ON THE SOLUTION OF THE BOLTZMANN EQUATION AT THE UPSTREAM SINGULAR POINT OF AN INFINITELY STRONG SHOCK WAVE

by

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ABSTRACT

The solution of the Boltzmann equation at the upstream singular point of an infinitely strong shock wave is examined, for the case of Maxwell molecules. The fluid velocity, u, is used as the independent variable, and $\frac{\partial f}{\partial u}$ is expanded at the upstream singular point in terms of the eigenfunctions of the linearized Boltzmann collision operator, where f is the velocity distribution function. The expansion coefficients are the velocity-derivatives of the eigenfunction moments of f, and are shown to satisfy an infinite system of nonlinear algebraic equations of the form $[A]\bar{\bar{\xi}} = \bar{b}$, where the elements of $\bar{\bar{\xi}}$ are the unknown expansion coefficients, and where $[A]$ is an upper-triangular, non-singular matrix, in which every element along the principal diagonal involves a single unknown. The nonlinearity of the problem is due to this unknown. It is shown that setting certain of the $\bar{\bar{\xi}}$ elements to zero to close the equations for solution (Grad's method) fails to yield a solution of this system to any order of closure.

Expressions for the velocity derivatives of the eigenfunction moments of the Mott-Smith distribution are developed, and used for certain of the $\bar{\bar{\xi}}$ elements to close the equations for solution (Elliott and Baganoff's method). The solution based on this method is carried to closure order 22 with no apparent convergence. A technique for extracting a rapidly convergent solution from the original solution sequence is proposed and carried out with success. The tentative results are physically reasonable.

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TABLE OF CONTENTS

LIST OF FIGURES

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CHAPTER 1

INTRODUCTION

The Boltzmann equation may be regarded either as a reduction of the Liouville equation or as an extension of the conservation equations of fluid dynamics. As an extension of the conservation equations, it goes beyond the use of simplifying assumptions such as the Navier - Stokes relation or the Fourier heat conduction law. However, the price paid for better representation of non-equilibrium gas dynamic situations is an overwhelming increase in the complexity of the mathematics. The problem considered here, related to the structure of a strong shock wave, is particularly worthwhile in that it affords an opportunity to explore techniques of solving the Boltzmann equation with a minimum of mathematical difficulty. Aside from the fact that the flow is steady and one-dimensional, a major simplfication occurs if the fluid properties in the wings of the shock are examined, as the kinetic variables approach their equilibrium values. In the upstream wing of an infinitely strong shock, i.e. allowing the upstream Mach number to become infinitely large, even further simplification takes place. Despite this, the solution is found to be quite sensitive to the particular method of approximation used. The problem will likely remain as one of the most stringent tests of various approximation techniques employed in gas dynamics while at the same time allowing examination of very high orders of approximation with little mathematical complexity.

The problem of shock structure was first considered by Taylor (1910), who obtained a closed-form analytic solution of the Navier - Stokes equations for a vanishingly weak shock. Morduchow and Libby (1949) unsuccessfully attempted to solve the Navier - Stokes equations in a shock wave of arbitrary strength. Gilbarg and Paolucci (1953) later showed that if the fluid velocity u is used, rather than the spatial variable x, as the independent variable in a shock wave, the Navier - Stokes equations can be solved for a solution curve in, say, the temperature-velocity (T-u) plane and then integrated to obtain the spatial variation of T, u, or any other variable. The situation is illustrated in figure 1.

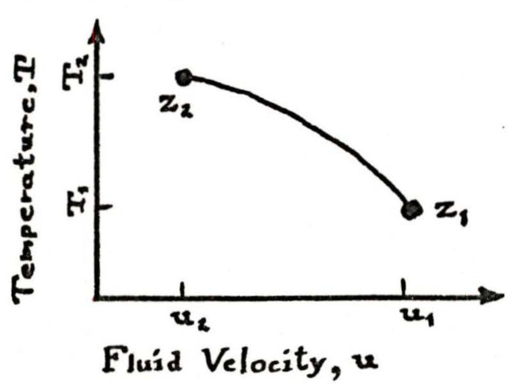


Figure 1. General form of the solution curve in the temperature-velocity plane.

Gilbarg and Paolucci (1953) showed that for the Navier - Stokes equations, z_1 and z_2 are singular points, z_1 is an unstable node and z_2 is a saddle point. Morduchow and Libby (1949) tried to solve for the T-u curve by integrating from the upstream singular point z_1, and found they could not satisfy the Rankine - Hugoniot conditions. They attributed their failure to a defect in the Navier - Stokes equations. Gilbarg and Paolucci (1953) correctly pointed out that the integration must be performed starting from the downstream singular point z_2 in order to obtain the T-u curve for the shock.

Since the gradients $\frac{dT}{dx}$ and $\frac{du}{dx}$ tend to zero in the wings of the shock, the points z_1 and z_2 are always singular, no matter what equation or set of equations is solved. Thus an analysis of the flow near the singular points, while interesting in its own right, is an essential first step in the more general problem of shock wave structure.

Elliott and Baganoff (1974) have carried out the singular point analysis for the Boltzmann equation. Their work is based on the method of moments. In it they derive a nonlinear integral equation for $\left.\frac{\partial f}{\partial u}\right)_s$, where f is the velocity distribution function, and the subscript s takes on the values 1 and 2 at the upstream and downstream singular points, respectively. From this equation they form a system of moment equations (involving velocity-derivatives of the various moments) which they solve by using Grad's method [Grad (1949)]. Although the solution based on this method converges very slowly upstream, even for weak shock waves, Elliott and Baganoff (1974) showed that the rate of convergence could be improved considerably if Grad's method were modified to incorporate the Mott-Smith distribution function [Mott-Smith (1951)] as the first approximation to f.

In the present work, we shall carry the application of the method used by Elliott and Baganoff (1974) a step forward and consider the flow near the upstream singular point of an infinitely strong shock wave. As a result of several crucial simplifications which occur, the solution can be easily examined to any desired order of approximation, the only practical limitation being the numerical accuracy of the computations. Although the flow near the downstream singular point is no less interesting, the simplification due to the strength of the shock does not occur there, and we shall therefore not consider this case. [Elliott and Baganoff (1974) have shown that the downstream flow is adequately represented by the solution based on Grad's method.]

Two important objectives are served by the present work. The first deals with the answer to the fundamental question as to whether the Boltzmann equation itself is capable of describing the flow in a strong shock wave. Various aspects of this question are discussed by Cercignani (1969), among others. The second, more practical objective is the determination of precise limit values for the upstream moment derivatives or moment ratios. Such information is essential in order to explore the possibility, suggested by Elliott and Baganoff (1974), of developing nonlinear constitutive relations among the higher moments of f.

CHAPTER 2

DEVELOPMENT OF THE FUNDAMENTAL EQUATION AND SUMMARY OF BACKGROUND

For steady, one-dimensional flow under zero external force the Boltzmann equation can be written

(1.) $$(u + c_x)\left[\frac{\partial(\rho f)}{\partial u} - \frac{\partial(\rho f)}{\partial c_x}\right] = \mathcal{C}(\rho f) \Big/ \frac{du}{dx} ,$$

where

u is the fluid velocity

$\vec{c} = (c_x, c_y, c_z)$ is the thermal velocity of a molecule,

ρ is the mass density, and

$\mathcal{C}(\rho f)$ is the nonlinear Boltzmann collision operator.

Let $f^{\circ} = (2\pi RT)^{-3/2} exp(-\frac{c^2}{2RT})$ be the Maxwellian distribution, where R is the ordinary gas constant and T is the local temperature. Then, following Elliott and Baganoff (1974), we expand f in a Taylor series of the form $\rho f = \rho_s f_s^{\circ}[1 + (u - u_s)h_s]$, where only the term of order $(u - u_s)$ has been retained. Note that

$$\left.\frac{\partial(\rho f)}{\partial u}\right|_s = \rho_s f_s^{\circ} h_s ,$$

and hence if

$$\langle\Phi\rangle = \int \Phi(\vec{c})\, f\, d^3c$$

is a general moment of f, then we have

(2.) $$\left.\frac{d}{du} \rho \langle\Phi\rangle\right|_s = \rho_s \int \Phi f_s^{\circ} h_s d^3c .$$

Substituting the expansion for ρf in equation 1, and noting that $\mathcal{C}(\rho f^{\circ}) = 0$, we find, after considerable manipulation

$$(3.)\qquad (\tilde{M}_s + V_x)(\tilde{M}^{-1} u_s h_s + 2 V_x) = \omega_s J(u_s h_s) \; .$$

Here

$\tilde{M}_s = u_s(2RT_s)^{-1/2} = \sqrt{5/6}\, M_s$, where M_s is the Mach number;

$V_x = c_x(2RT_s)^{-1/2}$ is a nondimensional thermal velocity (note the suppression of s);

J is the standard linearized collision operator discussed by Uhlenbeck and Ford (1953), among others.

The quantity ω_s appearing in equation 3 is defined by

$$(4.)\qquad \omega_s = \frac{16}{9A_2} \frac{\tau/\tau^{\circ})_s}{\frac{u_s}{P_s}\frac{d\tau}{du}\Big)_s} \; .$$

Here τ is the xx component of the viscous stress tensor, p is the pressure and

$$\tau^{\circ} = \frac{4}{3}\mu \frac{du}{dx}$$

is the Navier - Stokes expression for τ, where μ is the coefficient of viscosity. A_2 is a constant whose numerical value is 2.7406... . For the details in the derivation of equation 3, the reader is referred to Elliott and Baganoff (1974).

From equation 2 we see that $\frac{u_s}{P_s}\frac{d\tau}{du}\Big)_s$ is a moment of h_s. Further, Elliott and Baganoff (1974) have shown that

$\frac{\tau}{\tau_0})_s$ can be expressed as a linear combination of moments of h_s. Therefore, ω_s is a rational function of moments of h_s, and equation 3 is a nonlinear integral equation for h_s in spite of the fact that J is a linear operator.

Wang Chang and Uhlenbeck (1952) have determined the eigenvalues and eigenfunctions of the operator J. The eigenfunctions are orthonormal with respect to the weight function e^{-V^2}, and for a one-dimensional flow are given by

(5.) $$\Psi_{r\ell} = \sqrt{\frac{r!\,(\ell+\frac{1}{2})}{\pi\,(\ell+\frac{1}{2}+r)!}}\; V^{\ell}\, P_{\ell}(\cos\theta)\, S^{r}_{\ell+\frac{1}{2}} ,$$

where $S^{r}_{\ell+\frac{1}{2}} = \sum_{j=0}^{r} (-1)^{j}\, V^{2j} \frac{(\ell+\frac{1}{2}+r)!}{j!\,(r-j)!\,(\ell+\frac{1}{2}+j)!}$ is the Sonine polynomial, and P_ℓ is the Legendre polynomial, with $V_x = |V|\cos(\theta)$. Following Wang Chang and Uhlenbeck (1952), Elliott and Baganoff (1974) have expanded $u_s h_s$ in terms of the $\Psi_{r\ell}$'s:

$$u_s h_s = \pi^{3/4} \sum_{r,\ell} \xi_{r\ell}\, \Psi_{r\ell} .$$

As a consequence of (2.), the expansion coefficients $\xi_{r\ell}$ are related to the eigenfunction moments by

(6.) $$\xi_{r\ell} = \pi^{3/4} \frac{u_s}{\rho_s} \frac{d}{du} \rho \langle \Psi_{r\ell} \rangle \Big)_s .$$

Substituting the expansion into equation 3, multiplying by $\Psi_{r\ell}\, e^{-V^2}$, and integrating, we obtain the matrix equation

(7.) $$\sum_{r',\ell'} \left[\tilde{M}_s (\omega_s \lambda_{r\ell} - 1)\, \delta_{r\ell, r'\ell'} - M_{r\ell, r'\ell'} \right] \xi_{r\ell} = b_{r\ell},$$

as given by Elliott and Baganoff (1974). Here

$$M_{r\ell,r'\ell'} \equiv \int v_x e^{-v^2} \Psi_{r\ell} \Psi_{r'\ell'} d^3v \,,$$

$$b_{r\ell} \equiv 2\pi^{-3/4} \tilde{M}_s \int v_x(\tilde{M}_s + v_x) e^{-v^2} \Psi_{r\ell} d^3v \,,$$

$\delta_{r\ell,r'\ell'}$ is the Kronecker delta and $\lambda_{r\ell}$ is the eigenvalue corresponding to $\Psi_{r\ell}$. The $\lambda_{r\ell}$'s have been tabulated up to order $2r + \ell = 36$ by Alterman et al. (1962). (The tabulated values must be multiplied by the factor $1.25A_2$ if definition 4 is used for ω_s.) The only non-zero $b_{r\ell}$'s are $b_{00} = \tilde{M}_s$, $b_{01} = \sqrt{2}\,\tilde{M}_s^2$, $b_{10} = -2\tilde{M}_s/\sqrt{6}$, and $b_{02} = 2\tilde{M}_s/\sqrt{3}$. The $M_{r\ell,r'\ell'}$'s are given by Wang Chang and Uhlenbeck (1952) and are

$$\begin{aligned} M_{r\ell,r'\ell'} = {} & (\ell+1)\sqrt{\frac{r+\ell+3/2}{(2\ell+1)(2\ell+3)}}\ \delta_{r,r'}\ \delta_{\ell+1,\ell'} \\ & - (\ell+1)\sqrt{\frac{r}{(2\ell+1)(2\ell+3)}}\ \delta_{r-1,r'}\delta_{\ell+1,\ell'} \\ & + \ell\sqrt{\frac{r+\ell+1/2}{(2\ell-1)(2\ell+1)}}\ \delta_{r,r'}\ \delta_{\ell-1,\ell'} \\ & - \ell\sqrt{\frac{r+1}{(2\ell-1)(2\ell+1)}}\ \delta_{r+1,r'}\ \delta_{\ell-1,\ell'} \,. \end{aligned}$$

Figure 2 shows the location of all nonzero elements of the matrix in equation 7. The "D" entries arise from the term involving the Kronecker delta, and the "1", "2", "3", and "4" entries from the corresponding term in the above expression for $M_{r\ell,r'\ell'}$.

Owing to the presence of ω_s in the "D" terms of the

		$2r'+l'$	0	1	2		3		4			5			6			
		l'	0	1	0	2	1	3	0	2	4	1	3	5	0	2	4	6
		r'	0	0	1	0	1	0	2	1	0	2	1	0	3	2	1	0
$2r+l$	l	r																
0	0	0	D	1														
1	1	0	3	D	4	1												
2	0	1		2	D		1											
	2	0		3		D	4	1										
3	1	1			3	2	D		4	1								
	3	0				3		D		4	1							
4	0	2					2		D			1						
	2	1					3	2		D		4	1					
	4	0						3			D		4	1				
5	1	2							3	2		D			4	1		
	3	1								3	2		D			4	1	
	5	0									3			D			4	1
6	0	3										2			D			
	2	2										3	2			D		
	4	1											3	2			D	
	6	0												3				D

Figure 2.

Location of the nonzero elements in the matrix of the fundamental equation. (equation 7.)

matrix, equation 7 is an infinite system of nonlinear algebraic equations in the $\xi_{r\ell}$'s, since ω_s depends on several of the $\xi_{r\ell}$'s by virtue of equation 6. Inversion of the full matrix is therefore impossible. We then agree to truncate the system at a certain order n by eliminating all equations for which $2r+\ell > n$. The structure of the matrix in figure 2 shows that the truncated system is not closed, since the n^{th} order equations contain $\xi_{r\ell}$'s of order n+1. We must therefore resort to a method of closure using approximate information. That is to say, we must find a method by which the $\xi_{r\ell}$'s of order n+1 can either be evaluated numerically, or expressed as functions of the $\xi_{r\ell}$'s of order n and lower.

Grad (1949) has developed a logical method for closing the set of equations at any level of truncation. He expands f in a series of Hermite polynomials of the form

$$f = f^{o} \sum_{\nu} a_{\nu} H_{\nu} \ ,$$

where H_{ν} is a tensor polynomial of degree ν,* and a_{ν} is a coefficient to be determined. It follows from the orthogonality of the Hermite polynomials that

$$a_{\nu} = \langle H_{\nu} \rangle \ .$$

To obtain closure at order n, Grad sets $a_{\nu} = 0$ for $\nu > n+1$, which implies for $\nu = n+1$ that

$$\langle H_{n+1} \rangle = 0 \ . \tag{8.}$$

* Only axially symmetric contractions of Grad's H_{ν}'s need be considered here due to problem simplification.

Grad has since outlined a proof [Grad (1958)] showing the equivalence of his method to the expansion method of Wang Chang and Uhlenbeck (1952) used here. The particular property of importance is

$$H_\nu = \sum_{r,\ell} \gamma_{r\ell}^{(\nu)} \Psi_{r\ell} \quad ,$$

where the $\gamma_{r\ell}^{(\nu)}$'s are constant tensors, with

$$\gamma_{r\ell}^{(\nu)} = 0, \quad 2r+\ell \neq \nu .$$

Thus H_ν is a linear combination of the eigenfunctions $\Psi_{r\ell}$ of order ν alone. Since the $\Psi_{r\ell}$'s are linearly independent, equation 8 implies

$$\langle \Psi_{r\ell} \rangle = 0, \quad 2r+\ell = n+1 .$$

Since $\langle \Psi_{r\ell} \rangle = 0$ when $r \neq 0$ and $l \neq 0$, equation 6 gives

$$(9.) \qquad \langle \Psi_{r\ell} \rangle = 0, \; 2r+\ell = n+1 .$$

Closure of the truncated set by Grad's method, at order n, is thus accomplished by means of the substitution 9.

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 $r = \ell = 0$ is identically satisfied. Thus after closure at any order, there is always one less $\xi_{r\ell}$ coefficient than the number of equations to be satisfied. The extra unknown is ω_s and it completes the system.

Properties of the solution based on Grad's method of closure have been investigated for shock waves of moderate strength by Elliott and Baganoff (1974), who found that the solution converges rapidly at the subsonic singular point, but very slowly at the supersonic singular point. Moreover, for every order, there exists a critical value of the shock Mach number above which the solution is physically meaningless. Elliott and Baganoff (1974) then showed that the rate of convergence upstream is accelerated if the Mott-Smith distribution [Mott-Smith (1951)], f_{ms}, is used as the first approximation to f and the Hermite polynomial series is used to correct the error. That is

$$f = f_{ms} + f^{\circ}\sum_{\nu} a_{\nu} H_{\nu} ,$$

from which follows

$$a_{\nu} = \langle H_{\nu} \rangle - \langle H_{\nu} \rangle_{ms} ,$$

where $\langle \Phi \rangle_{ms} = \int \Phi \, f_{ms} \, d^3c$. Closure at order n now gives

$$\langle H_{n+1} \rangle = \langle H_{n+1} \rangle_{ms} ,$$

and since $\langle \Psi_{r\ell} \rangle_{ms} = 0$ when $r \neq 0$ and $\ell \neq 0$, we have

$$\xi_{r\ell} = (\xi_{r\ell})_{ms} , \quad 2r+\ell = n+1$$

as the closure relations for the n^{th} order solution.

CHAPTER 3

FORMULATION OF THE PROBLEM AT THE UPSTREAM SINGULAR POINT IN AN INFINITELY STRONG SHOCK

Elliott and Baganoff (1974) have determined that $\xi_{r\ell}$ increases upstream as $M_1^{2r+\ell}$ as the shock Mach number M_1 becomes large. This observation follows from the definitions of the $\xi_{r\ell}$'s in terms of the derivatives of the moments of f, together with the scaling of the low-order derivatives with M_1 implied by the form of the conservation equations. It will also be seen that the $\xi_{r\ell}$'s computed from the Mott-Smith distribution function display this property. The problem under consideration is the solution of equation 7, the fundamental equation, at the upstream singular point (s=1) in an infinitely strong shock wave ($M_1 \rightarrow \infty$). From the deduced dependence on M_1, $\xi_{r\ell} \rightarrow \infty$ as $M_1 \rightarrow \infty$, and we therefore must introduce bounded variables before the limit $M_1 \rightarrow \infty$ is taken. Since the combination $\tilde{\xi}_{r\ell} \equiv \xi_{r\ell}/M_1^{2r+\ell}$ is bounded for all values of M_1, let every equation in the set (7.) be divided by $M_1^{2r+\ell+1}$. From figure 2 we see that we then may write the nth order equations (the set for which $2r + \ell = n$) as

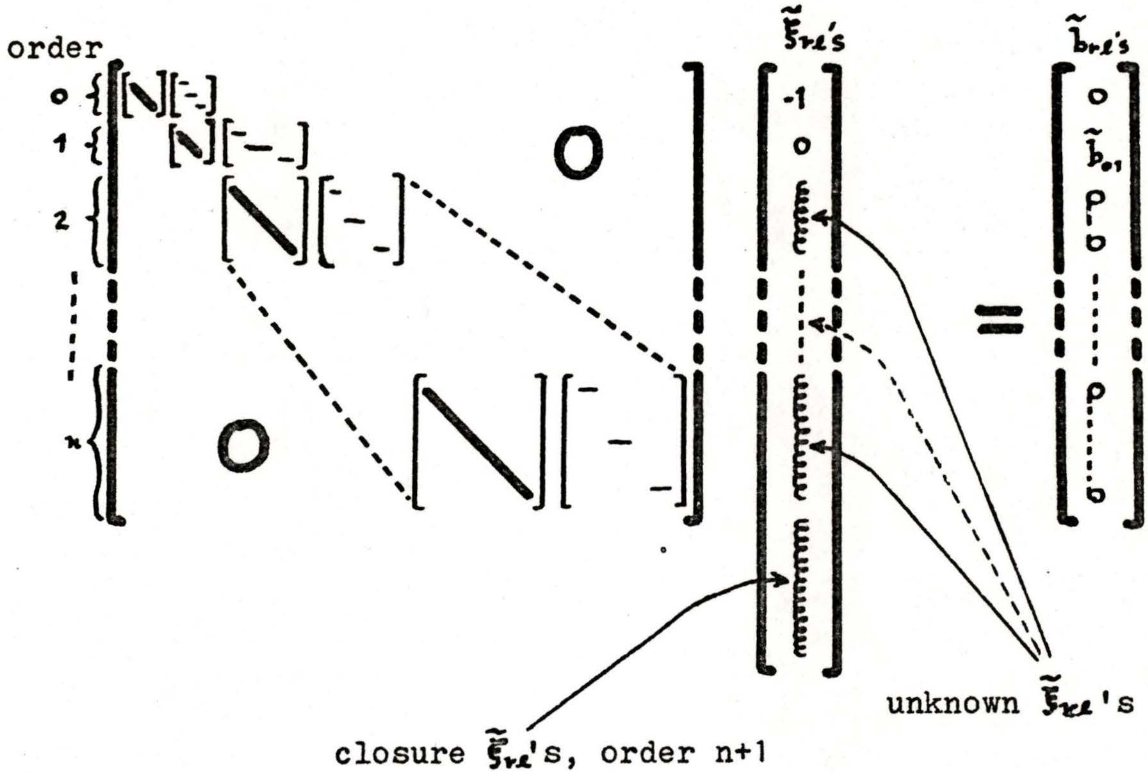
$$\sum_{\substack{r'\ell' \\ 2r'+\ell'=n-1}} M_{r\ell,r'\ell'}(M_1^{-1}\tilde{\xi}_{r'\ell'}) + \sum_{\substack{r'\ell' \\ 2r'+\ell'=n}} \sqrt{5/6}\,(\omega_1 \lambda_{r'\ell'} - 1)\,\tilde{\xi}_{r'\ell'}\,\delta_{r\ell,r'\ell'}$$
$$+ \sum_{\substack{r'\ell' \\ 2r'+\ell'=n+1}} M_{r\ell,r'\ell'}\,\tilde{\xi}_{r'\ell'} = \tilde{b}_{r\ell} ,$$

where $\tilde{b}_{r\ell} \equiv \tilde{b}_{r\ell}/M_1^{2r+\ell+1}$ and where we have made use of the fact that $\tilde{M}_1 = \sqrt{5/6}\, M_1$. As $M_1 \to \infty$, the contribution from the first summation goes to zero since $\xi_{r'\ell'}$ is already bounded. In addition, the only surviving $\tilde{b}_{r\ell}$ in the limit is $\tilde{b}_{01} = 5/6\sqrt{2}$. It can thus be seen from figure 2 that the important simplification achieved by considering the limiting case of the infinitely strong shock wave is the conversion of equation 7 to upper-triangular form.

Before proceeding with the solution of the upper-triangular system, let us strengthen the physical justification for the use of the method developed by Elliott and Baganoff (1974) by examining the solution based on Grad's method. Wang Chang and Uhlenbeck (1952) have shown that the eigenvalues of J are all negative and decrease with order $(2r+\ell)$. From physical considerations, we have

$$\tau/\tau^0)_1 > 0 \quad \frac{u}{\rho}\frac{d\tau}{du}\Big)_1 > 0, \text{ and hence } \omega_1 > 0 .$$

Thus $(\omega_1 \lambda_{r\ell} - 1) < 0$ for all r and ℓ. This in turn implies that the diagonal sub-matricies in figure 3 have no zero elements along their diagonals, and are thus non-singular. Employing Grad's closure method at order n, we set the $\tilde{\xi}_{r\ell}$'s of order n+1 to zero. From figure 3 and the discussion above, the order n equations



LEGEND

represents the diagonal submatricies of figure 2 with $\tilde{M}_1$ replaced by $\tilde{M}_1/M_1 = \sqrt{5/6}$

represents the superdiagonal submatricies of figure 2 consisting of the "1" and "4" terms.

Figure 3.

The fundamental equation for the upstream case, $M_1 \to \infty$

give

$$\tilde{\xi}_{r\ell} = 0, \quad 2r + \ell = n,$$

and we may continue to backsolve the set, order by order obtaining $\tilde{\xi}_{r\ell} = 0$ by virtue of the non-singularity of the diagonal matrices , until we reach the equation for which r=0 and ℓ=1. This equation will then yield a nonzero value for $\tilde{\xi}_{01}$ since $\tilde{b}_{01}$ is nonzero. But as noted earlier, $\tilde{\xi}_{01}$ is zero by definition of the thermal velocity, and so we arrive at a contradiction. Grad's method is therefore worthless in treating the present problem.

Turning back to the method of solution used by Elliott and Baganoff (1974), we find the monomial moments of the Mott-Smith distribution function,

$$f_{ms} = \frac{u-u_2}{u_1-u_2}\alpha_1 e^{-\beta_1 G_1^2} - \frac{u-u_1}{u_1-u_2}\alpha_2 e^{-\beta_2 G_2^2} ,$$

where $\beta_s = (2RT_s)^{-1}$, $G_s^2 = (c_x + u - u_s)^2 + c_y^2 + c_z^2$,

and $\alpha_s = (2\pi R T_s)^{-3/2} = \left(\frac{\beta_s}{\pi}\right)^{3/2}$.

The general expression for a monomial moment of this distribution function is

$$\langle c_x^\ell c^{2m} \rangle_{ms} = \frac{u-u_2}{u_1-u_2}\alpha_1 \int (c_x + Z_1)^\ell \left[(c_x+Z_1)^2 + c_\perp^2\right]^m e^{-\beta_1 c^2}\, d^3c$$

$$- \frac{u-u_1}{u_1-u_2}\alpha_2 \int (c_x + Z_2)^\ell \left[(c_x+Z_2)^2 + c_\perp^2\right]^m e^{-\beta_2 c^2}\, d^3c ,$$

where $z_1 = -u + u_1,$

$z_2 = -u + u_2,$

and $c_\perp^2 = c_y^2 + c_z^2 .$

The integrations are most easily performed in cylindrical coordinates and yield

$$\langle c_x^{\ell} c^{2m} \rangle_{ms} = \frac{1}{u_1 - u_2} \sum_{j=0}^{m} \sum_{\substack{k=0 \\ \text{even}}}^{\ell+2j} \Big[-z_2 z_1^{\ell+2j-k} \beta_1^{-m+j-k/2} + z_1 z_2^{\ell+2j-k} \beta_2^{-m+j+k/2} \Big] \frac{(\ell+2j)!\, m!}{(\ell+2j-k)\, 2^k \left(\frac{k}{2}\right)!\, j!} .$$

With $B_{jk} = \frac{(\ell+2j)!\,m!}{(\ell+2j-k)!\,j!\,2^k\left(\frac{k}{2}\right)!}$, a simplification of the sums arises if the following indices are used:

$q = \frac{1}{2}\ell + j - \frac{1}{2}k , \quad \nu = m ,$

$p = j + \frac{1}{2}k$, and $\quad n = \ell + 2m.$

We may re-cast the moment in the form

$$\langle c_x^{n-2\nu} c^{2\nu} \rangle_{ms} = \frac{1}{u_1 - u_2} \sum_{q=0}^{n/2} \Big[-z_2 (2RT_1)^{n/2-q} z_1^{2q} + z_1 (2RT_2)^{n/2-q} z_2^{2q} \Big] \sum_{\substack{p=|n/2-\nu-q| \\ \text{increment } p \text{ by } 2}}^{n/2+\nu-q} B_{qp} .$$

We have finally

$$\langle c_x^{n-2\nu} c^{2\nu} \rangle_{ms} = \frac{u-u_2}{u_1-u_2} \sum_{q=0}^{n/2} \bar{A}_q (RT_1)^{n/2-q} (u-u_1)^{2q} - \frac{u-u_1}{u_1-u_2} \sum_{q=0}^{n/2} \bar{A}_q (RT_2)^{n/2-q} (u-u_2)^{2q},$$

with

$$\mathcal{A}_q = \frac{\nu!\,2^\nu}{(2q)!} \sum_{\substack{p=|n/2-\nu-q| \\ \text{increment } p \text{ by } 2}}^{n/2+\nu-q} \frac{(n/2+q-\nu+p)!}{2^p\,(p/2+q/2-n/4+\nu/2)!\,(p/2-q/2+n/4-\nu/2)!}.$$

In order to determine the derivatives of the moments with respect to the fluid velocity u, it is convenient to handle the moments of odd and even order separately. For the odd moments, let n+1 be the order under consideration. Differentiation yields

$$\begin{aligned}
\frac{u}{u_1^{n+1}} \frac{d}{du} \langle c^{2\nu} c_x^{n+1-2\nu} \rangle_{ms} = {} & \frac{2\tilde{u}-\tilde{u}_2-1}{1-\tilde{u}_2} \sum_{j=0}^{n/2} \mathcal{A}_j \left(\frac{3}{5M_1^2}\right)^{n/2-j} (\tilde{u}-1)^{2j} \\
& + \frac{2(\tilde{u}-\tilde{u}_2)(\tilde{u}-1)}{1-\tilde{u}_2} \sum_{j=1}^{n/2} \mathcal{A}_j \left(\frac{3}{5M_1^2}\right)^{n/2-j} (\tilde{u}-1)^{2j-1} \\
& + \frac{(-2\tilde{u}+\tilde{u}_2+1)\,\tilde{u}_2^n}{1-\tilde{u}_2} \sum_{j=0}^{n/2} \mathcal{A}_j \left(\frac{3}{5M_2^2}\right)^{n/2-j} \left(\frac{\tilde{u}}{\tilde{u}_2}-1\right)^{2j} \\
& + \frac{2(1-\tilde{u})(\tilde{u}-\tilde{u}_2)\,\tilde{u}_2^{n-1}}{1-\tilde{u}_2} \sum_{j=1}^{n/2} j\mathcal{A}_j \left(\frac{3}{5M_2^2}\right)^{n/2-j} \left(\frac{\tilde{u}}{\tilde{u}_2}-1\right)^{2j-1},
\end{aligned}$$

where $\tilde{u} = u/u_1$ and $\tilde{u}_s = u_s/u_1$.

For the even moments, let n be the order under consideration. We have

$$\begin{aligned}
\frac{u_1}{u_1^{n+1}} \frac{d}{du} \langle c^{2\nu} c_x^{n-2\nu} \rangle_{ms} = {} & \frac{1}{1-\tilde{u}_2} \sum_{j=0}^{n/2} \mathcal{A}_j \left(\frac{3}{5M_1^2}\right)^{n/2-j} (\tilde{u}-1)^{2j} \\
& + 2\,\frac{\tilde{u}-\tilde{u}_2}{1-\tilde{u}_2} \sum_{j=1}^{n/2} \mathcal{A}_j \left(\frac{3}{5M_1^2}\right)^{n/2-j} (\tilde{u}-1)^{2j-1} \\
& - \frac{\tilde{u}}{1-\tilde{u}_2} \sum_{j=0}^{n/2} \mathcal{A}_j \left(\frac{3}{5M_2^2}\right)^{n/2-j} \left(\frac{\tilde{u}}{\tilde{u}_2}-1\right)^{2j} \\
& + 2\,\frac{1-\tilde{u}}{1-\tilde{u}_2} \sum_{j=1}^{n/2} j\mathcal{A}_j \left(\frac{3}{5M_2^2}\right)^{n/2-j} \left(\frac{\tilde{u}}{\tilde{u}}-1\right)^{2j-1}.
\end{aligned}$$

Evaluating both expressions at the upstream limit $\tilde{u} = 1$, we see that the only terms surviving in either expression arise from the third summation in the expression, and from the first term of the first summation. For the case under study, $M_1 \to \infty$, this single term also vanishes. From the Rankine - Hugoniot equations, we have $\tilde{u}_2 \to 1/4$ and $M_2^2 \to 1/5$ as $M_1 \to \infty$. Inserting these limits in the remaining expressions, we have, for the odd moments

$$\lim_{M_1 \to \infty} \frac{u}{u^{n+1}} \frac{d}{du} \langle c^{2\nu} c_x^{n+1-2\nu} \rangle_{ms} \Big)_1 = 4^{-n} 3^{n/2} \sum_{j=0}^{n/2} A_j 3^j ,$$

and for the even moments,

$$\lim_{M_1 \to \infty} \frac{u}{u^n} \frac{d}{du} \langle c^{2\nu} c_x^{n-2\nu} \rangle_{ms} \Big)_1 = -4^{-n+1} 3^{n/2-1} \sum_{j=0}^{n/2} A_j 3^j .$$

Note at this point that

$$\frac{d}{du} \langle v^{2\nu} v^{n-2\nu} \rangle \propto M_1^n$$

for both cases, since $\hat{c} = \sqrt{2RT_1}\, \vec{v}$.

Since $\langle \Psi_{r\ell} \rangle \big)_s = 0$ when $r \neq 0$ and $\ell \neq 0$, we have from (6.)

$$\xi_{r\ell} = \pi^{3/4}\, u \frac{d}{du} \langle \Psi_{r\ell} \rangle \Big)_s .$$

After substituting the series for the Legendre and Sonine polynomials as indicated in equation 5, we have, at the upstream singular point

$$\xi_{r\ell} = \pi^{3/4} \sqrt{\frac{r!\,(\ell+1/2)!}{\pi\,(\ell+1/2+r)!}} \sum_{k=0}^{[\ell/2]} \frac{(-1)^k (2\ell-2k)!}{2^\ell k!\,(\ell-k)!\,(\ell-2k)!} \cdot \sum_{j=0}^{r} (-1)^j \frac{(\ell+1/2+r)!}{j!\,(r-j)!\,(\ell+1/2+j)!} \left[u \frac{d}{du} \langle v^{2j+2k} v_x^{\ell-2k} \rangle \right]_1 .$$

When we form $\tilde{\xi}_{r\ell}$ by dividing by $M_1^{2r+\ell}$, note that in the second sum only the term for which $j=r$ survives as $M_1 \to \infty$. After performing this division by $M_1^{2r+\ell}$ and using the limiting expressions for the monomial moments we finally obtain

$$(10.)\quad \lim_{M_1\to\infty} (\tilde{\xi}_{r\ell})_{ms} = -\sigma\sqrt{\ell+\tfrac{1}{2}}\,(-1)^r\, 5^{\ell/2+r}\, \frac{4}{3} \sum_{k=0}^{[\ell/2]} \frac{(-1)^k (2\ell-2k)!\,(k+r)!}{k!\,(\ell-k)!\,(\ell-2k)!} \cdot$$

$$\frac{2^{-\frac{7}{2}\ell-4r+k}}{\sqrt{\pi}\, r!\,(\ell+\frac{1}{2}+r)!} \sum_{q=q_0}^{\ell/2+r} 3^{[q]} \sum_{\substack{j=\left|\frac{\ell}{2}-k-q\right| \\ \text{increment } j \text{ by } 2}}^{k+2r+\frac{\ell}{2}+q} \frac{\pi^{3/4}\,(j+q+\ell/2-k)!}{(2q)!\,2^j \left(\frac{j}{2}+\frac{q}{2}-\frac{\ell}{4}+\frac{k}{2}\right)! \left(\frac{j}{2}-\frac{q}{2}+\frac{\ell}{4}-\frac{k}{2}\right)!},$$

where $\sigma = 1$ and $q_0 = 0$ when ℓ and n are even,

$\sigma = \sqrt{3}$ and $q_0 = \frac{1}{2}$ when ℓ and n are odd, and

$[q]$ is the largest integer less than q.

Equation 10 provides the information necessary to close the upper triangular system of figure 3 at any order of truncation. Recall that since the $r = \ell = 0$ equation is identically satisfied, there is always one more equation than the number of $\tilde{\xi}_{r\ell}$'s to be determined. The solution is accomplished by using a Newton-Raphson method for finding the value of ω_1 that gives the optimum solution vector for the overdetermined set of equations in the $\tilde{\xi}_{r\ell}$'s. When the $\tilde{\xi}_{r\ell}$'s have been found, the quantities of physical interest are easily determined by inversion of (6.) to obtain the monomial moments. Several of these transformations are listed by Elliott and Baganoff (1974).

CHAPTER 4

RESULTS AND DISCUSSION

FORTRAN programs were developed to carry out the solution. The program to determine the limit values of the various $(\tilde{\xi}_{r\ell})_{ms}$ deserves special note. Expression 10 has several problems inherent in its numerical evaluation. One of these problems is the computation of extremely large factorials. The first factor in the numerator in the sum over k shows that for k=0 and ℓ=n we must evaluate (2n)!. This was accomplished by always working with the logarithms of the factorials. The most difficult problem is the extreme range in magnitude of the numbers found in the interleaving sums. This problem was attacked in two ways. The highest precision available (approximately 16 digits) was used throughout the calculations, and a special subroutine was designed to form the best possible sum of a set of numbers on a floating point binary computer. Despite this, it was found that order 23 was the operational limit. Beyond this order, for large values of ℓ, the number of terms in the sum over k, combined with the alternating sign of each term, result in large cancellations that reduce the number of significant digits in the final sum to nil.

One of the principal tests of the quality of the closure information is to check for convergence of the low-order $\tilde{\xi}_{r\ell}$'s, as the order of closure, n, is increased (cf. figure 3). If the Mott-Smith distribution function were nearly correct the convergence would be very rapid, where it will later be seen that the sense of "nearly correct" is not yet well determined. The type of convergence expected in this case is seen in figure 4, in which $\tilde{\xi}_{04}$ is depicted. Evidently the value of this particular moment is quite accurately predicted by the Mott-Smith distribution in this solution process, but it is the only variable found to be convergent. The typical behavior of the eigenfunction moments is seen in figures 5 and 6, which show the $\tilde{\xi}_{r\ell}$'s of orders 6 and 11 respectively, normalized to their Mott-Smith values. To summarize the properties of this behavior, all* $\tilde{\xi}_{r\ell}$'s increase in magnitude as the order of closure is increased, except for $\tilde{\xi}_{02}$ whose magnitude decreases, and $\tilde{\xi}_{03}$, which increases to order 9 and then decreases. This behavior is reflected in the physical variables $(\langle c_1^3\rangle/\langle c^2 c_1^2\rangle)_1$ $[=(-\sqrt{6}\,\tilde{\xi}_{03} + 3\xi_{11})/(5\xi_{11})]$ shown in figure 7, and $(\tau u/q)_1$ $[= 2^{3/2}\,\xi_{02}/(3\xi_{11})]$ shown in figure 8. Here $q = \frac{1}{2}\rho\langle c^2 c_1\rangle$ is the heat flux.

* based on inspection to eigenfunction order 15, and closure order 22.

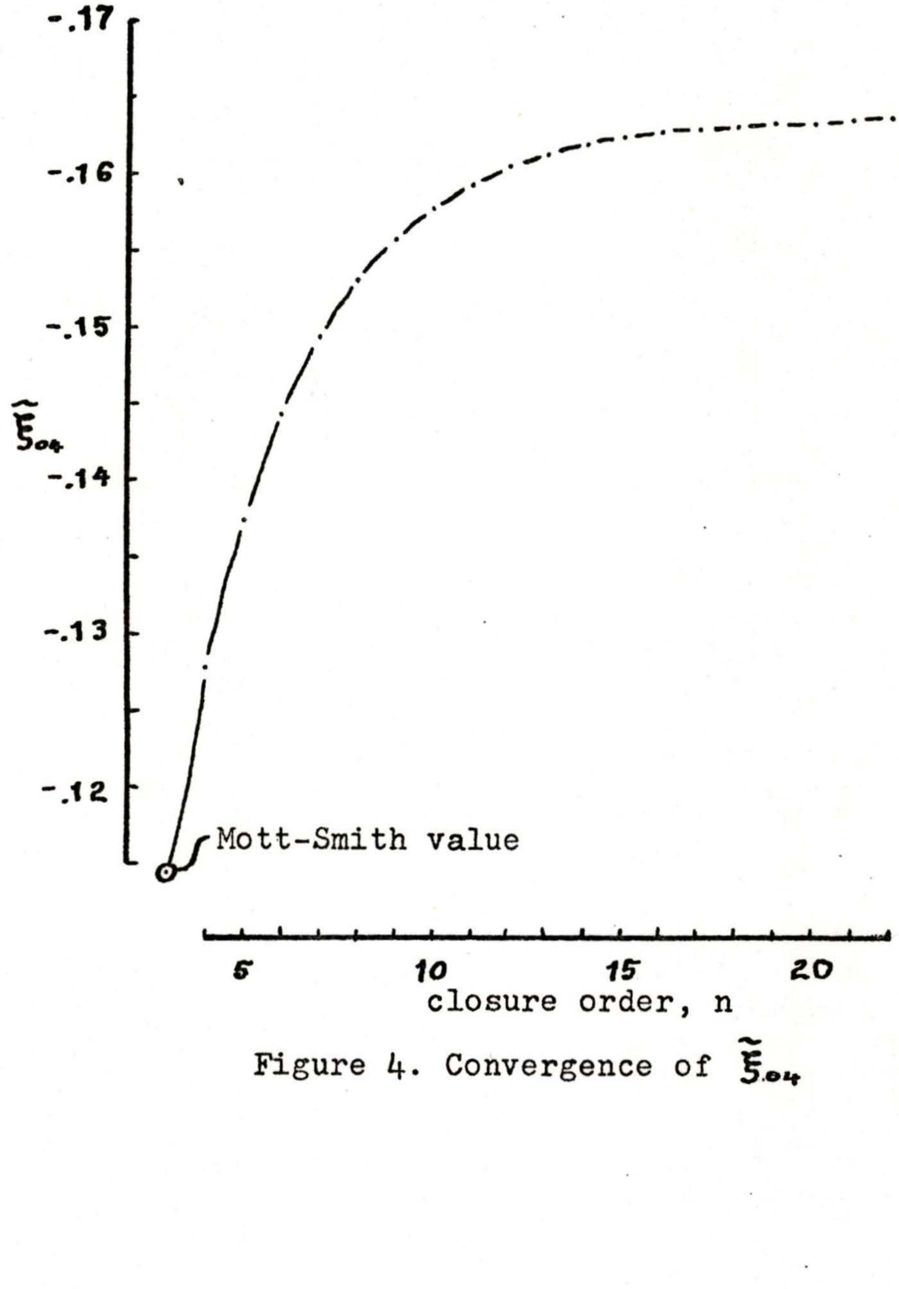


Figure 4. Convergence of $\tilde{\xi}_{04}$

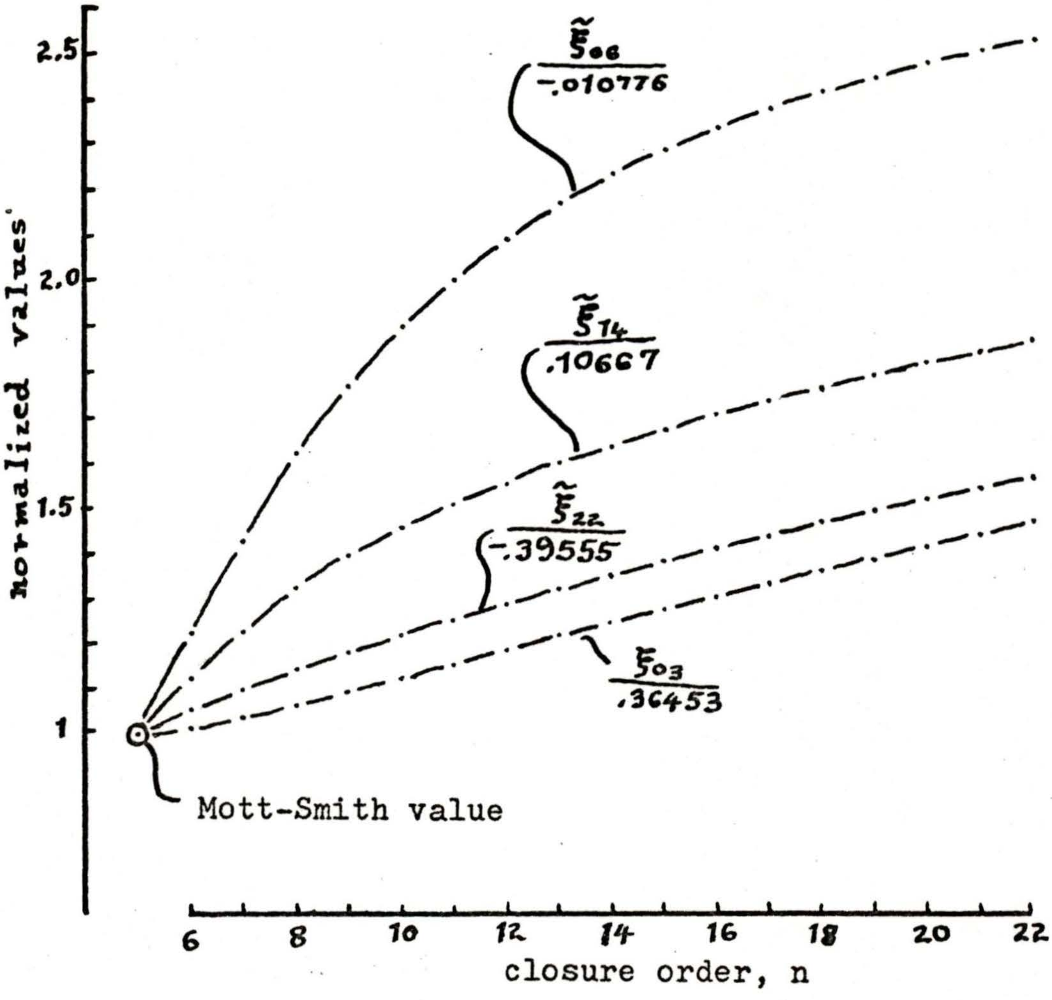


Figure 5.

Behavior of the $\tilde{\xi}_{rl}$'s of order 6.

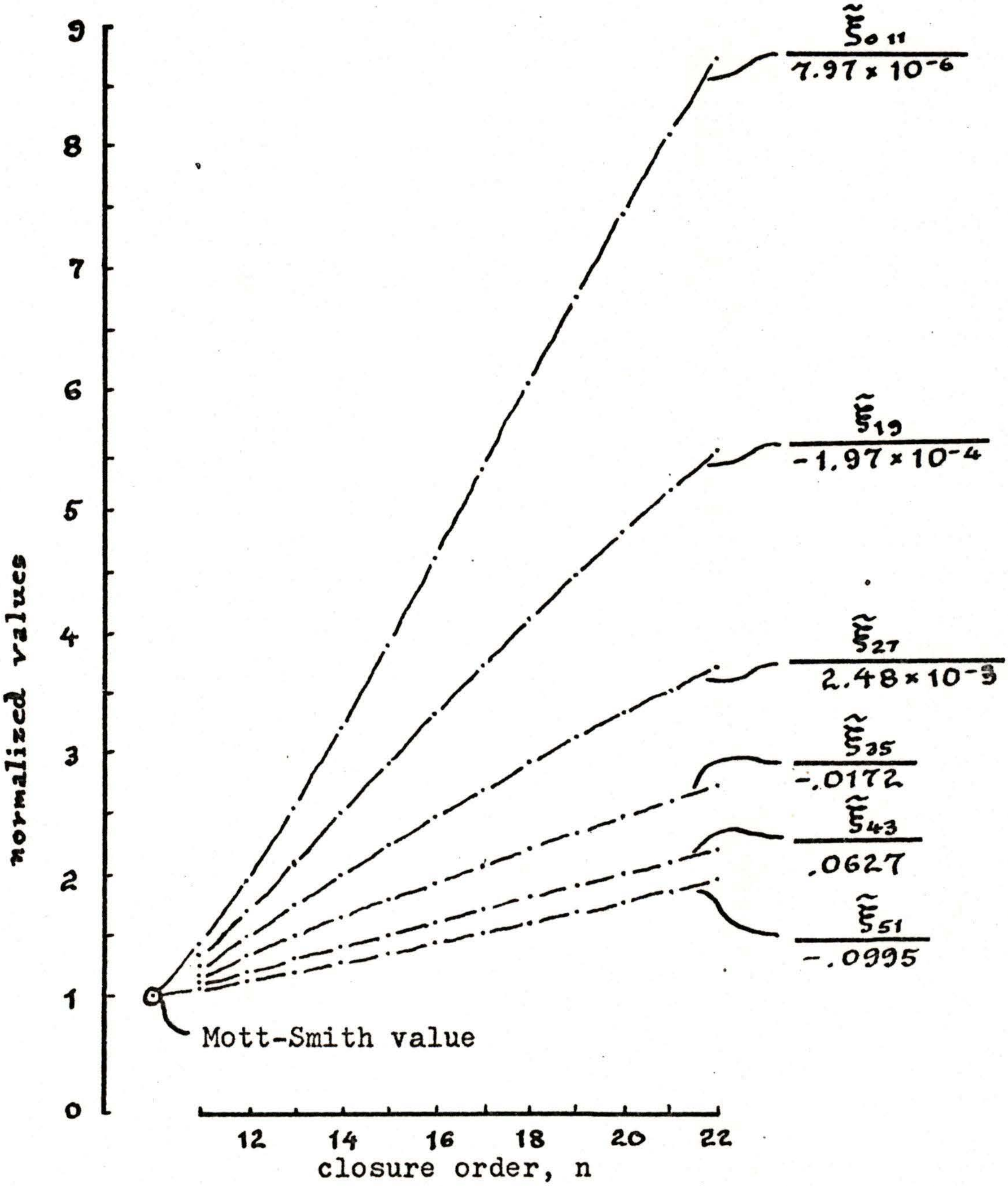


Figure 6.

Behavior of the $\tilde{\xi}_{r\ell}$'s of order 11.

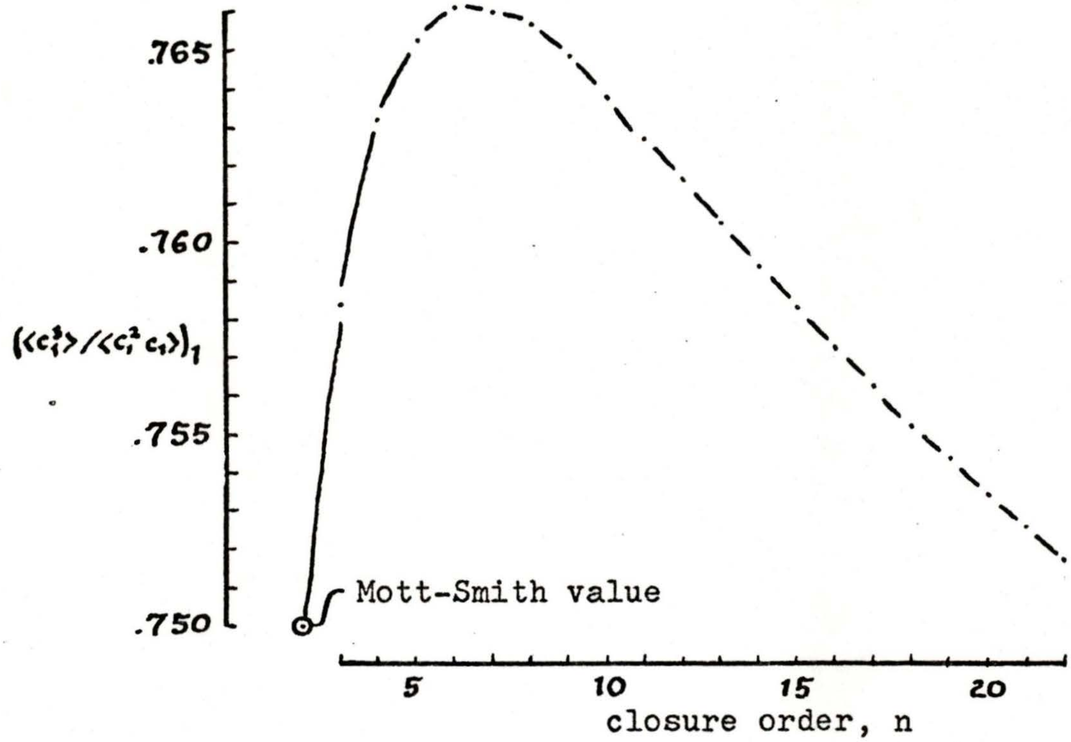


Figure 7. Behavior of $(\langle c_1^3\rangle / \langle c^2 c_1\rangle)_1$

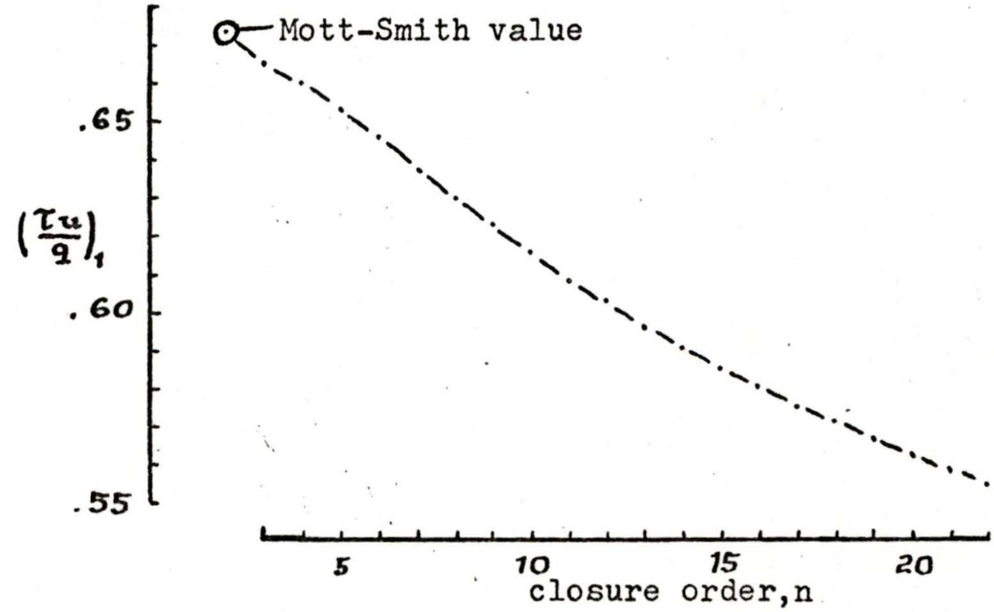


Figure 8. Behavior of $\left(\frac{\tau u}{q}\right)_1$

The similar behavior exhibited by the $\tilde{\xi}_{r\ell}$'s and the fact that they all tend to vary linearly with the order of solution closure suggests that some useful information may be extracted from an apparently divergent (or optimistically slowly convergent) solution. This line of reasoning led in turn to a computational experiment, the results of which were successful, but which, in view of the ad hoc procedure used, must be regarded as still of a preliminary nature.

Specifically, consider the variable $\tilde{\xi}_{o\ell}$ (chosen arbitrarily) as a single unknown parameter,and express the general $\tilde{\xi}_{r\ell}$ as a linear function of $\tilde{\xi}_{o\ell}$ by

(11.) $$\tilde{\xi}_{r\ell} = a_{r\ell}\,\tilde{\xi}_{o\ell} + c_{r\ell} \; .$$

Given the solution $\tilde{\xi}_{r\ell}$'s to any two consecutive orders of closure, equation 11 may be solved for each $a_{r\ell}$ and $c_{r\ell}$. Suppose that $a_{r\ell}^{(n)}$ and $c_{r\ell}^{(n)}$ are the values obtained from the solutions to closure orders n and n+1. It is found that the coefficients $a_{r\ell}^{(n)}$ and $c_{r\ell}^{(n)}$ converge quite rapidly as n is increased. Typical cases are shown in figures 9 and 10 where $a_{12}^{(n)}$ and $c_{12}^{(n)}$ are displayed.

We next make the hypothesis that the limit values of the various $a_{r\ell}^{(n)}$ and $c_{r\ell}^{(n)}$ are exact, even though they were obtained from a sequence of inexact solutions. If this be the case, then every $\tilde{\xi}_{r\ell}$ can be expressed

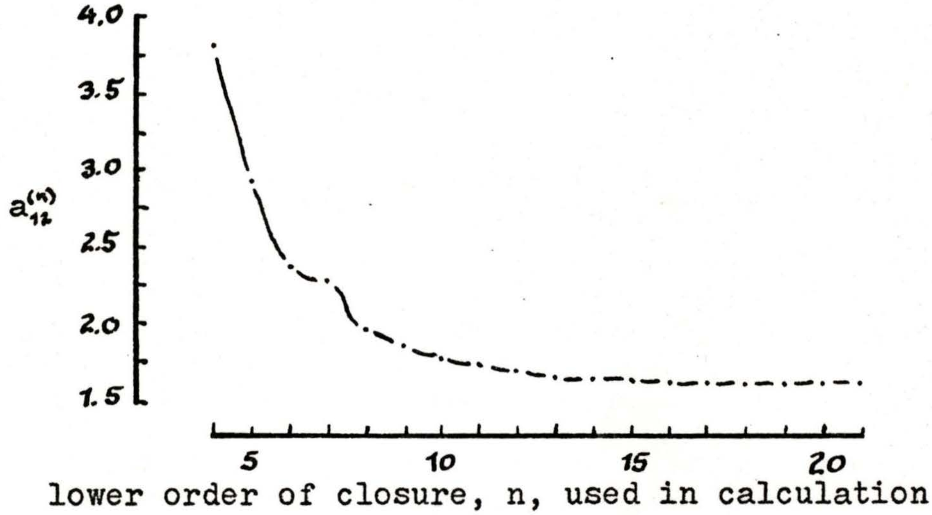


Figure 9. Convergence of $a_{12}^{(n)}$

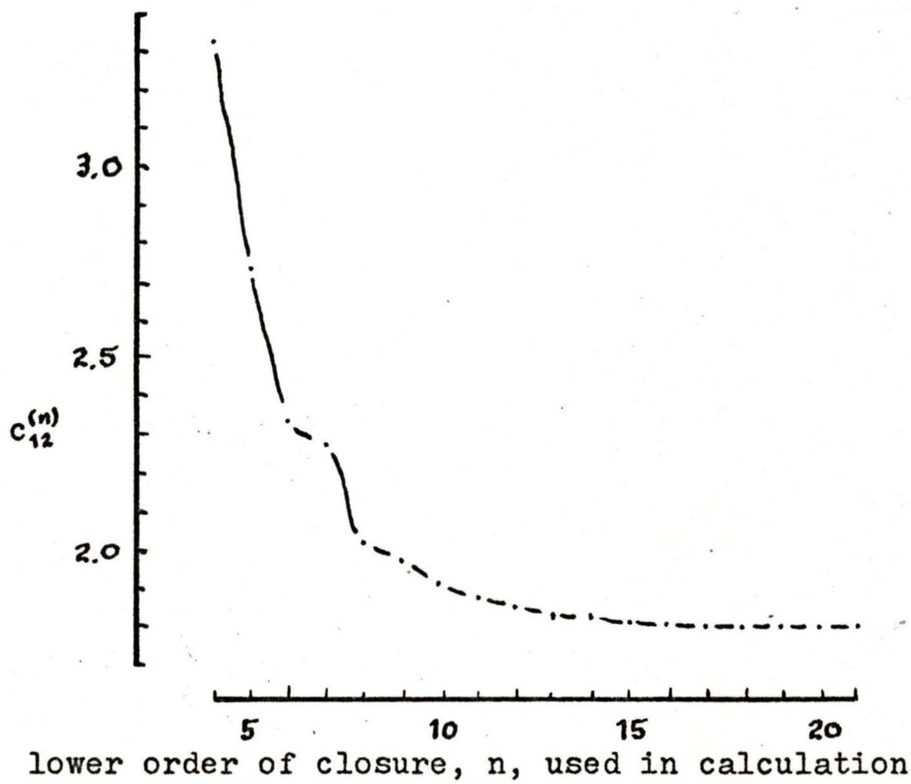


Figure 10. Convergence of $c_{12}^{(n)}$

exactly in terms of $\tilde{\xi}_{02}$ by means of equation (11). We can then return to the matrix of the fundamental equation (figure 3), pick any two equations, and solve them for $\tilde{\xi}_{02}$ and ω_1. A necessary condition for our hypothesis to be correct is that the values obtained for $\tilde{\xi}_{02}$ and ω_1 be independent of the choice of equations, and this is indeed found to be the case.

As an example, let us display values obtained from equations $r=0$, $\ell=3$, and $r=0$, $\ell=2$. A quadratic equation for ω_1 will always be obtained and its solution in this case is $\omega_1 = .843 \pm .006$, where the second term arises from a non-zero discriminant which may be expected to vanish upon insertion of more accurate $a_{r\ell}$'s and $c_{r\ell}$'s on the physical grounds that only one solution is realizable. The accuracy may be increased by increasing the order of closure (22 was the highest used in this case). In this way the limit values of the $a_{r\ell}$'s and $c_{r\ell}$'s can be determined with greater accuracy. The solution for $\tilde{\xi}_{02}$ corresponding to the above value of ω_1 is found to be $\tilde{\xi}_{02} = -.6565 \pm .0012$. Knowing $\tilde{\xi}_{02}$ and the $a_{r\ell}$'s and $c_{r\ell}$'s we may then obtain any of the $\tilde{\xi}_{r\ell}$'s, and hence the physical variables of interest. The results for low-order quantities are as follows, where for later discussion, the values computed from f_{ms} are given in parentheses.

$\left(M^{-2}\frac{u}{T}\frac{dT}{du}\right)_1$ = -.9086 (-.833)

$\left(M^{-2}\frac{u}{p}\frac{d\tau}{du}\right)_1$ = .7581 (.833)

$\left(M^{-2}\frac{1}{p}\frac{dq}{du}\right)_1$ = 1.362 (1.25)

$\left(\frac{\tau u}{q}\right)_1$ = .557 (.667) (cf. fig. 8)

$\left(\langle c_1^3\rangle/\langle c^2 c_1\rangle\right)_1$ = .752 (.75) (cf. fig. 7)

$\left(M^{-2}\,\tau/\tau^0\right)_1$ = .287

Note that $\left(M^{-2}\,\tau/\tau^0\right)_1$ is a moment of f so its value for f_{ms} is not given.

We again emphasize that the above results must be viewed as preliminary. Final justification for their use can be given only after the numerical accuracy of the entire calculation is increased, and certainly not until an adequate explanation can be given as to why the method used apparently works so well. Even with these reservations, the results are encouraging in that all the quantities listed have physically correct algebraic signs. In addition, the ratio $\left(\langle c_1^3\rangle/\langle c^2 c_1\rangle\right)_1$ satisfies the condition $0 < \left(\langle c_1^3\rangle/\langle c^2 c_1\rangle\right)_1 < 1$ proposed by Baganoff and Nathenson (1970).

An annoying question comes to mind if the above results are compared with the corresponding values based on f_{ms} which are given in parentheses. In all cases the discrepency is of the order of 10% or less. Why then does the solution based on f_{ms} converge so slowly (if at all)? It might be thought that a ten percent error evidenced by the low order moments in the first approximation for f could easily be corrected by just a few terms in the Hermite polynomial series.

Another interesting question can be raised with regard to the solution based on Grad's method: since the method fails for $M_1 \to \infty$, there must exist a critical finite value of the upstream Mach number above which the solution does not yield physically acceptable results to any order of closure. What is this value, and why does it exist? That the Grad solution to equation 7 for $M_1 \to \infty$ is unphysical is seen in that it requires a sub-diagonal form of the matrix, which in turn requires the relation $\xi_{r\ell} \propto M_1^{-2r-\ell+k}$ as $M_1 \to \infty$, with $k \geqslant 3$.

In conclusion, it is felt that once the ad hoc method used in obtaining the final results is well understood and can be rigorously justified, the first truly nonlinear exact solution to the Boltzmann equation may be proclaimed. It is ironic that this should also be the solution of a classic problem in gas dynamics for which the degree of nonequilibrium is so strong.

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APPENDIX A

FORTRAN PROGRAM WRITTEN TO GENERATE $\tilde{\xi}_{r\ell}$'S FROM THE MOTT-SMITH DISTRIBUTION FUNCTION

This program evaluates expression 10 to order 37, although the $\tilde{\xi}_{r\ell}$'s are only accurate to order 23, as discussed in chapter 4. Necessary logarithms of factorials are stored in the following array

$$F(K) = \log_e(K!) \ .$$

Similarly, for the integer-plus-one-half factorials

$$FH(K) = \log_e((K+\tfrac{1}{2})!/\sqrt{\pi}) \ .$$

Final $(\tilde{\xi}_{r\ell})_{ms}$ values are stored in the array E(I) for punching on cards. Here I is an index calculated by

$$I = \left[\tfrac{1}{4}(2r + \ell)^2\right] - r \ ,$$

where the brackets represent the largest integer less than the contained term. This is the standard ordering used in figure 2 and by many authors.

The subroutine SUM is also shown. Particulars are included at the top of the listing. Its purpose is to minimize loss of significant bits (also digits) due to the size of interim sums calculated in the adding of a column.

```
$WATFIV
C           MOTT-SMITH SHOCK END CONDITIONS ...TO BE USED FOR CLOSURE
            DOUBLE PRECISION DLOG,DEXP,L5,L2,F,FH,FA,FHA,DSQRT,T,TL,TA,TB,E,
           1 EEL,AK ,EL,R ,DABS,S,W,SL,SLH
            DIMENSION E(381),F(75),FH(38)
            DIMENSION SL(75),SLH(38)
            COMMON S(39,4),W,M,LU
            L5=DLOG(5.DO)
            L2=DLOG(2.DO)
            FA=0
            FHA=DLOG(.5DO)
            F(1)=C
            FH(1)=FHA
            DO10 K=1,37
            AK=K
            SL(K)=DLOG(AK)
            SLH(K)=DLOG(AK+.5DO)
         10 CONTINUE
            DO 15 K=38,74
             AK=K
            SL(K)=DLOG(AK)
         15 CONTINUE
            M=1
            DO17 I=1,76
            IP=I+1
            DO16 K=1,I
         16 S(K,1)=SL(K)
            LU=I
            CALL SUM
         17 F(IP)=W
            DO 19 I=1,37
            IP=I+1
            DO18 K=1,I
         18 S(K,1)=SLH(K)
            LU=I+1
            S(IP,1)=FH(1)
            CALL SUM
         19 FH(IP)=W
C
            IP=1
            L=0
            IR=0
            I=1
         20 LH=L/2
            EL=L
            IRP=IR+1
            LRP=L+IR+1
            LHP=LH+1
            R=IR
            EEL=EL+.5
            E(I)=-(-1.DO)**IR*(4.DO/3.DO)*DSQRT(EEL)
            TL=(R+EL/2.DO)*L5+(-4.DO*R-7.DO*EL/2.DO)*L2-.5DO*(F(IRP)+FH(LRP))
            T=0
            DO 250 KP=1,LHP
            K=KP-1
            AK=K
            HLMK=EL/2.0-AK
            HHLMK=HLMK/2.0
            ITLMTK=2*L-2*K+1
            KPR=K+IR+1
            LMK=L-K+1
            LMTK=L-2*K+1
            IRPHL=IR+LHP
            TA=0

            DO 200 IQP=1,IRPHL
            IQ=IQP-1
            Q=IQ -LH
            Q=Q+EL/2.0
            ITQ=Q*2.0+1.0
            TB=0
            FA=EL/2.0-AK-Q
            IAJ=DABS(FA)+1
            TN=Q+HLMK+1
            TD=-HHLMK+Q/2.0
            IND=2.0*R+EL/2.0+AK-Q+1.0
            IM=0
```

```
      DO 70  J=IAJ,IND,2
      JM=JM+1
      AJ=J-1
      NUM=AJ+TN
      IDN1=AJ/2.0+TD+1.0
      IDN2=AJ/2.0-TD+1.0
      IF(NUM*IDN1*IDN2*ITQ)  30,30,50
   30 WRITE(6,40) NUM,IDN1,IDN2,ITQ ,K,TD,Q,AJ
   40 FORMAT(   5(2X,I3),3(3X,F9.2))
   50 CONTINUE
      S(1,4)=F(NUM)
      S(2,4)=-F(IDN1)
      S(3,4)=-F(IDN2)
      S(4,4)=-F(ITQ)
      S(5,4)=-AJ*L2
      LU=5
      M=4
      CALL  SUM
      FHA=W
      IF(FHA+16.D1)  55,55,60
   55 S(JM,3)=0
      GO TO 70
   60 S(JM,3)=DEXP(FHA)
   70 CONTINUE
C
      M=3
      LU=JM
      CALL  SUM
      S(IQP,2)=3.D0**Q*W
  200 CONTINUE
      S(1,4)=F(ITLMTK)
      S(2,4)=F(KPR)
      S(3,4)=-F(KP)
      S(4,4)=-F(LMK)
      S(5,4)=-F(LMTK)
      S(6,4)=TL
      M=4
      LU=6
      CALL  SUM
      FHA=W
      LU=IRPHL
      M=2
      CALL  SUM
      S(KP,1)=(-2.D0)**K*W*DEXP(FHA)
  250 CONTINUE
      LU=LHP
      M=1
      CALL  SUM
      E(I)=E(I)*W
      IF(IP-4)  280,260,280
  260 KP=I-IP+1
      WRITE(6,270)(E(K),K=KP,I),L,IR
  270 FORMAT(4(2X,D18.11),2(3X,I3))
      WRITE(7,470)(E(K),K=KP,I)
  470 FORMAT(4(2X,D18.11))
      IF(I-16)  8100,8020,8100
 8020 IF(DABS(E(8)-.6027D0)-1.D-3)  8100,8100,8800
 8100 CONTINUE
      IP=1
      GO TO 290
  280 IP=IP+1
  290 CONTINUE
C        INDEX INCREMENT
      IF(IR) 350,350,300
  300 IR=IR-1
      L=L+2
      I=I+1
      GO TO 20
  350 IF(L-37) 370,400,400
  370 IR=(L+1)/2
      L=1+2*LH-L
      I=I+1
      GO TO 20
  400 KP=I-IP+1
      WRITE(6,270)(E(K),K=KP,I)
      WRITE(7,470)(E(K),K=KP,I)
 8800 CONTINUE
      STOP
      END
```

```
      SUBROUTINE  SUM
C     THE BEST POSSIBLE SUM ROUTINE FOR BINARY MACHINE & FLOATING POINT
C     SUM OF THE FIRST LU NUMBERS OF S(K,J) IS LEFT IN TSMAL, J SELECTS
C       WHICH COLUMN TO ADD.
C     FIRST ARRANGE IN ASSCENDING MAGNITUDE
      DOUBLE PRECISION S,TSMAL,DABS
      DOUBLE PRECISION      TMP
      COMMON S(39,4),TSMAL,J,LU
        ICF=1
      LUM=LU-1
      LUMM=LU-2
C       HANDLE THE TRIVIAL CASES=NO CHOICE OF ADDITION ORDER
      IF(LUMM) 9020,9030,9035
 9020 TSMAL=S(1,J)
      GO TO 9401
 9030 TSMAL = S(1,J)+S(2,J)
      GO TO 9401
 9035 CONTINUE
C       BACK TO WORK- ORDER TERMS BY MAGNITUDE
      DO 9100 K=1,LUM
      IS=K
      KP=K+1
      TSMAL=S(K,J)
      DO 9060 I=KP,LU
      IF(DABS(S(I,J))-DABS(TSMAL)) 9040,9060,9060
 9040 TSMAL=S(I,J)
      IS=I
 9060 CONTINUE
      S(IS,J)=S(K,J)
      S(K,J)=TSMAL
 9100 CONTINUE
C       ALTERNATE ENTRY HERE IF TERMS ARE ALREADY ASCENDING ORDERED
 9101 CONTINUE
      DO 9400 K=1,LUMM
      KP=K+1
      KPP=K+2
      IF(ICF.EQ.0) GO TO 9105
C
      JCS=-1
      DO 9900 JC=KP,LU
      IF(S(JC,J).GT.(2.D0*S(K,J))) GO TO 9910
      IF(S(JC,J)*S(K,J).GT.0.D0) GO TO 9900
      JCS=JC
 9900 CONTINUE
      ICF=0
 9910 IF(JCS.LT.0) GO TO 9105
      TMP=S(JCS,J)
      JTP=JCS-K
      IF(JTP.EQ.0) GO TO 9105
      DO 9950 JC=1,JTP
      JJC=JCS-JC
      JCP=JJC+1
 9950 S(JCP,J)=S(JJC,J)
      S(KP,J)=TMP
C
 9105 CONTINUE
      TSMAL=S(K,J)+S(KP,J)
      DO 9200 I=KPP,LU
      IM=I-1
      IF(DABS(S(I,J))-DABS(TSMAL )) 9110,9150,9150
 9110 S(IM,J)=S(I,J)
      IF(I-LU) 9200,9120,9200
 9120 S(I,J)=TSMAL
      GO TO 9200
 9150 S(IM,J)=TSMAL
      GO TO 9400
 9200 CONTINUE
 9400 CONTINUE
      TSMAL=       S(KPP,J) +S(KP,J)
 9401 CONTINUE
      RETURN
      END
```

APPENDIX B

FORTRAN PROGRAM WRITTEN TO SOLVE THE FUNDAMENTAL EQUATION SYSTEM

This program solves the upper-triangular form of equation 7 ($M_1 \rightarrow \infty$) for the unknown $\tilde{\xi}_{r\ell}$'s and $\omega_1/(1.25A_2)$ (cf. figure 3). It reads the $(\tilde{\xi}_{r\ell})_{ms}$ values needed for closure into the array E(I), where the index, I, is discussed in appendix A. The eigenvalues were taken directly from Alterman et al. (1962) and placed on two separate decks for checking purposes. In this program they are placed into the array EL(I). Terms "1" and "4" are stored in arrays T1(I) and T4(I), where I is the equation index. A Newton - Raphson method is used to determine ω_1 . The variable W(JRC) is used to store $\omega_1/(1.25A_2)$, where JRC is the order of closure. Equation r=0, ℓ=1 is to be satisfied by the Newton-Raphson method. The error in satisfying this equation is stored in DE as defined on line 74 of the listing. The final results, the unknown $\tilde{\xi}_{r\ell}$'s are stored in array EF(I), from which other variables of interest are calculated.

```
C      SOLVE FOR SHOCK END CONDITIONS UPSTREAM FOR LARGE M
      DIMENSION EF(380),IDL(379),EL(361),IF(380),E(380),T1(361),T4(361),
     1 W(39),ID(379)
      DOUBLE PRECISION EL,E,EF,BT,W,R2,ELL,R,T1,T4,WF,WN,DSORT,DABS,
     1 DF,DEF,WTR,R3,R56,C56
      READ(5,20)(ID(I),IDL(I),I=1,379)
   20 FORMAT(7(I9,I1,1X))
      C56=5.D0/6.D0
      R56=DSQRT(C56)
      R3= DSQRT(3.D0)
      TDC= 9.D0/(1.25D0*15.D0)
      IR=0
      L=0
      DO80 I=1,379
      IF(ID(I)-800000000) 60,60,40
   40 IR=(ID(I)-900000000)/1000000
      L=0
      GO TO 80
   60 J=(2*IR+L+2)*(2*IR+L+2)/4-IR
      L=L+1
      EL(J)=ID(I)
      ELL=IDL(I)
      EL(J)=-EL(J)/1.D8-ELL/1.D9
   80 CONTINUE
      R2=DSQRT(2.D0)
      JOTP=36
C      JOTP IS HIGHEST ORDER CONSIDERED . NOW READ CLOSURE TERMS
      READ(5,100) (E(J),J=1,380)
  100 FORMAT(4(2X,D18.11))
C     FIND OFF DIAGONAL ELEPHANTS
      JRR=1
      R=0
      ELL=1.D0
      I=2
  120 CONTINUE
      T4(I)=0.D0
      IF(ELL)140,160,140
  140 T4(I)=   ELL*DSQRT((R+1.D0)/((2.D0*ELL-1.D0)*(2.D0*ELL+1.D0)))
  160 T1(I)=-(ELL+1.D0)*DSQRT((R+ELL+1.5D0)/((2.D0*ELL+1.D0)*(2.D0*ELL
     1 +3.D0)))
      I=I+1
      IF(R) 180,200,180
  180 R=R-1.D0
      ELL=ELL+2.D0
      GO TO 120
  200 CONTINUE
      JRR=JRR+1
      IF(JRR-JOTP-1) 220,240,240
  220 R=JRR/2
      ELL=-2*(JRR/2)+JRR
      GO TO 120
  240 CONTINUE
      WTR=1.D-3
      W(3)=.535D0
      JRC=3
C     TO SOLVE FOR ONE COMPLETE ANSWER SET AT ORDER JRC
  250 ITOP=(JRC+3)*(JRC+3)/4
      IBOT=(JRC+2)*(JRC+2)/4+1
      ITSA=IBOT-1
      IBSA=(JRC+1)*(JRC+1)/4+1
      DO260 I=IBOT,ITOP
  260 EF(I)=E(I)*(-1.D0)**(JRC+1)
      ISF=1

C      ATTEMPT MATRIX SOLVE WITH GUESSED W
  270 JRR=JRC
      IBOT=IBSA
      ITOP=ITSA
  280 IBS=(JRR+1)/2+1
      DO 300 IT=IBOT,ITOP
      I=IT+IBS
      IM=I-1
      IF(T4(IT)) 294,287,294
  287 BT=T1(IT)*EF(I)
      GO TO 300
  294 BT=T1(IT)*EF(I)+T4(IT)*EF(IM)
  300 EF(IT)=-BT/((W(JRC)*EL(IT)-1) *R56)
      IF(JRR-2) 320,340,320
  320 JRR=JRR-1
      ITOP=IBOT-1
      IBOT=(JRR+1)*(JRR+1)/4+1
      GO TO 280
```

```
C       CLOSURE VERIFICATION (W GUESS CORRECT)
  340 DE=-R2*C56+T4(2)*EF(3)+T1(2)*EF(4)
      IF(ISF-1) 400,360,360
  360 WF=W(JRC)
      W(JRC)=W(JRC)+WTR
      DEF=DE
      ISF=0
      GO TO 270
  400 CONTINUE
      IF(DABS(DE)-1.D-11)420,440,440
  420 IF(DABS(W(JRC)-WF)-1.D-11)480,440,440
  440 WN=W(JRC)-(W(JRC)-WF)*DE/(DE-DEF)
      WF=W(JRC)
      W(JRC)=WN
      DEF=DE
      GO TO 270
C       SUCCESSFUL GUESS AT W.  COMPLETE SOLUTION FOR ORDER JRC SITS IN EF
  480 CONTINUE
      WRITE(6,500)JRC,W(JRC),(EF(J),J=3,10)
  500 FORMAT('  ORDER #',I2,' W = ',D18.11,/,4(2X,D18.11),/,4(2X,D18.11)
     1 ,/)
      EF(3)=-R2*EF(3)/R3
      EF(4)=-2.D0*EF(4)/R3
      EF(5)=-R3*EF(5)/R2
      EF(5)=5.D0*(EF(6)+EF(5))/5.D0
      EF(1)=.5D0*EF(6)/EF(5)
      EF(2)=W(JRC)*TOC*EF(4)
      WRITE(6,505)(EF(J),J=1,2)
  505 FORMAT('  S(111)/S(1) = ',E13.6,'  TAU/TAU(0) = ',E13.6,/,40X,
     1   'GRADIENTS')
      WRITE(6,506)(EF(J),J=3,6)
  506 FORMAT(             '  TEMP = ',E13.6,' TAU = ',E13.5,' Q = ',
     2  E13.6,' S(111) = ',E13.6)
      WRITE(6,508)
  508 FORMAT(1X,100('*'),/)
      IF(JRC-JOTP) 510,2000,2000
  510 JRM1=JRC
      JRM2=JRC-1
      JRM3=JRC-2
      JRC=JRC+1
      IF(JRC-5) 520,540,560
  520 W(JRC)=W(JRM1)
      GO TO 250
  540 WTR=.5D0*(W(JRM1)-W(JRM2))
      GO TO 580
  560 WTR=W(JRM1)-2.D0*W(JRM2)+W(JRM3)
  580 W(JRC)=2.D0*W(JRM1)-W(JRM2)
      IF(DABS(WTR)-1.D-8) 600,250,250
  600 WTR=2.D-8
      GO TO 250
 2000 CONTINUE
      STOP
      END
```

Sample Output

```
ORDER # 3 W =  0.464578239900 00
 0.102202245390 01  -0.720696655310 00  -0.102202245390 01   0.330522170670 00
-0.641862372080 00   0.602747450790 00  -0.114363289800 00   UUJUJJUUUUUUUUUUUU

S(111)/S(1) =  0.758433D 00   TAU/TAU(0) =  0.174015D 00
                                        GRADIENTS
TEMP = -0.834478D 00 TAU =  0.832189D 00 Q =  0.125172D 01 S(111) =  0.189869D 01
****************************************************************************************************

ORDER # 4 W =  0.502824726830 00
 0.102524273370 01  -0.718419583550 00  -0.102524273370 01   0.341789618380 00
-0.638289788930 00   0.624157254430 00  -0.127872948550 00   0.647953520350 00

S(111)/S(1) =  0.753319D 00   TAU/TAU(0) =  0.187705D 00
                                        GRADIENTS
TEMP = -0.837107D 00 TAU =  0.829559D 00 Q =  0.125566D 01 S(111) =  0.191694D 01
****************************************************************************************************

ORDER # 5 W =  0.537264077540 00
 0.103088591610 01  -0.714429251030 00  -0.103088591610 01   0.347925144980 00
-0.643688382570 00   0.639418290880 00  -0.137452832580 00   0.660928071690 00

S(111)/S(1) =  0.755341D 00   TAU/TAU(0) =  0.199448D 00
                                        GRADIENTS
TEMP = -0.841715D 00 TAU =  0.824952D 00 Q =  0.126257D 01 S(111) =  0.193260D 01
```

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