMAT(M,N)=IMAT(M+1,N-2) +1
      GO TO 30
   80 IF (N-1.EQ.ORDER) GO TO 100
      IF (ICNTR.EQ.1) GO TO 90
      ICNTR=1
      M=MMAX
```

```
      N=2
      IMAT(M,N)=IMAT(1,2*MMAX-1) +1
      GO TO 30
   90 MMAX=MMAX+1
      N=1
      M=MMAX
      IMAT(M,N)=IMAT(1,2*MMAX-2) +1
      ICNTP=0
      GO TO 30
      END
C
C
C COMPUTE MATRIX ELEMENTS P(K,M)
      SUBROUTINE CALCP
      IMPLICIT INTEGER(A-Z)
      REAL*8 DFAC,P(49,49)
      DIMENSION PW(49),PWX(49),EQ(49)
      COMMON/AREA2/  P,PW,PWX,EQ,IMAX
      DO 20 K=1,IMAX
      DO 10 M=1,IMAX
      IF(EQ(K)+EQ(M).EQ.1) GOTO 5
      P(K,M)=DFAC(PW(K)+PW(M)+PWX(K)+PWX(M)+1)/(PWX(K)+PWX(M)+1)
      GOTO 10
    5 P(K,M)=0.
   10 CONTINUE
   20 CONTINUE
      RETURN
      END
```

APPENDIX B

FORTRAN PROGRAM FOR SOLVING THE SYSTEM OF MOMENT EQUATIONS

This program solves the system of moment equations (2.6) for truncation at orders 3-11 inclusive. Either Grad's closure or closure based on the relations (1.13) can be specified. The matrix elements γ_{ijk} needed for the closure relations (1.13) are read from the tape output of the previous program. A streamlined version of this program was used to solve the system for truncation at orders 12 and 13.

As with the previous program, a general outline is included at the top of the listing and more specific information is appropriately distributed throughout the listing. It should be noted that this listing is not complete in the sense that it does not contain a listing of the subroutine LINRD. Information about this subroutine can be obtained from the University of Victoria Computing Center.

```
C
C
C THIS PROGRAM SOLVES THE "WANG CHANG" SYSTEM OF MOMENT EQUATIONS AT THE
C SINGULAR POINTS IN A SHOCK WAVE. IT ALLOWS FOR TRUNCATION AT ORDERS
C 3-11 INCLUSIVE AND CLOSES THE SYSTEM USING THE "RATIONAL TRUNCATION
C AND COORDINATE STRAINING PROCEDURE" WHERE THE NECESSARY CLOSURE MATRIX
C ELEMENTS ARE COMPUTED BY AN AUXILIARY PROGRAM. THE DETERMINANT OF THE
C AUGMENTED MATRIX IS USED TO ITERATIVELY DETERMINE W (I.E., "OMEGA").
C
C THE FOLLOWING NOTATIONS AND DEFINITIONS ARE USED:
C
C      AW IS THE LEFT-HAND-SIDE MATRIX OF COEFFICIENTS
C
C      AUG IS THE AUGMENTED MATRIX WITH THE RIGHT-HAND-SIDE VECTOR B AS
C      THE ADDITIONAL COLUMN AND "EQUATION 2" AS THE ADDITIONAL ROW
C
C      TNOT AND TSTAR ARE THE UPPER AND LOWER SUBMATRICES, RESPECTIVELY,
C      AND ARE ACHIEVED FROM THE PRODUCTS OF GNOT AND GSTAR WITH THE
C      VECTOR "S" FOR EACH PAIR OF VALUES OF THE STRAINING PARAMETERS
C
C      MS IS THE SINGULAR POINT MACH NUMBER AND THE PROGRAM IS RUN FOR
C      VALUES OF MS FROM MSTART TO MSTOP IN STEPS OF MINC
C
C      ALPAMS AND BETAMS ARE STRAINING PARAMETERS. (THEY ARE THE "LAMBDA"
C      AND "MU" DEFINED IN THE THESIS.) THE FIVE AVAILABLE STRAINING
C      OPTIONS ARE DETERMINED BY THE VALUE OF ISTRN AND, IN ADDITION,
C      GRAD CLOSURE IS ACHIEVED BY GIVING ISTRN THE VALUE 0
C
      IMPLICIT REAL*8(A-H,S-Z),INTEGER(I-R)
      REAL*8 MS,MSTART,MSTOP,MINC,ROOT56
      DIMENSION AUG(41,41),AW(41,41),B(41),DNORM(47),EIGRL(40),
     &GNOT(21,21,21),GSTAR(7,21,28),IAEXP(28),IBEXP(28),IDF(47),
     &LMAT(47),NMAT(47),RMAT(47),TNOT(21,21),TSTAR(7,21),ZETA(40)
      EQUIVALENCE(AUG,AW)
      COMMON AW,B,B1,B2,SQRT3,SQRT23,MS,ORDER,IMAX,IIMAX,IPRNTR
      COMMON/AREA1/ ROOT56,EIGRL
      COMMON/AREA2/ TNOT,TSTAR,NMAT,LMAT,RMAT,IDIMT,DNORM,IDF,IGRAD
      COMMON/AREA3/ WBEGIN,WSTOP,WSTEP,MPKNTR,MBSTEP
      COMMON/AREA4/ ZETA,DSTNXT,ITCOMP,ITKNTR
      COMMON/AREA5/ NDUP(47),NORD
C
      KDIMG(I)=(I/2+2)*(I/2+1)/2
      ALPHA1(X)=1.D0
      BETA1(X)=1.D0
      ALPHA2(X)=X/DSQRT(2.D0)
      BETA2(X)=X/DSQRT(2.D0)
      ALPHA3(X)=X/DSQRT(2.D0)
      BETA3(X)=1.D0/DSQRT(2.D0)
      ALPHA4(X)=DSQRT(X**2+3.D0)/2.D0/DSQRT(2.D0)
      BETA4(X)=DSQRT(X**2+3.D0)/2.D0/DSQRT(2.D0)
      ALPA5(X)=DSQRT((X**2+3.D0)*(5.D0*X**2-1.D0))/(4.D0*DSQRT(2.D0)*X)
      BETA5(X)=DSQRT((X**2+3.D0)*(5.D0*X**2-1.D0))/(4.D0*DSQRT(2.D0)*X)
C
      ITPDRV=4
      IREADR=5
      IPRNTR=6
      WINC=.1D-03
      WDUMMY=1.D0
      IGRAD=0
C
      SQRT3=DSQRT(3.D0)
      SQRT23=DSQRT(2.D0/3.D0)
      ROOT56=DSQRT(5.D0/6.D0)
```

```
C       SUPPRESS UNDERFLOW ERROR MESSAGES
        IERN=208
        CALL ERRSET(IERN,256,-1)
C
        READ(IREADR,5) ISTRN
      5 FORMAT(17X,I2)
        IF(ISTRN .EQ. 0) IGRAD=1
        IF(ISTRN .EQ. 0) ISTRN=1
        READ(IREADR,10) (IDF(I),I=1,47)
     10 FORMAT(12I6)
        READ(IREADR,15) (EIGRL(I),I=1,40)
     15 FORMAT(3D25.16)
        READ(IREADR,20) ORDER
     20 FORMAT(6X,I2)
        NORD=ORDER
C
C       COMPUTE THE DIMENSIONS OF THE VARIOUS MATRICES
        IMAX=ORDER-1+(ORDER/2)*((ORDER+1)/2)
        IIMAX=IMAX+1
        IDIMT=(2*((ORDER+1)/2)-ORDER/2)*((ORDER+2)/2)/2
        IDIMGS=(ORDER+3)/2
        KMAXGN=KDIMG(ORDER-1)
        KMAXGS=KDIMG(ORDER+1)
C
C       IN RMAT(I), LMAT(I) AND NMAT(I), STORE THE VALUES OF R, L, AND
C       2R+L CORRESPONDING TO THE SINGLE SUBSCRIPT I. (THESE VALUES WILL
C       BE TWICE DISPLACED FROM THEIR CORRECT VALUES SINCE, HERE, I REFERS
C       TO THE ROW (OR COLUMN) OF THE L.H.S. MATRIX THAT HAS HAD THE FIRST
C       TWO ROWS AND COLUMNS REMOVED)
        KNTR=0
        R=0
        L=0
        RMAX=0
        DO 140 I=1,49
        IF(I.LE.2) GO TO 110
        RMAT(I-2)=R
        LMAT(I-2)=L
        NMAT(I-2)=2*R+L
        NDUP(I-2)=2*R+L
    110 IF(R.EQ.0) GO TO 120
        R=R-1
        L=L+2
        GO TO 140
    120 IF(KNTR.EQ.1) GO TO 130
        KNTR=1
        R=RMAX
        L=1
        GO TO 140
    130 RMAX=RMAX+1
        L=0
        R=RMAX
        KNTR=0
    140 CONTINUE
C
C       READ THE MATRIX ELEMENTS, GAMMA(I,J,K), FROM TAPE
        REWIND ITPDRV
        IGN=1
        IGS=1
        DO 80 I=1,49
        IF(I-2) 25,26,27
     25 LMATI=0
        GO TO 30
     26 LMATI=1
```

```
      GO TO 30
   27 LMATI=LMAT(I-2)
   30 IF((ORDER-LMATI)/2*2 .NE. ORDER-LMATI) GO TO 40
      DO 35 IJ=1,42
   35 READ(ITPDRV)
      GO TO 80
   40 JGN=1
      JGS=1
      DO 70 J=1,42
      IF(J-2) 45,46,47
   45 LMATJ=0
      GO TO 50
   46 LMATJ=1
      GO TO 50
   47 LMATJ=LMAT(J-2)
   50 IF((LMATJ-LMATI)/2*2 .EQ. LMATJ-LMATI) GO TO 55
      READ(ITPDRV)
      GO TO 70
   55 IF(I.GT.IMAX+2) GO TO 60
      READ(ITPDRV) (GNOT(IGN,JGN,K),K=1,KMAXGN)
      JGN=JGN+1
      GO TO 65
   60 READ(ITPDRV) (GSTAR(IGS,JGS,K),K=1,KMAXGS)
      JGS=JGS+1
   65 IF(JGN.GT.IDIMT .OR. JGS.GT.IDIMT) GO TO 75
   70 CONTINUE
   75 IF(I.GE.IMAX+2+IDIMGS) GO TO 85
      DO 76 JJ=J,41
   76 READ(ITPDRV)
      IF(I-(IMAX+2)) 77,80,78
   77 IGN=IGN+1
      GO TO 80
   78 IGS=IGS+1
   80 CONTINUE
   85 REWIND ITPDRV
C
      READ(IREADR,90) MSTART,MSTOP,MINC
   90 FORMAT(3D20.8)
      READ(IREADR,100) WBEGIN,WSTOP,WSTEP,MFSTEP
  100 FORMAT(3D20.8,I10)
      WORIG=WBEGIN
C
C     PRINT INFORMATION CONCERNING THE USER'S CHOICE OF PARAMETERS
      WRITE(IPRNTR,400) ORDER
  400 FORMAT('1'/'-','ORDER OF SOLUTION:',I4)
      IF(MSTART .GE. 1.D0) GO TO 420
      WRITE(IPRNTR,410)
  410 FORMAT('-','DOWNSTREAM SINGULAR POINT')
      GO TO 440
  420 WRITE(IPRNTR,430)
  430 FORMAT('-','UPSTREAM SINGULAR POINT')
  440 IF(IGRAD .NE. 1) GO TO 460
      WRITE(IPRNTR,450)
  450 FORMAT('-','GRAD CLOSURE')
      GO TO 600
  460 WRITE(IPRNTR,470)
  470 FORMAT('-','STRAINING USED:')
      GO TO (480,500,520,540,560),ISTRN
  480 WRITE(IPRNTR,490)
  490 FORMAT('0',5X,'NO STRAINING (LAMBDA=MU=1)')
      GO TO 600
  500 WRITE(IPRNTR,510)
  510 FORMAT('0',5X,'ISOTROPIC STRAINING WITH LAMBDA=MU=M/SQRT(2)')
```

```
      GO TO 600
  520 WRITE(IPRNTR,530)
  530 FORMAT('0',5X,'ANISOTROPIC STRAINING WITH LAMBDA=M/SQRT(2) AND ',
     &'MU=1/SQRT(2)')
      GO TO 600
  540 WRITE(IPRNTR,550)
  550 FORMAT('0',5X,'ISOTROPIC STRAINING WITH LAMBDA=MU=SQRT(M**2+3)/',
     &'(2*SQRT(2))')
      GO TO 600
  560 WRITE(IPRNTR,570)
  570 FORMAT('0',5X,'ISOTROPIC STRAINING WITH LAMBDA=MU=SQRT((M**2+3)',
     &'+(5*M**2-1))/(4*SQRT(2)*M)')
  600 CONTINUE
C
C     FORM VECTORS IAEXP(K) AND IBEXP(K) CONTAINING THE POWERS TO WHICH
C     "LAMBDA" AND "MU" ARE RAISED IN THE K'TH ELEMENT OF THE VECTOR "S"
      IALPHA=0
      IBETA=0
      ISIZE=1
      DO 160 K=1,KMAXGS
      IAEXP(K)=IALPHA
      IBEXP(K)=IBETA
      IF(IBETA.EQ.0) GO TO 150
      IALPHA=IALPHA+2
      IBETA=IBETA-2
      GO TO 160
  150 IBETA=2*ISIZE
      IALPHA=0
      ISIZE=ISIZE+1
  160 CONTINUE
C
C     STORE THE NORMALIZATION CONSTANTS FOR THE EIGENFUNCTIONS IN THE
C     VECTOR DNORM(J)
      SQRTPI=.17724538509055160D1
      JEND=IMAX+IDIMGS
      DO 180 J=1,JEND
      R=RMAT(J)
      L=LMAT(J)
      IFAC=1
      IF(R.EQ.0) GO TO 170
      DO 165 I=1,R
  165 IFAC=IFAC*I
  170 DNORM(J)=DSQRT(IFAC*(L+.5D0)*SQRTPI/DGAMMA(L+R+1.5D0))
  180 CONTINUE
C
      MS=MSTART
      MPRNTR=0
      WRITE(IPRNTR,190)
  190 FORMAT('1')
  200 B1=-DSQRT(5.D0)*MS/3.D0
      B2=DSQRT(1.D1)*MS/3.D0
      GO TO (201,202,203,204,205),ISTRN
  201 ALFAMS=ALPHA1(MS)
      BETAMS=BETA1(MS)
      GO TO 208
  202 ALFAMS=ALPHA2(MS)
      BETAMS=BETA2(MS)
      GO TO 208
  203 ALFAMS=ALPHA3(MS)
      BETAMS=BETA3(MS)
      GO TO 208
  204 ALFAMS=ALPHA4(MS)
      BETAMS=BETA4(MS)
```

```
      GO TO 208
  205 ALFAMS=ALFAS(MS)
      BETAMS=BETAS(MS)
C     FORM THE CLOSURE MATRICES TNOT AND TSTAR FROM GNOT AND GSTAR
  208 DO 250 J=1,IDIMT
      DO 220 I=1,IDIMT
      TNOT(I,J)=0.D0
      DO 210 K=1,KMAXGN
      IF(GNOT(I,J,K).EQ.0.) GO TO 210
      TNOT(I,J)=TNOT(I,J)+GNOT(I,J,K)*(ALFAMS**IAEXP(K))*(BETAMS**
     &IBEXP(K))
  210 CONTINUE
  220 CONTINUE
      DO 240 I=1,IDIMGS
      TSTAR(I,J)=0.D0
      DO 230 K=1,KMAXGS
      IF(GSTAR(I,J,K).EQ.0.) GO TO 230
      TSTAR(I,J)=TSTAR(I,J)+GSTAR(I,J,K)*(ALFAMS**IAEXP(K))*(BETAMS**
     &IBEXP(K))
  230 CONTINUE
  240 CONTINUE
  250 CONTINUE
C     CONSTRUCT THE L.H.S. COLUMN VECTOR (AGAIN NOTING DISPLACEMENT OF
C     THE INDEX)
      B(1)=B1
      B(2)=B2
      DO 255 I=3,IIMAX
  255 B(I)=0.D0
      IF(MS.NE.MSTART) GO TO 260
C     CONSTRUCT (AND CLOSE) THE AUGMENTED MATRIX USING DUMMY VALUE OF
C     W FOR DIAGONAL ELEMENTS
      CALL FORMAW(WDUMMY)
      GO TO 270
  260 CALL CLOSAW(WDUMMY)
C     CONSTRUCT TABLE OF VALUES OF THE DETERMINANT OF THE AUGMENTED
C     MATRIX AND SEARCH FOR APPROXIMATE LOCATION OF FIRST ROOT
  270 CALL DETMAP(1,JCOMP,WINIT)
      IF(JCOMP.NE.1) GO TO 275
      WRITE(IPRNTR,272) MS,WSTOP
  272 FORMAT('-','MACH NO.=',F8.4/' ','NO ROOTS FOUND FOR W LESS THAN ',
     &D25.16)
      GO TO 315
  275 WRITE(IPRNTR,276)
  276 FORMAT('0')
C     PERFORM FIRST ITERATION
      CALL ITER8(1,WINIT-WINC,WINIT,WNEW)
      WOLD=WINIT
      W=WNEW
C     PERFORM SECOND AND SUBSEQUENT ITERATIONS
  280 CALL ITER8(2,WOLD,W,WNEW)
      IF(ITKNTR.GT.20) GO TO 282
      WOLD=W
      W=WNEW
C     WHEN THE VALUE OF W HAS BEEN DETERMINED TO 15 FIGURES OF ACCURACY
C     (AND SUBSEQUENTLY THE SYSTEM OF EQUATIONS SOLVED), COMPUTE THE
C     PHYSICAL MOMENTS OF INTEREST
      IF(ITCOMP.EQ.1) GO TO 290
      GO TO 280
  282 WRITE(IPRNTR,285) MS
  285 FORMAT('0','MACH NO.=',D25.16,'   TOO MANY ITERATIONS WITHOUT ',
     &'CONVERGENCE ')
      GO TO 310
  290 DEMA=-SQRT23*ZETA(1)/MS**2
```

```
      DRMG=-2.D0*ZETA(2)/DSQRT(3.D0)/MS**2
      DRMD=-DSQRT(1.5D0)*ZETA(3)/MS**3
      DRMS=.6D0-DSQRT(6.D0)*ZETA(4)/5.D0/ZETA(3)
      DRMT=-9.D0*W*ZETA(2)/8.D0/SQRT3/MS**2
      WRITE(IPRNTR,295) MS,W,DETNXT
  295 FORMAT('-','MACH NO.=',F8.4/' ','FINAL W:',D25.16,20X,'DET. OF ',
     &'AUGMENTED MATRIX:',D25.16)
      WRITE(IPRNTR,300) (ZETA(I),I=1,IMAX)
  300 FORMAT('0','EIGENFUNCTION MOMENTS (STARTING WITH ZETA(3)):'/(' ',
     &7D18.8))
      WRITE(IPRNTR,305) DRMA,DRMG,DRMD,DRMS,DRMT
  305 FORMAT('0','PHYSICAL MOMENTS:'/' ','ALPHA=',D23.10/' ','GAMMA=',
     &D23.10/' ','DELTA=',D23.10/' ','S111/S1=',D21.10/' ','T/T0/M**2=',
     &D19.10)
C     SEARCH TABLE FOR ADDITIONAL ROOTS
  310 CALL SEARCH(2,JCOMP,WINIT)
      IF(JCOMP.EQ.1) GO TO 315
      GO TO 275
C     MODIFY UPPER LIMIT OF UPSTREAM ROOT SEARCH IN ACCORDANCE WITH
C     OBSERVED DEPENDENCE ON MACH NUMBER
  315 IF(WSTOP .GT. 0.D0) WSTOP=WINIT+1.D0
      MS=MS+MINC
C
C     MODIFY STARTING VALUE OF W FOR DOWNSTREAM ROOT SEARCH IN ACCORDANCE
C     WITH OBSERVED FUNCTIONAL DEPENDENCE ON MACH NUMBER.
      IF(MS .LE. .8D0) WBEGIN=-8.D0-(.8D0-MS)*1.D1
      IF(MS .GT. .8D0 .AND. MS .LT. .91D0) WBEGIN=-9.D0+(.8D0-MS)*4.D1
      IF(MS .GE. .91D0 .AND. MS .LT. 1.D0) WBEGIN=WORIG
C
      IF(MS.GT.MSTOP) GO TO 320
      IF(MPKNTR.EQ.MPSTEP) MPKNTR=0
      MPKNTR=MPKNTR+1
      GO TO 200
  320 WRITE(IPRNTR,330)
  330 FORMAT('1')
      STOP
      END
C
C
C THIS SUBROUTINE CONSTRUCTS AND CLOSES THE LHS MATRIX OF COEFFICIENTS
      SUBROUTINE FORMAW(W)
      IMPLICIT REAL*8(A-H,S-Z),INTEGER(I-R)
      REAL*8 MS,S1,S2,ROOTS6,RMTRMS
      INTEGER S1,S4
      LOGICAL DEFINR/.TRUE./,DETER/.FALSE./,REFINE/.TRUE./
      DIMENSION AUG(41,41),AW(41,41),B(41),C(6,7),CTTIN(6,21),DNORM(47),
     &EIGRL(40),IDF(47),IWRK(83),LMAT(47),RMAT(47),TNOT(21,21),
     &TNOTIN(21,21),TSTAR(7,21),VALUE(2),WRK1(41),WRK2(41),WRK3(41),
     &WRK4(41,41)
      EQUIVALENCE(AUG,AW)
      COMMON AW,B,S1,S2,SQRT3,SQRT23,MS,ORDER,IMAX,IIMAX,IPRNTR
      COMMON/WRKBLK/ IWRK,WRK1,WRK2,WRK3,WRK4
      COMMON/AREA1/ ROOTS6,EIGRL
      COMMON/AREA2/ TNOT,TSTAR,NMAT,LMAT,RMAT,ICIVT,DNORM,IDF,IGRAD
C
      A1(R,L)=-1.D0*(L+1.D0)*DSQRT((R+L+1.5D0)/(2.D0*L+1.D0)/(2.D0*L
     &+3.D0))
      A4(R,L)=L*DSQRT((R+1.D0)/(2.D0*L-1.D0)/(2.D0*L+1.D0))
C     CONSTRUCT OFF-DIAGONAL ELEMENTS
      DO 10 J=1,IMAX
      DO 5 I=1,IMAX
      AW(I,J)=0.D0
    5 CONTINUE
```

```
   10 CONTINUE
      DO 12 I=1,IMAX
      R=RVAT(I)
      L=LMAT(I)
      N=NMAT(I)
      IF(I.GT.34) GO TO 12
      S1=(N+3)/2
      S4=(N+1)/2
      AW(I,I+S1)=A1(R,L)
      AW(I+S1,I)=AW(I,I+S1)
      IF(L.EQ.0) GO TO 12
      AW(I,I+S4)=A4(R,L)
      AW(I+S4,I)=AW(I,I+S4)
   12 CONTINUE
C
C     ALTERNATE ENTRY TO AVOID RECONSTRUCTION OF OFF-DIAGONAL ELEMENTS
      ENTRY CLOSAW(W)
C     COMPUTE THE INVERSE OF TNOT
      DO 20 I=1,IDIMT
      DO 15 J=1,IDIMT
      TNOTIN(J,I)=0.D0
   15 CONTINUE
      TNOTIN(I,I)=1.D0
   20 CONTINUE
      CALL LINRD(IDIMT,IER,TNOT,WRK1,IWRK,WRK2,WRK3,WRK4,21,TNOTIN,21,
     &IDIMT,VALUE,DEFINB,DETER,REFINE)
      IF(IER.NE.0) WRITE(6,21) IER
   21 FORMAT('0','FORMAW:',4X,'IER=',I2)
C
C     CONSTRUCT SUBMATRIX "C"
      IISTOP=(ORDER+2)/2
      JJSTOP=(ORDER+3)/2
      DO 30 II=1,IISTOP
      R=RMAT(II+IMAX-IISTOP)
      L=LMAT(II+IMAX-IISTOP)
      N=NMAT(II+IMAX-IISTOP)
      LOC1=II+JJSTOP-IISTOP
      LOC4=II+JJSTOP-IISTOP-1
      DO 25 JJ=1,JJSTOP
      C(II,JJ)=0.D0
   25 CONTINUE
      C(II,LOC1)=A1(R,L)
      IF(LOC4.EQ.0) GO TO 30
      C(II,LOC4)=A4(R,L)
   30 CONTINUE
C
C     COMPUTE MATRIX PRODUCT C*TSTAR*(INVERSE OF TNOT)
      DO 50 K=1,IISTOP
      DO 45 N=1,IDIMT
      R2=0.D0
      DO 40 L=1,JJSTOP
      R1=0.D0
      DO 35 M=1,IDIMT
      R1=TSTAR(L,M)*TNOTIN(M,N)+R1
   35 CONTINUE
      R2=DNORM(IMAX+L)/IDF(IMAX+L)*R1*C(K,L)+R2
   40 CONTINUE
      CTTIN(K,N)=R2
   45 CONTINUE
   50 CONTINUE
C
C     ADD THE CLOSURE MATRIX TO AW, REMEMBERING TO INCLUDE THE "NORMALI-
C     ZATION AND DIVIDING FACTORS"
```

```
      ISTART=IMAX-ORDER/2
      JSTOP=ISTART-1
      K=1
      DO 60 I=ISTART,IMAX
      N=2
      DO 58 J=1,JSTOP
      IF((ORDER-NMAT(J))/2*2 .EQ. (ORDER-NMAT(J))) GO TO 58
      IF(ORDER/2*2.NE.ORDER .AND. N.EQ.2) GO TO 55
      AW(I,J)=AW(J,I)+IDF(J)/DNORM(J)*CTTIN(K,N)
      IF(IGRAD .EQ. 1) AW(I,J)=AW(J,I)
   55 N=N+1
   58 CONTINUE
      K=K+1
   60 CONTINUE
C
C     INPUT ELEMENTS OF LAST ROW AND COLUMN OF AUGMENTED MATRIX
      AUG(1,IIMAX)=B1
      AUG(2,IIMAX)=B2
      AUG(IIMAX,1)=1.D0/SQRT3
      AUG(IIMAX,2)=-SQRT23
      DO 65 IJ=3,IMAX
      AUG(IJ,IIMAX)=0.D0
      AUG(IIMAX,IJ)=0.D0
   65 CONTINUE
      RMTRMS=-DSQRT(2.D0)*MS**2*5.D0/6.D0+DSQRT(.5D0)
      AUG(IIMAX,IIMAX)=-RMTRMS
C
C     CONSTRUCT DIAGONAL ELEMENTS OF AW
      ENTRY DIAG(W)
      DO 70 I=1,IMAX
      AW(I,I)=ROOT56*MS*(W*EIGRL(I)-1.D0)
   70 CONTINUE
      RETURN
      END
C
C
C THIS SUBROUTINE CONSTRUCTS A TABLE (MAP) OF THE VALUES OF THE DETER-
C MINANTS OF THE AUGMENTED MATRIX AND SEARCHES FOR APPROXIMATE LOCATIONS
C OF THE ROOTS. THE VALUES OF THE DETERMINANT ARE STORED IN DETMAT(K)
C AND THE CORRESPONDING VALUE OF W IS STORED IN WMAT(K)
      SUBROUTINE DETMAP(NTRY,JCOMP,WINIT)
      IMPLICIT REAL*8(A-H,S-Z),INTEGER(I-R)
      REAL*8 MS
      LOGICAL SOLVE/.FALSE./,DETER/.TRUE./,REFINE/.FALSE./
      DIMENSION AUG(41,41),AW(41,41),B(41),DETMAT(2000),IWRK(82),
     &VALUE(2),WMAT(2000),WRK1(41),WRK2(41),WRK3(41),WRK4(41,41)
      EQUIVALENCE(AUG,AW)
      COMMON AW,B,B1,B2,SQRT3,SQRT23,MS,ORDER,IMAX,IIMAX,IPRNTR
      COMMON/WRKBLK/ IWRK,WRK1,WRK2,WRK3,WRK4
      COMMON/AREA3/ WBEGIN,WSTOP,WSTEP,MPRNTR,MSTEP
C
      K=1
      W=WBEGIN
    5 CALL DIAG(W)
      CALL LINRD(IIMAX,IER,AUG,WRK1,IWRK,WRK2,WRK3,WRK4,41,3,41,1.
     &VALUE,SOLVE,DETER,REFINE)
      WMAT(K)=W
      DETMAT(K)=VALUE(1)*(1.0D1**VALUE(2))
      W=W+WSTEP
      IF(W.GT.WSTOP) GO TO 10
      K=K+1
      GO TO 5
   10 NPTS=K
```

```
C       REMOVE C'S FROM THE FOLLOWING CARDS IF OUTPUT OF TABLE IS DESIRED
C       IF(MPKNTR.NE.MPSTEP .AND. MPKNTR.NE.0) GO TO 30
C       WRITE(IPRNTR,20) MS
C    20 FORMAT('1','MACH NUMBER= ',F8.4)
C       WRITE(IPRNTR,25) (WMAT(I),DETMAT(I),I=1,NPTS)
C    25 FORMAT('0',D25.16,5X,D25.16)
C    30 CONTINUE
C
C       ALTERNATE ENTRY FOR LOCATING SECOND AND SUBSEQUENT ROOTS OF THE
C       DETERMINANT
        ENTRY SEARCH(NTRY,JCOMP,WINIT)
        IROOT=0
        JCOMP=0
        IF(NTRY.EQ.2) GO TO 35
        J=1
        W1=WMAT(1)
        DET1=DETMAT(1)
    35  W2=WMAT(J+1)
        DET2=DETMAT(J+1)
        IF(DET1/DABS(DET1)*DET2 .GT. 0.D0) GO TO 40
        WAVE=(W1+W2)/2
        CALL DIAG(WAVE)
        CALL LINPD(IIMAX,IER,AUG,WRK1,IWRK,WRK2,WRK3,WRK4,41,B,41,1,
       &VALUE,SOLVE,DETER,REFINE)
        DETAVE=VALUE(1)*(1.6D1**VALUE(2))
        DETEND=DET1
        IF(DETAVE/DABS(DETAVE)*DET2 .GE. 0.D0) DETEND=DET2
        IF(DET1/DABS(DET1)*DET2 .LT. 0.D0 .AND. DABS(DETAVE) .LT.
       &DABS(DETEND)) IROOT=1
    40  W1=W2
        DET1=DET2
        J=J+1
        IF(IROOT.EQ.0) GO TO 45
        WINIT=WAVE
        GO TO 50
    45  IF(J.LT.NPTS) GO TO 35
        JCOMP=1
    50  RETURN
        END
C
C
C THIS SUBROUTINE PERFORMS A SINGLE STEP OF A NEWTON-RAPHSON ITERATIVE
C PROCEDURE TO DETERMINE THE EXACT VALUE OF THE ROOT. IF THE ROOT IS
C SUCCESSFULLY DETERMINED TO AN ACCURACY OF 15 SIGNIFICANT FIGURES THEN
C THE SYSTEM OF MOMENT EQUATIONS IS SOLVED AND THE SOLUTION IS STORED
C IN THE VECTOR ZETA
        SUBROUTINE ITER8(NTRY,WPREV,WACW,WNEXT)
        IMPLICIT REAL*8(A-H,S-Z),INTEGER(I-R)
        REAL*8 MS
        LOGICAL SOLVE,DETER,REFINE
        DIMENSION AUG(41,41),AW(41,41),B(41),IWRK(82),VALUE(2),WRK1(41),
       &WRK2(41),WRK3(41),WRK4(41,41),ZETA(40)
        EQUIVALENCE(AUG,AW)
        COMMON AW,B,B1,B2,SQRT3,SQRT2,MS,ORDER,IMAX,IIMAX,IPRNTR
        COMMON/WRKBLK/ IWRK,WRK1,WRK2,WRK3,WRK4
        COMMON/AREA4/ ZETA,DETNXT,ITCOMP,ITKNTR
C
        SOLVE=.FALSE.
        REFINE=.FALSE.
        DETER=.TRUE.
        ITCOMP=0
        IF(NTRY.EQ.1) ITKNTR=1
        IF(NTRY.NE.1) GO TO 5
```

```
      CALL DIAG(WPREV)
      CALL LINRD(IIMAX,IER,AUG,WRK1,IWRK,WRK2,WRK3,WRK4,41,B,41,1,
     &VALUE,SOLVE,DETER,REFINE)
      DETPRV=VALUE(1)*(1.6D1**VALUE(2))
    5 CALL DIAG(WNOW)
      CALL LINRD(IIMAX,IER,AUG,WRK1,IWRK,WRK2,WRK3,WRK4,41,B,41,1,
     &VALUE,SOLVE,DETER,REFINE)
      DETNOW=VALUE(1)*(1.6D1**VALUE(2))
      WNEXT=WNOW-DETNOW*(WPREV-WNOW)/(DETPRV-DETNOW)
      IF(DABS(WNEXT-WNOW) .GT. 1.D-02) WNEXT=WNOW+.1D0*(WNEXT-WNOW)
C
C     TO OUTPUT ITERATION INFO., SUPPRESS "C'S" IN FOLLOWING 2 CARDS
C     WRITE(IPRNTR,10) ITKNTR,WNOW,DETNOW
C  10 FORMAT(' ','ITERATION:',I3,5X,'W=',D25.16,6X,'DET.=',D25.16)
C
      DETPRV=DETNOW
      ITKNTR=ITKNTR+1
      IF(DABS(WNEXT-WNOW) .GE. .1D-14) GO TO 20
      CALL DIAG(WNEXT)
      CALL LINRD(IIMAX,IER,AUG,WRK1,IWRK,WRK2,WRK3,WRK4,41,B,41,1,
     &VALUE,SOLVE,DETER,REFINE)
      DETNXT=VALUE(1)*(1.6D1**VALUE(2))
      SOLVE=.TRUE.
      REFINE=.TRUE.
      DETER=.FALSE.
      DO 15 I=1,IMAX
   15 ZETA(I)=B(I)
      CALL DIAG(WNEXT)
      CALL LINRD(IMAX,IER,AW,WRK1,IWRK,WRK2,WRK3,WRK4,41,ZETA,41,1,
     &VALUE,SOLVE,DETER,REFINE)
      ITCOMP=1
   20 RETURN
      END
```

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Title of Thesis

Solution of the Boltzmann Equation at the Singular Points in a Shock Wave by the Method of Rational Truncation and Coordinate Straining

Author [redacted]

ROY DANIEL MCGREGOR

July, 1976