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A NON-EQUILIBRIUM KINETIC DESCRIPTION OF SHOCK WAVE STRUCTURE*

- by -

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ABSTRACT

A formulation for the shock wave structure is devised by viewing the transition as a phenomenon in which non-equilibrium effects play an important role. The essence of the method is the approximation of Boltzmann's equation by a simpler kinetic model. Initially, the distribution function in Boltzmann's collision integral is expressed in terms of a function of deviation from local equilibrium. Then, by suitably transforming the complete collision term, the molecular velocities after collision are eliminated. At this stage the formulation of the method is specialized to hard sphere molecules and the problem of deriving a model equation thus reduces to one of assigning an expression for the deviation function. In the first instance, this function is chosen to be zero and an exploratory model is obtained which, when its variable collision frequency is replaced by its mean value, reduces identically to the Bhatnagar-Gross-Krook model. However, it is found that the exploratory model provides a somewhat crude representation of Boltzmann's equation and is shown to imply a Prandtl number very nearly equal to unity. A more accurate model is then derived by choosing for the deviation function the first order term of Chapman-Enskog's sequence, leading to the Navier-Stokes equations. Here, the specific form of Boltzmann's collision term is represented more accurately than hitherto and the model is found to possess all the known features of the Boltzmann equation. It is shown that this model contains a description of a gas in non-equilibrium state.

The application of the one-dimensional form of the model to the shock problem necessitates the definition of two half-range distributions and results subsequently in a set of three integral equations for the macroscopic variables of the flow. In these equations, the collision frequency of the loss term is replaced by a set of mean frequencies each of which characterizes a specific macroscopic quantity. The mean frequencies are independent of the molecular velocity and their expressions are obtained by satisfying the conservation requirements throughout the shock. The resulting shock equations are solved numerically for an Argon gas,

employing an iteration scheme which is initiated by the use of Navier-Stokes profile with a Prandtl number value of 2/3. The numerical method follows essentially the approach of Chahine (1965), and the computations are programmed on an I.C.T. Atlas computer. One iteration only to the flow variables is performed.

For weak shocks the iteration proves to be in very close agreement with Navier-Stokes solution for a Prandtl number of 2/3. Hence, in such cases, the model equation correctly represents the Boltzmann equation, and the assumptions underlying its derivation and application appear to be justified. At higher Mach numbers, the iteration predicts a progressively larger deviation from the Navier-Stokes solution, particularly upstream, where a long precursor develops rapidly, especially in the temperature profile. In addition, the density and velocity profiles exhibit a 'kink' at Mach numbers 5 and 10. It is argued that upstream the first iteration exaggerates the corrections in the profiles. The reason for this is attributed to the large values predicted by the Navier-Stokes solution for the Chapman-Enskog expansion parameters that also enter the present formulation. The first iteration, however, generally yields smaller values for these parameters and indicates that for strong shocks further iterations are necessary. Unlike the Navier-Stokes predictions, the results also show that for high Mach numbers the total enthalpy within the shock no longer remains sensibly constant. This reflects the non-equilibrium nature of the gas and exhibits the inadequacy at high Mach numbers of the Navier-Stokes description of the viscous and heat conduction effects.

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CONTENTS

LIST OF PRINCIPAL SYMBOLS

A	Parameter in the B.G.K. model
b	Impact parameter, see Fig. 1
$\vec{C}$	Random velocity (C_x, C_y, C_z)
$\bar{C}$	Mean random speed, $\sqrt{8RT/\pi}$
C_m	Most probable speed, $\sqrt{2RT}$
$\vec{c}$	Dimensionless random velocity
c_p, c_v	Specific heat capacities
$d\vec{V}$	Element of volume in $\vec{V}$-space, $dV_x dV_y dV_z$
F	Maxwellian distribution function
f	Molecular velocity distribution function
G	Boltzmann's gain term
$\vec{g}$	Dimensionless relative velocity (g_x, g_y, g_z)
H	Boltzmann's H-function
h_o, h_1, h_2	See eq. (5.24)
j_o, j_1	See eq. (5.22)
K_o, K_1, K_2, K_4	Weighting functions, see eqs. (3.23) to (3.26)
k	Coefficient of thermal conductivity
$k_o, \ldots, k_5$	Weighting functions, see Appendix 3
L	Boltzmann's loss term
l_o, l_1, l_2	See eq. (5.18)
M	Mach number
m	Molecular mass
n	Number density
P	Mean pressure, $(P_{xx} + P_{yy} + P_{zz})/3$
Pr	Prandtl number
Q	Molecular property (such as mC_x, mC_xC_y)

R	Gas constant
$\vec{r}$	Position vector (x,y,z)
s	Molecular force law index
T	Temperature
t	Time
t_x, t_{xx}	See eq. (5.5)
$\vec{U}$	Mean gas velocity (U_x,U_y,U_z)
$\vec{u}$	Dimensionless mean gas velocity
$\vec{V}$	Molecular velocity (V_x,V_y,V_z)
$\vec{v}$	Dimensionless molecular velocity
β =	$1/2RT$
ϵ	Impact angle, see Fig. 1
$\kappa_0, \ldots, \kappa_5$	Weighting functions, see Appendix 3
Λ_1	Maxwellian mean free path ahead of shock, see eq. (5.25)
λ	Mean free path
μ	Coefficient of viscosity
ρ	Density
σ	Molecular diameter
Φ	Deviation function from Maxwellian
$\overline{\Phi K_1}, \overline{\Phi K_2}, \overline{\Phi K_4}$	See eqs. (3.21) and (3.22)
ψ	Impact angle, see Fig. 1
ψ_i	Represents a summational invariant
$\vec{\Omega}$	Relative velocity $(\Omega_x, \Omega_y, \Omega_z)$

INTRODUCTION

Since the turn of the century, the problem of the normal shock wave structure in a monatomic gas has been the subject of many investigations. However, no general and reliable solution is available at present. The salient aspect of the problem is its geometric simplicity and lack of solid boundaries, which eliminates all difficulties due to interactions between gas and surfaces. The transition across the shock, which mainly takes place over a layer of the order of a mean free path in dimension, is highly non-uniform and is accompanied by effects of viscosity and heat conduction. These features of the shock problem have made it a kind of model problem for checking the validity of formulations for flows in which the gas state deviates from thermodynamic equilibrium.

In attempting to review the past work on shock structure, one notices that there has been a marked growth of activity in the last two decades. At the same time, no investigation has yet been undertaken to systematically compare and unify the various formulations. Here, a brief review of the existing methods is presented but, in view of the previous remark, the classification used should be regarded as somewhat arbitrary. The aim, however, is to show along which lines previous theories have been evolved and to give a presentation of some known solutions for the various special cases.

Early investigations of the problem were restricted to the Navier-Stokes equations with constant coefficients of viscosity and thermal conductivity. The study of the problem began with papers by Rankine (1870) and Hugoniot (1889) who established the general conditions relating the variables of the two end states, with Rankine in addition giving a solution for the case of heat conduction only. Rayleigh (1910) demonstrated, qualitatively, that a solution is possible for the general case and calculated for a discontinuous rarefaction wave a negative entropy change. This result was confirmed and amplified by Taylor (1910), who also gave a solution valid for weak shocks with both viscosity and heat conduction present. Becker (1922), still treating the coefficients of viscosity and thermal conductivity as constants, obtained an exact explicit solution for a shock of arbitrary strength for a Prandtl number value of 3/4. The results of Becker showed that weak shocks are a few mean free paths thick, while strong shocks have a very small thickness and are almost discontinuous. Later, Thomas (1944) remarked that if the viscosity coefficient is assumed to be proportional to the square root of the temperature, i.e. the gas molecules are rigid spheres, the limiting thickness would be finite. His treatment was subsequently generalised by Morduchow and Libby (1949), who showed that a variation of the form T^s results in a limiting thickness which vanishes if $s < 1/2$ or increases beyond bounds if $s > 1/2$. In 1953 Gilbarg and Paolucci demonstrated that the Navier-Stokes equations with the viscosity variation as a power of the temperature can be solved at all Mach numbers (above unity).

The second approach for developing shock wave descriptions has been through the use of the so-called higher continuum approximations which result from expansion solutions of the Boltzmann equation. Here, Wang Chang (1948), taking into account third order terms in the Chapman-Enskog expansion, showed that for shock thickness the series obtained converged very slowly unless the Mach number is very slightly greater than unity. Zoller (1951), using the Burnett (1935, 1936) thirteen moment equations, calculated shock thickness up to 30% greater than predicted by the Navier-Stokes equations. However, for a Mach number $M_1 > 1.23$ damped oscillations appeared in the solution and no results could be obtained for $M_1 > 2.36$. Later Sherman and Talbot (1959), using the exact Burnett equations, obtained solutions in the range $1 \leq M_1 \lesssim 2.1$ and thickness closer to those given by the Navier-Stokes equations. Grad (1949) expanded the distribution function in Hermite polynomials and obtained a set of thirteen moment equations as the basic gas equations. Applying this formulation, Grad (1952) calculated shock thickness even larger than Zoller's, but failed to obtain solutions for $M_1 > 1.65$. A comparison between the experimental shock profiles, obtained by Sherman (1955) and Talbot and Sherman (1959), and the various theoretical predictions leads to the conclusion that the Navier-Stokes equations are adequate for describing weak shocks, in the range $M_1 < 2.0$. None of the higher continuum methods is found to yield any better result. Sherman and Talbot (1960) also showed that for stronger shocks the distribution function leading to the Navier-Stokes equations became negative over part of its range.

The failure of the higher continuum approximations to yield an improvement on Navier-Stokes theory suggests that a reliable theory for high Mach numbers does not lie in the direction of adding more terms or moments in these methods. In 1951 Mott-Smith initiated a new approach for the study of strong shock waves by introducing the notion of a bimodal distribution function. Viewing the shock transition as a mixing of two streams, Mott-Smith represented the distribution function as the sum of two full-range Maxwellians with only the number density as a mixing parameter. To make the analytical problem determinate, he made use of the transfer equation of either V_x^2 or V_x^3, and the thickness obtained was substantially greater than that of the Navier-Stokes theory. Since for weak shocks the Navier-Stokes treatment is valid, it is concluded that the Mott-Smith theory is wrong in this limit. Further, this theory always yields a symmetric density profile, and has been criticized for its somewhat arbitrary nature and unsuitability for fitting into a general approximation scheme. Recently, however, Radin and Mintzer (1966) used Mott-Smith bimodal distribution as the weight function in a generalized orthogonal polynomial solution of the Boltzmann equation. They predicted the same shock thickness as that obtained by Mott-Smith by transporting V_x^2, but with the restriction to Mach numbers above 2.14. In Mott-Smith's treatment shock thickness calculations were made for the rigid sphere and Sutherland molecular models. Muckenfuss (1960) extended the calculation to molecules with an arbitrary inverse-power intermolecular force. Later, Glansdorff (1961) and Ziering et al (1961) modified and improved the Mott-Smith treatment. They obtained a better agreement with the weak shock solutions of Navier-Stokes equations, while for strong shocks the results remained in agreement with those of Mott-Smith. Nevertheless, from a theoretical point of view, the method of Mott-Smith and its variants still lacks rigorous justification and its relation to the Boltzmann equation has not been duly demonstrated.

Recently, some important results in the kinetic theory of shock wave structure have been obtained through the application of a model of the Boltzmann equation proposed by Bhatnagar et al (1954). Liepmann et al (1962, 1964) conducted on the basis of this model a revealing study of the problem and subsequently Anderson (1965a) and Chahine and Narasimha (1965) obtained exact numerical solutions for Mach numbers up to 10 and in Argon. Liepmann et al showed that the total enthalpy within the shock remained constant to within a few per cent, and demonstrated that for strong shocks the Navier-Stokes description ceased to apply in a region (notably extending upstream) of the transition layer. The numerical solutions were found to reproduce the Navier-Stokes profiles for weak shocks but progressively departed from them, particularly upstream, as the Mach number increased. The result of this was thicker and more unsymmetrical profiles, in particular the temperature profile, and the development of a long precursor upstream. The computed distribution function within the shock layer proved to be bimodal and the shock thickness obtained was 25% larger than the Navier-Stokes value at a Mach number of 10.

Experimental measurements in strong shocks are so far only available for density profiles. The recent measurements by Camac (1965) and Russell (1965) indicate that for maximum density slope thickness the experimental data roughly fall between the results of the model, Pr=1, and Mott-Smith results, Pr=2/3. The agreement with the predictions of the Mott-Smith theory is somewhat better, but then the Prandtl number implied in the model equation is the wrong one and the comparison depends on the criterion used. This indicates that the merit of a theoretical treatment is best judged by the profiles of the flow quantities it yields.

In the present investigation a systematic formulation is proposed for describing the shock structure, based on an approximation of Boltzmann's equation by simpler relationships. It is argued that, in general, non-equilibrium effects play an important role in this phenomenon. Consequently, this investigation is first directed towards obtaining an appropriate description of a gas in non-equilibrium state. To this end, the distribution function in Boltzmann's collision integral is represented in terms of a deviation function about a local Maxwellian, and a model equation is then derived by prescribing an expression for the deviation function. It turns out that the model advanced by Bhatnagar et al is contained in the present formulation as a special case. The model obtained is finally applied to the shock problem and profiles of the macroscopic quantities are computed for specific cases.

To make this study self-contained, the salient aspects of the kinetic theory required for the development of the non-equilibrium description are presented in Chapters 1 and 2. In Chapter 3 the Boltzmann equation is transformed and suitably expressed for the approximation of its collision term, and in Chapter 4 the model equation is derived and investigated. Then, in Chapter 5, the new kinetic description is applied to the shock problem resulting in a set of integral equations for the macroscopic variables. The numerical method used for evaluating the integral equations is given in Chapter 6, followed by the results and concluding remarks in Chapter 7.

1. BASIC EQUATIONS OF KINETIC THEORY OF GASES

This chapter is devoted to the presentation of the basic concepts and equations of the kinetic theory. Apart from introducing our notation, the aim is to provide the necessary foundations for the subsequent study without, however, dwelling on details or intricate aspects of principles since these are dealt with at length in the special works. In particular, we shall discuss, in sufficient detail, the Boltzmann equation, its equilibrium solution and Maxwell's transfer equation, and conclude the chapter with an analysis of molecular encounters. The presentation, and in fact the entire present work, is confined to a homogeneous and monatomic gas, having translational energy only.

1.1 Molecular Velocity Distribution Function

We consider a medium of 'gas' as being made up of a large number of molecules, and represent by n the number of these in unit volume, and by $\vec{V},(V_x,V_y,V_z)$, the velocity of a molecule relative to some fixed axes. We introduce the physical element of volume $d\vec{r}$(=dxdydz) selected in such a way that its dimensions are very small compared with those over which variations of the physical parameters of the gas are significant, yet large enough to contain a great number of molecules so that the mean values of certain quantities in this element make sense.

The determination of the gas properties from the motion of its molecules requires not only the knowledge of their number density in the element of volume but, more specifically, the number of molecules which have velocities within a given range. For this purpose, a so-called velocity distribution function, $f(\vec{V},\vec{r},t)$, is defined which expresses the probable number density of molecules which, at time t, are situated in the volume element $d\vec{r}$ enclosing the point $\vec{r}$, and have velocities lying in the range $d\vec{V}$ around $\vec{V}$ (that is, between V_x and $V_x + dV_x$, V_y and $V_y + dV_y$ and V_z and $V_z + dV_z$). The definition of the velocity distribution function involves probability concepts, and any result in which it appears will be a result as to the probable, or average, behaviour of the gas.

The element $fd\vec{r}d\vec{V}$ represents the total number of molecules included in an element of volume $d\vec{r}d\vec{V}$ in phase space. The function f is positive and from its definition it must satisfy

$$n(\vec{r},t) = \int f(\vec{V},\vec{r},t)\, d\vec{V}, \qquad (1.1)$$

the integration being carried over the whole (three dimensional) velocity space. Further integration w.r.t. $d\vec{r}$ over the whole volume would yield the total number of molecules in the container.

In (1858-1859) Maxwell introduced the concept of the molecular velocity distribution function and discovered the law it obeys in a uniform gas in equilibrium; later he derived the equation of transfer of a molecular property. Boltzmann, in (1872), gave his famous integro-differential equation which f must satisfy, and derived Maxwell's results directly from it. Hilbert's application (1910) of the theory of integral equations to the kinetic theory enabled Chapman and Enskog in (1917) to derive solutions for the distribution function of non-uniform gases. The methods and results of Chapman and Enskog will be summarised in Chapter 2 and will subsequently serve as a basis for our description of a gas in non-equilibrium state.

1.2 The Boltzmann Equation

The velocity distribution function satisfies an integro-differential equation, named after Boltzmann, which occupies a focal position in the kinetic theory since it can serve to determine this function. Here, we derive this equation and outline its underlying assumptions.

We call 'molecules of class A' these which, at time t, are situated in the volume element $d\vec{r}$ and have velocities lying in the range $d\vec{V}$ around $\vec{V}$. Similarly, define as molecules of class B those which have velocity $\vec{V}_1$ in the range $d\vec{V}_1$. We require the change, in time dt, of the number of molecules of class A, in the volume element $d\vec{r}$, relative to some axes. This change is due to:

1. increase in f during dt, due to its dependence on time
2. molecular flux through the sides of the volume element $d\vec{r}$
3. acceleration of molecules in presence of an external force field which alters their velocity in time dt, in between encounters
4. molecular encounters resulting in changes in velocities.

The first three contributions may be accounted for by noting that $\vec{V}$ is the velocity of the coordinates $\vec{r}$ of a molecule, and $\vec{X}$, the external force per unit mass, is the velocity of $\vec{V}$ since $\vec{X} = d\vec{V}/dt$. If we introduce coordinate axes moving with the molecules A, we have in such axes

$$\frac{df}{dt} = (\frac{\partial}{\partial t} + \vec{V}.\frac{\partial}{\partial \vec{r}} + \vec{X}.\frac{\partial}{\partial \vec{V}})f, \tag{1.2}$$

which is a generalised Euler derivation. This rate of change is balanced by the change Δf due to molecular encounters; hence

$$\frac{df}{dt} = \Delta f, \tag{1.3}$$

and there remains to express Δf explicitly.

Consider an encounter between an A type molecule with velocity $\vec{V}$ and a B type molecule with velocity $\vec{V}_1$ and let their initial relative velocity be $\vec{\Omega}=\vec{V}_1-\vec{V}$. We fix the coordinate axes on the centre O of molecule A and pass through it a plane P perpendicular to $\vec{\Omega}$ (see Fig. 1); the projection of $\vec{\Omega}$ on plane P determines a point with polar coordinates (b,ϵ). The relative velocity $\vec{\Omega}$ is then a function of $\vec{V}$ and $\vec{V}_1$ and its position depends on b and ϵ. The number of molecules per unit volume such as B is $f(\vec{V}_1)d\vec{V}_1$ of which during time dt only the fraction

$$f(\vec{V}_1)d\vec{V}_1\ \Omega\ dt\ bdb\ d\epsilon$$

can pass through the element $bdbd\epsilon$. This, then, is also the probability that our single molecule of class A shall experience an encounter within the interval of time dt and lose its velocity. Since each unit volume contains $f(\vec{V})d\vec{V}$ molecules of class A, the total number of molecules of this class lost due to molecular encounters in the element $d\vec{r}$ in the time dt is

$$\int_{\vec{V}_1}\int_{b}\int_{\epsilon} f d\vec{V}\ d\vec{r}\ dt\ f_1\ d\vec{V}_1\ \Omega\ bdbd\epsilon$$

where, for brevity, f is used for $f(\vec{V})$, etc. In this expression the integrations extend over all possible values of the variables leading to an actual encounter, with an appreciable change in the molecular velocity.

After the encounter the molecule with velocity $\vec{V}$ takes the velocity $\vec{V}'$ (function of $\vec{V}$, $\vec{V}_1$, b and ϵ) and similarly the velocity $\vec{V}_1$ becomes $\vec{V}_1'$. Let us now consider an inverse encounter with initial velocities $\vec{V}'$ and $\vec{V}_1'$ and the same values of b and ϵ taken in a plane perpendicular to the new relative velocity $\vec{\Omega}'$. In such an encounter the final velocities will be $\vec{V}$ and $\vec{V}_1$ and there will be a gain in the number of molecules of class A. The gain in class A molecules due to such a cause is

$$\int_{\vec{V}_1'}\int_{b}\int_{\epsilon} f'\, d\vec{V}'\, d\vec{r}\, dt\, f_1'\, d\vec{V}_1'\, \Omega'\, b\,db\,d\epsilon,$$

where, again, f' for example signifies $f(\vec{V}')$. It will be shown later that for perfectly elastic encounters with complete conservation of energy and momentum, $\Omega=\Omega'$. In addition, it can be shown that the Jacobian relating the sixfold elements $d\vec{V}\, d\vec{V}_1$ and $d\vec{V}'\, d\vec{V}_1'$ is equal to unity, i.e. $d\vec{V}'\, d\vec{V}_1' = d\vec{V}\, d\vec{V}_1$.

Using these results to simplify the gain term and finally taking the difference between the gain and loss terms, the change Δf is determined and the complete Boltzmann equation takes the form

$$\left(\frac{\partial}{\partial t} + \vec{V}.\frac{\partial}{\partial \vec{r}} + \vec{X}.\frac{\partial}{\partial \vec{V}}\right)f = \int (f'f_1' - ff_1)\Omega b\,db\,d\epsilon\; d\vec{V}_1 . \qquad (1.4)$$

An analysis of the derivation of the Boltzmann equation shows that the following assumptions are used:

i) Small range of intermolecular forces-Molecules are assumed to be influenced by forces of interaction only along a small portion of their paths.

ii) Binary encounters.

iii) Slowly varying f - The variation of f within the boundaries of the element $d\vec{r}$ is assumed to be infinitesimal and f remains constant over a distance comparable to the size of the molecule.

iv) Molecular chaos - This means that the history of a molecule prior to an encounter is completely ignored and that there is no correlation between two encountering molecules before they enter each other's field.

1.3 Equilibrium State

Consider a simple uniform gas, with no external forces acting upon it, for which f depends on t alone; and define a function the variation of which will indicate the trend of the state of the gas as time progresses.

If the state of the gas is changing, then at the end of an interval of time dt the fractional change in the number of a certain class of molecules in $d\vec{r}$ is $\delta f/f$, or $\delta(\log f)$. That is, the variation in logf is a measure of the contribution of this class of molecules to the general change of state. The mean of logf is represented by an H-function

$$H = \int f \log f \, d\vec{V}, \qquad (1.5)$$

whose variation, dH/dt, indicates the trend of the state of the gas. Using Boltzmann's equation, (1.4), it can be shown that

$$\frac{dH}{dt} = \int \log(ff_1/f'f_1') \, (f'f_1' - ff_1) \, \Omega \, b db d\epsilon \, d\vec{V} \, d\vec{V}_1. \qquad (1.6)$$

Since $\log(ff_1/f'f_1')$ is always opposite in sign to $(f'f_1'-ff_1)$, it follows

$$\frac{dH}{dt} \leqslant 0 \qquad (1.7)$$

and H can never increase. This is known as Boltzmann's H-theorem.

Chapman and Cowling (p.70) show that H cannot decrease indefinitely, it must then tend to a limit corresponding to a state of the gas in which $dH/dt=0$, and $f=F$. This, in fact, is the necessary and sufficient condition for equilibrium. By (1.6), it entails $F'F_1' = FF_1$ for all values of $\vec{V}$, $\vec{V}_1$; or

$$\log F' + \log F_1' = \log F + \log F_1, \qquad (1.8)$$

and from Boltzmann's equation $dF/dt = 0$. Thus, the state of the gas is steady as well as uniform, the gain and loss terms are equal and molecular encounters no longer affect the distribution function.

If a function $\Phi(\vec{V})$ is such that $\Phi+\Phi_1 = \Phi'+\Phi_1'$ for an encounter, then clearly it is a solution of (1.8). For two encountering molecules of same mass the initial and final velocities are related by the conservation requirements of momentum and energy

$$\vec{V} + \vec{V}_1 = \vec{V}' + \vec{V}_1'; \quad V^2 + V_1^2 = V'^2 + V_1'^2. \qquad (1.9)$$

With $\vec{V}$ and $\vec{V}_1$ being given, these four equations, together with the additional parameters b and ϵ specifying the orientation of an encounter, are all that is necessary to determine the six components of the molecular velocities after the encounter. It follows that the general solution for logF can only be of the form

$$\log F = \alpha_o + \vec{\alpha}.\vec{V} + \alpha_4 V^2, \qquad (1.10)$$

involving five constants. The function logF is called a summational invariant. The equilibrium distribution function may also be written in the form

$$F = A \exp\{-\beta(\vec{V}-\vec{U})^2\} \qquad (1.11)$$

where A, β, U_x, U_y, U_z are five new constants. By satisfying eq. (1.1), we find $A = n\,(\beta/\pi)^{3/2}$. The quantity $\vec{V}fd\vec{V}$ is the sum of all the velocities of class A molecules in $d\vec{r}$. Integrating over all possible classes in $d\vec{r}$, and dividing by the total number density, the mean velocity is obtained. For F we have

$$(1/n)\int_{-\infty}^{+\infty} \vec{V}F\, d\vec{V} = (1/n)\int_{-\infty}^{+\infty} (\vec{V}-\vec{U})F d\vec{V} + (1/n)\int_{-\infty}^{+\infty} \vec{U}F\, d\vec{V} = \vec{U} \qquad (1.12)$$

since the term involving $(\vec{V}-\vec{U})$ vanishes. The velocity $\vec{U}$ is then the mean velocity, and can be related to $\vec{V}$ by the introduction of the peculiar or random velocity

$$\vec{C} = \vec{V} - \vec{U}. \qquad (1.13)$$

Clearly, the mean value of the random velocity, that is each component, is zero. By similar reasoning, the quantity β may be determined from a calculation of the mean value of C^2 for the equilibrium state; we find $\overline{C^2} = 3/2\beta$. But $\overline{C^2}/2$ is the mean kinetic energy per unit mass of molecule measured with respect to the mean velocity $\vec{U}$ and is therefore used to define a temperature T by

$$RT = \overline{C^2}/3; \qquad \beta = (2RT)^{-1}, \qquad (1.14)$$

where R is the gas constant per unit mass. The equilibrium distribution F becomes

$$F = n(1/2\pi RT)^{3/2}\exp(-C^2/2RT) \qquad (1.15)$$

which is known as the Maxwellian distribution function.

When the distribution is Maxwellian, the peculiar velocity is characterized by certain mean values which are readily found. In particular, we shall make use of the quantities

$$\bar{C} = \sqrt{8RT/\pi}, \quad C_m = \sqrt{2RT}, \qquad (1.16)$$

which represent, respectively, the mean random speed and the most probable speed, possessed by the greatest number of molecules.

A concept of fundamental importance in the kinetic theory is that of the mean free path, λ, which can be defined as the average distance that a molecule travels between successive collisions. If the molecules constituting the gas are assumed to be rigid elastic spheres of diameter σ, the so-called differential collision cross section $b\,db\,d\epsilon$ is equal to $\sigma^2 \sin\psi \cos\psi\, d\epsilon$. On the assumption of a Maxwellian distribution, the calculation of the mean free path proceeds by determining the total distance travelled by the molecules in the volume element $d\vec{r}$ during dt - which is $n d\vec{r}\, \bar{C}\, dt$ - and the corresponding total number of collisions

$$(1/2)\,\{\int FF_1\, \Omega\, d\vec{V}_1\, d\vec{V} \sin\psi \cos\psi\, d\psi\, d\epsilon\} d\vec{r}\, dt,$$

which is simply half the total number of free paths. The Maxwellian mean free path is found to be

$$\lambda = 1/\sqrt{2}\,\pi\, n\, \sigma^2. \tag{1.17}$$

1.4 Maxwell's Transfer Equation and General Equations of Motion

Consider the integral

$$\Delta Q = \int Q(\vec{V})\,(f'f_1'-ff_1)\Omega\, b\,db\,d\epsilon\; d\vec{V}_1\; d\vec{V}, \tag{1.18}$$

obtained by multiplying the Boltzmann collision term by a function of velocity $Q(\vec{V})$ and then integrating. The quantity ΔQ is independent of the molecular velocities. It can be shown, by interchanges of the role of the molecular velocities, that the following symmetry relations result for ΔQ:

$$\begin{aligned}\Delta Q &= (1/4)\int (Q + Q_1 - Q' - Q_1')(f'f_1'-ff_1)\Omega\; b\,db\,d\epsilon\; d\vec{V}_1\; d\vec{V}\\ &= (1/2)\int (Q' + Q_1' - Q - Q_1)\; ff_1\Omega\; b\,db\,d\epsilon\; d\vec{V}_1\; d\vec{V}\\ &= \int (Q' - Q)\; ff_1\Omega\; b\,db\,d\epsilon\; d\vec{V}_1\; d\vec{V}.\end{aligned} \tag{1.19}$$

Consider the problem of transfer of a quantity Q which, as above, depends solely on the velocity of a molecule, as for instance V_x^2, V_xV_y. At a point $\vec{r}$ and time t, Q has the mean value

$$\bar{Q} = (1/n)\int Qf\; d\vec{V}. \tag{1.20}$$

If the Boltzmann equation is multiplied by $Q(\vec{V})$ and integrated, on the assumption of no external forces, the following expression, known as Maxwell's transfer equation, results:

$$\frac{\partial}{\partial t}(n\bar{Q}) + \frac{\partial}{\partial x}(n\overline{V_xQ}) + \frac{\partial}{\partial y}(n\overline{V_yQ}) + \frac{\partial}{\partial z}(n\overline{V_zQ}) = \Delta Q, \tag{1.21}$$

where ΔQ is given by eq. (1.19). The change ΔQ vanishes when Q represents a summational invariant since in this case $Q+Q_1=Q'+Q_1'$. Hence, by putting successively $Q=1,\vec{V},V^2$, eq. (1.21) yields the conservation equations of mass, momentum and energy. Expressed concisely in Chapman and Cowling's notation, these equations read:

Mass: $$\frac{Dn}{Dt} + n\frac{\partial}{\partial\vec{r}}\cdot\vec{U} = 0, \tag{1.22}$$

Momentum: $$n\frac{D\vec{U}}{Dt} = -\frac{\partial}{\partial\vec{r}}\cdot(n\overline{\vec{C}\vec{C}}), \tag{1.23}$$

Energy: $$n\frac{D\overline{C^2}}{Dt} = -2n\left(\overline{\vec{C}\vec{C}} : \frac{\partial\vec{U}}{\partial\vec{r}}\right) - \frac{\partial}{\partial\vec{r}}\cdot(n\overline{\vec{C}C^2}), \tag{1.24}$$

where D/Dt is a mobile operator given by

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{U}.\frac{\partial}{\partial \vec{r}}. \qquad (1.25)$$

Equations (1.22, 23, 24) are the fundamental kinetic relations governing the flow of a gas; they exhibit the dependence of its state on the mean values of the peculiar velocity and are true for any molecular model satisfying the assumptions of the theory.

The kinetic equations of motion can be identified with the hydrodynamic equations by relating the kinetic variables with the basic thermodynamic quantities - density, pressure and temperature. From the usual definition of density, we have $\rho = n\,m$, where m is the mass of molecule. Further, we have obtained the equation (1.23) of momentum transfer in the form

$$n\frac{DU_x}{Dt} = -\frac{\partial}{\partial x}(n\,\overline{C_x^2}) - \frac{\partial}{\partial y}(n\,\overline{C_xC_y}) - \frac{\partial}{\partial z}(n\,\overline{C_xC_z}), \qquad (1.26)$$

etc. In hydrodynamics the equations of motion, in the absence of external forces, are given by

$$\rho\frac{DU_x}{Dt} = -\frac{\partial}{\partial x}(P_{xx}) - \frac{\partial}{\partial y}(P_{xy}) - \frac{\partial}{\partial z}(P_{xz});\ P_{xy} = P_{yx}, \qquad (1.27)$$

etc., where P_{xx}, P_{xy}, P_{xz}, ..., are the stress components exerted at $\vec{r}$,t upon the gas. Comparison of equations (1.26) with (1.27) suggests that the expressions $\rho\overline{C_x^2}$, $\rho\overline{C_xC_y}$, $\rho\overline{C_xC_z}$, ..., are equivalent to P_{xx}, P_{xy}, P_{xz}, ..., and that the conditions in (1.27) are automatically satisfied. Accordingly, the hydrostatic pressure P, defined as the mean of the three normal pressures, is $\rho\overline{C^2}/3$. Combining this with (1.14) the kinetic theory yields

$$P = \rho RT, \qquad (1.28)$$

which is the equation of state of a perfect gas. Finally, the definition of the kinetic temperature is consistent with the thermodynamic one and the kinetic temperature is the same as the absolute temperature of thermodynamics.

The kinetic definitions of the hydrostatic pressure and temperature are applicable whether the state of the gas is in equilibrium or not. This is equally true in hydrodynamics, except that the Stokes' hypothesis is implied in the definition of the pressure. For future analysis, it is relevant for us to examine how this hypothesis is introduced in the equations of hydrodynamics.

In a gas at rest the pressure at a point is constant irrespective of orientation, and the normal stresses are equal

$$P_{xx} = P_{yy} = P_{zz} = P, \quad P_{xy} = P_{xz} = P_{yz} = 0. \qquad (1.29)$$

If, on the other hand, the gas is in motion so that one layer moves relative to an adjacent layer, shear stresses occur and the pressure intensity is, in general, no longer the same in all directions at a point. The pressure system then depends on the viscosity of the gas and on the mean velocity gradients. For a small departure from equilibrium, and using the methods of the theory of elasticity, the following expressions for the stresses can be derived:

$$\begin{aligned} P_{xx} &= P + \tfrac{2}{3}\mu \frac{\partial}{\partial \vec{r}}.\vec{U} - 2\mu\frac{\partial U_x}{\partial x}; \quad P_{xy} = -\mu\left(\frac{\partial U_y}{\partial x} + \frac{\partial U_x}{\partial y}\right) = P_{yx}, \\ P_{yy} &= P + \tfrac{2}{3}\mu \frac{\partial}{\partial \vec{r}}.\vec{U} - 2\mu\frac{\partial U_y}{\partial y}; \quad P_{yz} = -\mu\left(\frac{\partial U_z}{\partial y} + \frac{\partial U_y}{\partial z}\right) = P_{zy}, \qquad (1.30) \\ P_{zz} &= P + \tfrac{2}{3}\mu \frac{\partial}{\partial \vec{r}}.\vec{U} - 2\mu\frac{\partial U_z}{\partial z}; \quad P_{zx} = -\mu\left(\frac{\partial U_x}{\partial z} + \frac{\partial U_z}{\partial x}\right) = P_{xz}, \end{aligned}$$

where μ is the coefficient of viscosity and P is introduced through

$$\frac{P_{xx} + P_{yy} + P_{zz}}{3} = p - \left(\frac{3\mu' + 2\mu}{3}\right)\frac{\partial}{\partial \vec{r}}.\vec{U} = P. \qquad (1.31)$$

In this formula μ' is termed the second coefficient of viscosity and p, the non-viscous hydrostatic pressure, is independent of the velocity gradients. Then, to assume that $P = p$, is to assume that

$$3\mu' + 2\mu = 0, \qquad (1.32)$$

that is, the gas is Stokesian and $(P_{xx} + P_{yy} + P_{zz})/3$ is the hydrostatic pressure of a gas whether it is (so-called) perfect or real.

Before this section is concluded, we investigate the transfer equations corresponding to a Maxwellian distribution function. Using eqs. (1.20) and (1.15) we find

$$\overline{C_x^2} = \overline{C_y^2} = \overline{C_z^2} = \overline{C^2}/3, \qquad (1.33)$$

$$\overline{C_xC_y} = \overline{C_xC_z} = \overline{C_yC_z} = \overline{C_x^3} = \overline{C_xC_y^2} = \overline{C_xC_z^2} = \ldots = 0. \qquad (1.34)$$

By substituting these results in the conservation equations of mass, momentum and energy and then integrating we find that the flow of the gas is isentropic. It must be emphasized, however, that this solution corresponds to a quasi-Maxwellian distribution and not to a real continuous solution of the Boltzmann equation.

Likewise, as an example of the use of the transfer equation itself we calculate the transfer of V_x^2 and V_xV^2, denoted respectively by ΔV_x^2 and ΔV_xV^2, corresponding to a Maxwellian distribution. Using eq. (1.21) and applying the conservation equations we determine

$$\Delta V_x^2 = n\frac{\overline{C^2}}{3}\{2\frac{\partial U_x}{\partial x} - \frac{2}{3}\frac{\partial}{\partial\vec{r}}.\vec{U}\} \tag{1.35}$$

$$\Delta V_xV^2 = 2\frac{\overline{C^2}}{3}n\left[U_x(2\frac{\partial U_x}{\partial x} - \frac{2}{3}\frac{\partial}{\partial\vec{r}}.\vec{U}) + U_y(\frac{\partial U_y}{\partial x} + \frac{\partial U_x}{\partial y}) + U_z(\frac{\partial U_z}{\partial x} + \frac{\partial U_x}{\partial z}) + \frac{5}{6}\frac{\partial\overline{C^2}}{\partial x}\right]. \tag{1.36}$$

These expressions will be referred to in Chapter 2.

1.5 Dynamics of a Binary Encounter

In this section we consider the collision term of the Boltzmann equation (1.4) and aim at expressing it explicitly. For this purpose, the velocities before and after a molecular encounter must be related. The equations of a binary encounter, introduced earlier by eq. (1.9), are governed by the conservation of momentum and energy, and are independent of the specific inter-molecular forces. In order to make this system of equations complete, two additional parameters, such as b and ϵ, are required. Since the positions of the relative velocities $\vec{\Omega}$, $\vec{\Omega}'$ also depend on the geometry of the encounter, we are led to introduce

$$\vec{\Omega} = \vec{V}_1 - \vec{V};\ \vec{\Omega}' = \vec{V}_1' - \vec{V}', \tag{1.37}$$

as new parameters. The first relation of eq. (1.9) may then be expressed as

$$\vec{V}' = \vec{V} + (\vec{\Omega} - \vec{\Omega}')/2;\ \ \vec{V}_1' = \vec{V}_1 - (\vec{\Omega} - \vec{\Omega}')/2, \tag{1.38}$$

and from the second relation we determine

$$(\vec{\Omega} - \vec{\Omega}')/2 = \vec{k}(\vec{\Omega}.\vec{k}), \tag{1.39}$$

where $\vec{k}$ is a unit vector in the direction of $(\vec{\Omega} - \vec{\Omega}')$, i.e. in the direction of the change in the relative velocities. Hence, eq. (1.38) becomes

$$\vec{V}' = \vec{V} + \vec{k}\,(\vec{\Omega}.\vec{k});\ \ \vec{V}_1' = \vec{V}_1 - \vec{k}\,(\vec{\Omega}.\vec{k}), \tag{1.40}$$

which is the desired solution of (1.9). If eq. (1.39) is multiplied by $\vec{k}$, it reduces to

$$\vec{k}.\vec{\Omega}' = -\,\vec{k}.\vec{\Omega}, \tag{1.41}$$

hence $\Omega = \Omega'$, that is, the relative speed is unchanged by encounter.

The direction of $\vec{k}$ is called the apse-line and, in view of (1.41), passes through O′ (Fig. 1), the intersection of the two asymptotes, and bisects the angle between them. If we denote by ψ the angle between $\vec{\Omega}$ and $\vec{k}$, inspection of Fig. 1 reveals that ψ and ϵ are polar angles specifying the direction of the unit vector $\vec{k}$ about $\vec{\Omega}$. The final velocities $\vec{V}'$ and $\vec{V}_1'$ of eq. (1.40) may, therefore, be expressed in terms of $\vec{V}$, $\vec{V}_1$, ψ and ϵ. Further, the angles ψ and ϵ may be introduced in Boltzmann's equation as variables of integration substituting b and ϵ. Keeping Ω constant, we can write

$$\Omega b db d\epsilon = \tau d\vec{k}, \tag{1.42}$$

where $d\vec{k}$ represents an element of solid angle

$$d\vec{k} = \sin\psi d\psi d\epsilon, \tag{1.43}$$

and τ is a function which depends on the molecular law of interaction,

$$\tau = \Omega\ b\left|\partial b/\partial\psi\right| / \sin\psi. \tag{1.44}$$

Substitute $\tau d\vec{k}$ for $\Omega b db d\epsilon$ in eq. (1.4) we obtain

$$df/dt = \int (f'f_1' - ff_1)\tau d\vec{k} d\vec{V}_1 \tag{1.45}$$

as an alternative expression for the Boltzmann equation. The variables ψ, ϵ enter explicitly into the argument of f, but the determination of ψ, or the so-called deflection angle $\chi = \pi - 2\psi$, depends on the molecular model adopted. Several models may be envisaged, such as the rigid elastic spherical molecule, molecules that are centres of force and molecules possessing both attractive and repulsive fields. All these models are assumed to have spherical symmetry.

The determination of the angle ψ follows an analysis of the relative trajectory of two encountering molecules. The relative motion of the second molecule about the first is the same as the motion of a particle of unit mass about a fixed centre of force. Let r, θ be the coordinates in the plane of the relative motion, (Fig. 2), the equations of angular momentum and energy for the particle have the form

$$r^2\dot{\theta} = \text{constant} = \Omega b \tag{1.46}$$

$$(\dot{r}^2 + r^2\dot{\theta}^2)/2 + \Phi' = \text{constant} = \Omega^2/2.$$

Here $\Phi' = 2\Phi/m$, where Φ is the potential function. The integration of (1.46) gives the orbit in the form of the relation $\theta = f(r)$, but since we are only interested in the angle between the two asymptotes, the shortest distance of approach, r_o, is given by $dr/d\theta = 0$ which corresponds to θ_o, half the required angle.

For rigid elastic molecules with diameter σ, we have $r_o = \sigma$ at the moment of contact, hence

$$\sin\psi = b/\sigma, \tag{1.47}$$

and knowing ψ the velocities after the collision are determinate. For molecules with a force of repulsion which follows a power law, m^2K/r^s, the potential is

$$\Phi' = 2\Phi/m = 2mK/(s-1)r^{s-1} \tag{1.48}$$

and the required θ_o is given by

$$\theta_o = \int_o^{\eta_o} \left[1-\eta^2-\frac{2}{(s-1)}\ \left(\frac{\eta}{\alpha}\right)^{s-1}\right]^{-\frac{1}{2}} d\eta;\ 1 - \eta_o^2 - \frac{2}{(s-1)}\ \left(\frac{\eta_o}{\alpha}\right)^{s-1} = 0; \tag{1.49}$$

where

$$\alpha = b\ \{\Omega^2/2mK\}^{1/s-1}. \tag{1.50}$$

The last expression permits us to replace b by α, in which case the Boltzmann equation takes the form

$$df/dt = (2mK)^{\frac{2}{s-1}} \int (f'f_1'-ff_1)\Omega^{\frac{s-5}{s-1}} \alpha d\alpha d\epsilon d\vec{V}_1. \tag{1.51}$$

In Chapter 2 this form is reconsidered and some of its implications are investigated.

For use in our later calculations, we derive the components of eq. (1.40), taking this opportunity to introduce a transformation which will be used subsequently. Consider eq. (1.40) and let us require its components in an arbitrary set of rectangular coordinates x, y, z. Let the unit vector $\vec{k}$ in the apse-line direction have the corresponding components k_α, and make the angle ψ with the relative velocity $\vec{\Omega}$. Introduce also coordinate axes $\tilde{k}_\alpha$ such that $\tilde{k}_z$ lies in the direction of $\vec{\Omega}$; hence

$$k_\alpha = \tilde{k}_x\xi_\alpha + \tilde{k}_y\eta_\alpha + \tilde{k}_z\zeta_\alpha \tag{1.52}$$

where ξ_α, η_α, ζ_α are the direction cosines. Express the unit vector $\vec{k}$ in terms of polar angles ψ, ϵ about $\vec{\Omega}$ as axis, thus:

$$\vec{k} = (\tilde{k}_x, \tilde{k}_y, \tilde{k}_z) = (\sin\psi\cos\epsilon,\ \sin\psi\sin\epsilon,\ \cos\epsilon). \tag{1.53}$$

Consider the fixed set of coordinates $\tilde{k}_\alpha$ and the moving set k_α, both coinciding initially. In order to obtain an arbitrary setting between them the latter set is rotated first about $\tilde{k}_z$, then about $\tilde{k}_y$ and finally about $\tilde{k}_x$ by the respective constant setting angles ϕ_o, θ_o, ψ_o, (see Fig.3). From the consideration of the various spherical triangles the direction cosines ξ_α, η_α, ζ_α may be related to these angles. We may choose $\phi_o=0$, implying that $\vec{\Omega}$, k_x, $\tilde{k}_x$ lie in the same plane, and from which the angle ϵ is measured. Expressing then the direction cosines in terms of ζ_α, and noting that $\zeta_\alpha = \Omega_\alpha/\Omega = (V_{1\alpha} - V_\alpha)/\Omega$, we can obtain

$$\begin{aligned}
&\xi_1 = (\Omega^2-\Omega_x^2)^{\frac{1}{2}}/\Omega; \quad && \xi_2 = -\Omega_x\Omega_y/\Omega(\Omega^2-\Omega_x^2)^{\frac{1}{2}}; \quad && \xi_3 = -\Omega_x\Omega_z/\Omega(\Omega^2-\Omega_x^2)^{\frac{1}{2}} \\
&\eta_1 = 0 \quad ; && \eta_2 = -\Omega_z/(\Omega^2-\Omega_x^2)^{\frac{1}{2}} \quad ; && \eta_3 = \Omega_y/(\Omega^2-\Omega_x^2)^{\frac{1}{2}} \qquad (1.54) \\
&\zeta_1 = \Omega_x/\Omega \quad ; && \zeta_2 = \Omega_y/\Omega \quad ; && \zeta_3 = \Omega_z/\Omega .
\end{aligned}$$

Using (1.52, 53, 54), the required components of $\vec{k}\,(\vec{\Omega}.\vec{k}) = \Omega\cos\psi\vec{k}$ are known and eq. (1.40) can be put in the form

$$\begin{aligned}
V'_\alpha - V_\alpha &= \Omega_\alpha\cos^2\psi + (\delta_\alpha/2)\sin 2\psi \\
V'_{1\alpha} - V_{1\alpha} &= -\Omega_\alpha\cos^2\psi - (\delta_\alpha/2)\sin 2\psi
\end{aligned} \qquad (1.55)$$

where

$$\begin{aligned}
\delta_x &= (\Omega^2-\Omega_x^2)^{\frac{1}{2}}\cos\epsilon \\
\delta_y &= -(\Omega_x\Omega_y\cos\epsilon + \Omega\Omega_z\sin\epsilon)/(\Omega^2-\Omega_x^2)^{\frac{1}{2}} \qquad (1.56) \\
\delta_z &= -(\Omega_x\Omega_z\cos\epsilon - \Omega\Omega_y\sin\epsilon)/(\Omega^2-\Omega_x^2)^{\frac{1}{2}}
\end{aligned}$$

and α represents x, y, or z. Equations (1.55) give the final velocity components of the two molecules in terms of the initial components and the geometry of the encounter.

The information we have derived regarding the mechanics and geometry of a molecular encounter forms the basis for subsequent evaluation of collision integrals, and a prelude to Chapter 3 where the full Boltzmann equation is transformed.

2. NON-UNIFORM STATE

In Chapter 1 the basic properties of Boltzmann's equation were investigated and its solution at equilibrium was determined. Next, we direct our attention to a state of a gas which departs from equilibrium only slightly, but which cannot be adequately described by the Maxwellian distribution function. In this chapter we present a concise, but systematic, treatment of Chapman-Enskog's method of solution, and their results which lead to the Navier-Stokes equations of continuum gas dynamics. The object is to obtain the near-equilibrium distribution and to gain some understanding of the concepts involved in its derivation. It is this solution that we shall use subsequently to formulate our description of a state removed from equilibrium. The chapter is concluded by an examination of the Bhatnagar-Gross-Krook model equation in which the collision integral is replaced by a simple relaxation approximation. This model will prove to be of particular relevance to the kinetic formulation presented in Chapter 4.

2.1 Near-Equilibrium State

Consider a gas which is not in equilibrium, in the sense discussed in Chapter 1; the collision term of Boltzmann's equation no longer vanishes and n, $\vec{U}$ and T vary from point to point. In order to determine an appropriate solution, assume that we can write

$$f = F(1+\Phi(\vec{r},\vec{V})), \tag{2.1}$$

F being the Maxwellian distribution and Φ is a small quantity of first order corresponding to a state of a gas slightly deviating from equilibrium; then

$$(f'f_1'-ff_1) = FF_1(\Phi'+\Phi_1'-\Phi-\Phi_1) \tag{2.2}$$

since $FF_1 = F'F_1'$ and second order terms are negligible. The resulting Boltzmann collision term involves a fivefold integration effected on first order quantities which must be equated to the first order terms of the derivative df/dt for which, it is verified, only F of the representation (2.1) will be responsible. In such an event the Boltzmann equation (1.4) becomes

$$d_oF/dt = \int FF_1(\Phi'+\Phi_1'-\Phi-\Phi_1)\Omega \text{ bdb } d\epsilon \; d\vec{V}_1, \tag{2.3}$$

where the subscript (o) is added to denote that only first order quantities of dF/dt are to be considered. However, there still remains some arbitrariness in the assumed distribution function. The physical meaning of the quantities n, $\vec{U}$ and T appearing in F is, at present, at our disposal; it need not necessarily be identical with that ascribed to them in the equilibrium state. However, it is convenient to conserve their significance at any point $\vec{r}$ as number density, mass velocity and temperature, as in equilibrium. This amounts to requiring that the following mean values taken with a Maxwellian distribution (symbolized by curly brackets) vanish by definition:

$$\{\bar{\Phi}\} = \{\overline{C_x\Phi}\} = \{\overline{C_y\Phi}\} = \{\overline{C_z\Phi}\} = \{\overline{C^2\Phi}\} = 0;\ \{\bar{\Phi}\} = (1/n)\int \Phi F d\vec{V} = 0. \qquad (2.4)$$

If it is required to specify a function of $\vec{V},\vec{r},t$ in terms of $\vec{C},\vec{r},t$, where $\vec{C} = \vec{V} - \vec{U}(\vec{r},t)$, the variables $\vec{r},t$ will appear in the new expression of the function not only explicitly but also implicitly through its dependence on $\vec{C}$. Observing this, we can derive a new expression for the derivative df/dt, eq. (1.2), of Boltzmann's equation; in Chapman and Cowling's notation we have

$$\frac{df}{dt} = \frac{Df}{Dt} + \vec{C}.\frac{\partial f}{\partial \vec{r}} + (\vec{X} - \frac{D\vec{U}}{Dt}).\frac{\partial f}{\partial \vec{C}} - \frac{\partial f}{\partial \vec{C}}\vec{C} : \frac{\partial \vec{U}}{\partial \vec{r}}, \qquad (2.5)$$

where D/Dt is defined by eq. (1.25) and the last term is a double product of two tensors equal to $\Sigma\Sigma\ C_j(\partial f/\partial C_i)\ (\partial U_i/\partial r_j)$.

In order to evaluate d_oF/dt from eq. (2.5), we require the first approximation D_o/Dt of the operator D/Dt. By inspecting the conservation equations (1.22,23,24) we are led to consider the simplified set

$$\frac{D_o n}{Dt} = - n\frac{\partial}{\partial \vec{r}}.\vec{U};\ \frac{D_o\vec{U}}{Dt} = \vec{X} - \frac{1}{\rho}\frac{\partial P}{\partial \vec{r}};\ \frac{D_oT}{Dt} = - \frac{2}{3}T\frac{\partial}{\partial \vec{r}}.\vec{U}, \qquad (2.6)$$

in which viscous and heat conductivity terms have been neglected since they are of second order (see eqs. (1.30)). To this approximation, the variation of temperature during the motion of the gas follows the adiabatic law. By using eqs. (2.5), (2.6) and the expression for the Maxwellian distribution (1.15), the required quantity d_oF/dt can be calculated. Thus

$$\frac{1}{F}\frac{d_oF}{d\,t} = (c^2 - \frac{5}{2})\vec{C}.\frac{\partial \log T}{\partial \vec{r}} + 2\vec{c}\overset{o}{}\vec{c}: \frac{\partial \vec{U}}{\partial \vec{r}};\quad \vec{c} = (1/2RT)^{\frac{1}{2}}\vec{C}. \qquad (2.7)$$

The symbol $c_i \overset{o}{} c_j = c_ic_j - \delta_{ij}\ c^2/3$ denotes a tensor for which the sum of the diagonal (i=j) components is zero, and $\vec{c}$ is a dimensionless peculiar velocity. The simplified equations (2.3) and (2.7) constitute the first approximation of Chapman-Enskog's method for solving the Boltzmann equation.

Reconsider the representation (2.1), but with a different viewpoint. Since Φ is assumed to be small it can be represented, a priori, by a power series expansion in the molecular velocity $\vec{C}$. In order to determine the series' coefficients, let us have a closer look at the hydrodynamic relations (1.30) which, too, are only valid for near-equilibrium conditions. The required distribution function should yield for $\rho\overline{C_x^2}$, $\rho\overline{C_xC_y}$, ..., expressions which are equivalent to the hydrodynamic P_{xx}, P_{xy}, ... Since the Maxwellian $\{\rho\overline{C_x^2}\} = P$, $\{\rho\overline{C_xC_y}\} = 0$, ..., it follows that in the calculated expressions for $\rho\overline{C_x^2}$, etc. the deviation function Φ will be responsible for the additional terms involving the gradients $\partial U_x/\partial x$, $\partial U_x/\partial y$, ... Hence, the coefficients of the series representing the small quantity Φ must be linear functions of the flow velocity gradients and also the temperature gradients.

Furthermore, the distribution function f is invariant under changes in the rectangular coordinate axes and remains unaltered in form and value. Since F is also invariant under such changes, the invariance of Φ follows from (2.1). Apart from C^2, the invariant flow quantities involving $\vec{C}$ and the first order space gradients are the following:

$$\frac{\partial}{\partial\vec{r}}.\vec{U}\ ;\quad \vec{C}.\frac{\partial T}{\partial\vec{r}}\ ;\quad \overset{\leftrightarrow}{CC}:\frac{\partial\overset{\leftrightarrow}{U}}{\partial\vec{r}}. \qquad (2.8)$$

Consequently, the power series expansion for Φ is of the form

$$\Phi = (\frac{\partial}{\partial\vec{r}}.\vec{U})\,A_1\Sigma\alpha_\nu C^{2\nu} - (\vec{C}.\frac{\partial T}{\partial\vec{r}})\,B_1\Sigma\beta_\nu C^{2\nu} + (\overset{\leftrightarrow}{CC}:\frac{\partial\vec{U}}{\partial\vec{r}})\,\Gamma_1\Sigma\gamma_\nu C^{2\nu}. \qquad (2.9)$$

This expression for the deviation function, obtained by considerations of invariance, is due to Lorentz, but was also taken up by Chapman who first succeeded in determining the coefficients. Hilbert and Enskog arrived at the same result by direct integration of the Boltzmann equation as expressed by eq. (2.3) above.

An interesting consequence is brought to light by subjecting the expansion (2.9) for Φ to the conditions (2.4) in order to retain the significance of n, $\vec{U}$ and T as in the equilibrium state. Applying the condition $\{\overline{C^2\Phi}\} = 0$, or $\{\overline{\Phi}\} = 0$, we obtain

$$\rho(\frac{\partial}{\partial\vec{r}}.\vec{U})\left[A_1\Sigma\alpha_\nu\{\overline{C^{2(\nu+1)}}\} + \frac{\Gamma_1}{3}\Sigma\gamma_\nu\{\overline{C^{2(\nu+2)}}\}\right] = 0 \qquad (2.10)$$

or essentially

$$A + \frac{\Gamma}{3} = 0, \tag{2.11}$$

A and Γ being the coefficients of the mass velocity gradients in (2.10). But suppose we calculate $\rho\overline{C_x^2}$, using the symbols A and Γ and applying the result (2.11), we get

$$\rho\overline{C_x^2} = m\int C_x^2 F(1+\Phi)\, d\vec{V} = P - \frac{2}{3}\left(\frac{\Gamma}{15}\right)\frac{\partial}{\partial\vec{r}}\cdot\vec{U} + 2\left(\frac{\Gamma}{15}\right)\frac{\partial U_x}{\partial x}. \tag{2.12}$$

Comparison of this expression with (1.30) reveals that $\rho\overline{C_x^2}$ is equivalent to P_{xx} and that

$$-\frac{\Gamma}{15} = \mu\ ;\ -\left(\frac{A}{3} + \frac{\Gamma}{15}\right) = \mu'. \tag{2.13}$$

Thus, the result (2.11) is in fact the Stokesian gas condition $3\mu' + 2\mu = 0$, given earlier by (1.32), and is always implied by the form of eq. (2.12).

The demonstration of this important result is achieved with no assumptions other than that Φ can be represented by a power series expansion. However, when use is made of the conditions (2.4), the meaning of n, $\vec{U}$ and T becomes definite, and in particular the temperature is related to the mean molecular energy. It is seen from (2.12), and two other similar expressions for $\rho\overline{C_y^2}$ and $\rho\overline{C_z^2}$, that the mean normal pressure $(\rho\overline{C_x^2} + \rho\overline{C_y^2} + \rho\overline{C_z^2})/3$ is equal to P, so that $P = \rho RT$ follows, and is independent of the velocity gradients, though the state of the gas is not in equilibrium.

2.2 Properties of a Gas Composed of 'Maxwellian Molecules'

Before proceeding to determine the coefficients of the expansion (2.9) for the deviation function Φ, we consider in the present section a special case which can be analysed without the specific knowledge of the distribution function. This is the case of a gas whose molecules are assumed to repel each other with a force inversely proportional to the fifth power (s=5) of the distances between their centres; such molecules are called Maxwellian molecules. For a power law force of repulsion, the simplified Boltzmann eq. (2.3) takes the form

$$d_o(\log F)/dt = (2mK)^{\frac{2}{s-1}}\int F_1(\Phi' + \Phi_1' - \Phi - \Phi_1)\Omega^{\frac{s-5}{s-1}}\alpha d\alpha d\epsilon\, d\vec{V}_1 \tag{2.14}$$

in which the differential collision cross section is that used in eq.(1.51).

For s=5, the relative velocity disappears from the integrand and a considerable simplification is thus produced. We note from (2.7) that $d_o\log F/dt$ contains terms in the molecular velocities of up to third order. Hence, if in the present case Φ is represented by the power series (2.9) we need only retain the quantities up to the same order in the velocities; the resulting expression for Φ will have a finite number of terms. However, Maxwell discovered that in this special case the kinetic theory can be developed without the actual determination of the distribution function. As an illustration of his method, we calculate the coefficient of viscosity.

Let ΔC_x^2 be the transfer of C_x^2, then by (1.19) and for an inverse power law

$$\Delta C_x^2 = (2mK)^{\frac{2}{s-1}} \iint f f_1 \Omega^{\frac{s-5}{s-1}}\, d\vec{V}_1 d\vec{V} \int_0^\infty \int_0^{2\pi} (C_x'^2 - C_x^2)\alpha\, d\alpha\, d\epsilon; \qquad (2.15)$$

by eq. (1.55),

$$C_x'^2 - C_x^2 = (C_x + \Omega_x \cos^2\psi + \tfrac{1}{2}(\Omega^2 - \Omega_x^2)^{\frac{1}{2}} \sin 2\psi \cos\epsilon)^2 - C_x^2, \qquad (2.16)$$

where Ω_x stands for $C_{1_x} - C_x$. For s=5 the power of Ω vanishes and eq. (2.15) reduces to an expression for finding mean values. The last two integrations readily yield

$$2\pi \int_0^\infty \{(C_{1_x}^2 - C_x^2)\cos^2\psi + {}^1/_8(-2\Omega_x^2 + \Omega_y^2 + \Omega_z^2)\sin^2 2\psi\}\, \alpha\, d\alpha;$$

the first term vanishes due to the symmmetry of C_{1_x} and C_x, and the second term may be further averaged, giving

$$\Delta C_x^2 = \sqrt{2mK}\, \frac{n^2}{2} A_2 \left(-2\overline{C_x^2} + \overline{C_y^2} + \overline{C_z^2}\right); \quad A_2 = \pi \int_0^\infty \sin^2 2\theta_o\, \alpha\, d\alpha. \qquad (2.17)$$

The quantity A_2 is a pure number, $2\theta_o$ is the angle between the initial and final relative velocities which, by (1.49), depends on α alone. Maxwell (Collected papers, <u>2</u>, 42) calculated $A_2 = 1.3682$.

In Chapter 1 the transfer eq. (1.21) was used to derive the expression (1.35) for the transfer of ΔV_x^2 based on a Maxwellian distribution. Since as far as (2.15) is concerned $\Delta V_x^2 = \Delta C_x^2$, where the difference is a collisional invariant, we equate ΔV_x^2 of (2.17) with that of (1.35) obtaining

$$-\rho\overline{C_x^2} + \tfrac{1}{3}\rho\overline{C^2} = \frac{2}{3}\ \frac{\rho\overline{C^2}/3}{nA_2(2mK)^{\frac{1}{2}}} \left(2\frac{\partial U_x}{\partial x} - \frac{2}{3}\frac{\partial . \vec{U}}{\partial \vec{r}}\right). \qquad (2.18)$$

Or, by comparison with the first equation of (1.30), we can write

$$\rho\overline{C_x^2} = P_{xx} = P + \frac{2}{3}\mu\frac{\partial . \vec{U}}{\partial \vec{r}} - 2\mu\frac{\partial U_x}{\partial x}, \tag{2.19}$$

having introduced μ as the coefficient of viscosity

$$\mu = \frac{2}{3}\frac{\rho\overline{C^2}/3}{nA_2(2mK)^{\frac{1}{2}}} = \frac{2}{3}\frac{mRT}{A_2(2mK)^{\frac{1}{2}}}. \tag{2.20}$$

This relation shows μ to be independent of the pressure; this in fact is a general result for perfect gases irrespective of the intermolecular force law. It also shows that for Maxwellian molecules μ is proportional to T. The preceding results were arrived at because the power of Ω in (2.15) vanishes when s=5; for other values of s the distribution function must be found first. As a crude approximation, a truncated form of the expansion representation (2.19) may be adopted, keeping terms up to the third order in the molecular velocity, and then the analysis presented above is followed. For hard sphere molecules, s=∞, this approach would yield

$$\mu = \frac{5}{16}\frac{m}{\sigma^2}\sqrt{\frac{RT}{\pi}} \tag{2.21}$$

as a first approximation to the coefficient of viscosity. Here σ is the molecular diameter and μ proves to be proportional to $\sqrt{T}$.

We proceed to determine the coefficient of thermal conductivity for Maxwellian molecules; we need to calculate the transfer of V_xV^2, i.e. ΔV_xV^2. Using the transfer equation

$$\Delta Q = \sqrt{(2mK)}\iint ff_1\, d\vec{V}_1\, d\vec{V}\int_0^{\infty}\int_0^{2\pi}(Q'-Q)\alpha\, d\alpha\, d\epsilon, \tag{2.22}$$

as we have done with ΔC_x^2, we find

$$\Delta V_xV^2 = 2\frac{\rho RTn}{\mu}\left[U_x\left(\frac{\overline{C^2}}{3} - \overline{C_x^2}\right) - \left(U_y\overline{C_xC_y} + U_z\overline{C_xC_z}\right) - \frac{1}{3}\overline{C_xC^2}\right]. \tag{2.23}$$

On the other hand, the methods of the transfer equation of Chapter 1 yielded for ΔV_xV^2 the relation (1.36), by comparison with (2.23) we see that

$$\frac{1}{2}\rho\overline{C_xC^2} = -\frac{15}{4}R\mu\frac{\partial T}{\partial x}. \tag{2.24}$$

When all the stress and heat components for Maxwellian molecules are worked out in this fashion and then substituted in the energy equation (1.24), the resulting equation will contain a term which represents the change of heat by conduction. Comparison of this term with Fourier's equation for heat transfer will indicate that a coefficient of thermal conductivity can be defined,

$$k = \frac{15}{4}R\mu = \frac{5}{2}c_v\mu, \qquad (2.25)$$

which is a function of the coefficient of viscosity and the specific heat only. The kinetic theory, in general, yields a relation of the form $k = f\,c_v\mu$, $f \simeq 2.5$. This means that for monatomic molecules the Prandtl number, $c_p\mu/k$, is always nearly equal 2/3.

2.3 The Chapman-Enskog Solution of the Boltzmann Equation

The procedure outlined in section (2.2), which has succeeded for the case of Maxwellian molecules, is unfortunately inapplicable for the general case. Expressions for the coefficients of viscosity and thermal conductivity can no longer be found without first determining the velocity distribution function.

In an attempt to determine the distribution function for a non-uniform gas, Enskog in 1911 applied the method of solution by series to the Boltzmann equation. He arrived at the form of the function but without evaluating its coefficients. Hilbert, in 1912, showed that if the molecules of the gas are rigid elastic spheres, the 'linearized' Boltzmann equation may be transformed into a linear orthogonal integral equation of the second kind with a symmetrical kernel, and deduced the existence of a unique solution. Finally, in 1917, the near-equilibrium solution was independently determined by Chapman and Enskog. Chapman's method was based on Maxwell's equation of transfer while Enskog made use of the Boltzmann equation. The two methods, however, led ultimately to precisely the same results. The present section is devoted to a brief discussion of Chapman's method and relevant results. In section (2.4) the so-called B.G.K. model will be investigated and some notions of Enskog's method will be presented there.

Initially, Chapman (1912) derived general expressions for the coefficients of viscosity and thermal conductivity based on the expansion

(2.9) but in which he retained the terms up to the third order only in the molecular velocity. This, we have indicated, is true for Maxwellian molecules but not for the general case. However, in his second paper of 1917, Chapman drops this approximation and the analysis is developed rigorously and in generality. He finds out that the error made in his first paper is very small.

Chapman considers Maxwell's equation of transfer of a property Q:

Rate of change of Q = Change in Q due to encounters.

The l.h.s. of this equality is given by the l.h.s. of eq. (1.21) which he always calculates on the basis of a Maxwellian distribution, as shown earlier. This part of the transfer equation is, therefore, determinate and requires no further elaboration.

For the evaluation of the r.h.s. of the equality, given conveniently by the third equality of (1.19), Chapman adopts the representation (2.1). He simplifies the product ff_1, $ff_1 = FF_1\ (1+\Phi+\Phi_1)$, since Φ is small, and omits the term FF_1 as its contribution to ΔQ is zero. Equation (1.19) reduces to

$$\Delta Q = \iint FF_1\ (\Phi+\Phi_1)\Omega\ d\vec{V}_1\ d\vec{V} \iint (Q'-Q)\ b db\ d\epsilon . \tag{2.26}$$

The deviation function Φ is next represented by the expansion (2.9) or, more conveniently, written in the form

$$\begin{aligned} \Phi = &- B_o\ (\vec{C}\cdot \frac{\partial \log T}{\partial \vec{r}}) \sum_{r=o}^{\infty} \frac{(RT)^{-r}}{1.3.5\ldots(2r+3)r}\,\beta_{r-1}\ C^{2r} \\ &- C_o\ (6\ \overset{o}{\vec{c}\vec{c}} : \frac{\partial \vec{U}}{\partial \vec{r}}) \sum_{r=o}^{\infty} \frac{(RT)^{-r}}{1.3.5\ldots(2r+5)}\,\gamma_r\ C^{2r} \end{aligned} \tag{2.27}$$

where, in the first line, when r=o the factor r in the denominator is to be omitted. The problem is to determine the coefficients β_r, γ_r and B_o, C_o.

Chapman applies the transfer equation as many times as the number of these coefficients by assigning separately to Q the following functions:

$$Q = \vec{C}C^{2\nu}\ ; \quad Q = \overset{o}{\vec{C}\vec{C}}\ C^{2\nu}\ ; \quad \nu = 0,1,2,\ \ldots \tag{2.28}$$

that is to say, $Q = C_x C^{2\nu}$, ..., $(C_x^2 - C^2/3)C^{2\nu}$, ... In this way he obtains an infinite number of linear algebraic equations relating the coefficients of the series (2.27). Recalling that (2.26) involves eight integrations, Chapman's method of integration proceeds on the following lines:

1) Assign Q to a function as given by (2.28).
2) Using the l.h.s. of (1.21), determine the Maxwellian rate of change of Q.
3) Subject Φ of (2.27) to the conditions (2.4).
4) Use (1.55) to express Q' in terms of $\vec{C}$, $\vec{C}_1$, ψ and ϵ.
5) Refer to (2.26), integrate w.r.t. ϵ.
6) Transform the variables $\vec{C}$, $\vec{C}_1$ to $\vec{\Omega}=\vec{C}_1-\vec{C}$, $\vec{G}=\vec{C}_1+\vec{C}$.
7) Express $\vec{G}$ in polar coordinates, integrate w.r.t. the three polar variables.
8) Express $\vec{\Omega}$ in polar coordinates, integrate w.r.t. the two polar angles.
9) Adopt a molecular model, establish relation between Ω and b (or ψ).
10) Integrate w.r.t. b or ψ.
11) Finally, integrate w.r.t. Ω and obtain ΔQ due to encounters.
12) Equate ΔQ with result of (2).
13) Repeat as many times as required (omitting steps (3) and (9)).

The following linear equations will ultimately be obtained

$$\sum_{r=0}^{\infty} \beta_r b_{r\nu} = 1; \quad \sum_{r=0}^{\infty} \gamma_r c_{r\nu} = 1; \quad \nu = 0, 1, 2, \ldots \tag{2.29}$$

with the coefficients $b_{r\nu}$ and $c_{r\nu}$ being completely determined in terms of the molecular data. Chapman solves for the β's and γ's by means of infinite determinants and finds that they are either pure numbers or simple functions of temperature, and also that

$$B_0 = \frac{9}{4} C_0, \quad \beta_{-1} = -\sum_{r=0}^{\infty} \beta_r/(1+r). \tag{2.30}$$

Once the distribution function is known the pressure at any point in the gas is found by calculating $\rho\overline{C_x^2}$, $\rho\overline{C_x C_y}$, etc. We calculate, for example,

$$\rho\overline{C_x^2} = P - C_0 \frac{2}{15} \rho RT \left(2\frac{\partial U_x}{\partial x} - \frac{\partial U_y}{\partial y} - \frac{\partial U_z}{\partial z}\right) \sum_{0}^{\infty} \gamma_r; \tag{2.31}$$

and by identification with (1.30) we obtain the general result

$$\mu = \frac{C_0}{5} \rho RT \sum_{0}^{\infty} \gamma_r. \tag{2.32}$$

This expression for μ may also be achieved by calculating, for example, $\rho\overline{C_x C_y}$. In Chapman's treatment B_o and C_o are so chosen that each is equal to $1/\rho$ multiplied into a function of $1/RT$, depending on the molecular model adopted. By (2.32), the general result that the coefficient of viscosity is independent of the pressure is thus affirmed. The quantity B_o is actually determined by Chapman for various models and, in short, may be put in the form

$$B_o = \frac{45}{4} \mu^{(1)}/P \tag{2.33}$$

where $\mu^{(1)}$ is the first approximation to the coefficient of viscosity of the particular molecular model. For Maxwellian molecules and hard spheres, for instance, $\mu^{(1)}$ is given by (2.20) and (2.21) respectively.

The coefficient of thermal conductivity is similarly obtained by determining $\rho\overline{C_x C^2}$, we get

$$\tfrac{1}{2} \rho\overline{C_x C^2} = - k \frac{\partial T}{\delta x}; \ k = \frac{3}{2} f\mu R; \ f = \frac{5}{2} \sum_o^\infty \beta_r / \sum_o^\infty \gamma_r . \tag{2.34}$$

For molecules which are point centres of force varying as r^{-s}, Chapman calculates the following table:

s	5	9	15	25	∞
$\sum_o^\infty \beta_r$	1	1.007	1.013	1.018	1.026
$\sum_o^\infty \gamma_r$	1	1.004	1.007	1.011	1.016
$\sum_o^\infty \beta_r / \sum_o^\infty \gamma_r$	1	1.003	1.006	1.077	1.010

He concludes that for all the molecular models he investigated the correction to $\mu^{(1)}$ of (2.33) does not exceed one or two per cent, and that f of eq. (2.34) is very nearly equal to 5/2 in the case of all likely models. The table shows that for Maxwellian molecules $\mu = \mu^{(1)}$. For hard spheres $\mu = 1.016\mu^{(1)}$; or, by (1.17) and (2.21), we have the well-known result

$$\mu = 0.499 \, \rho\bar{C}\lambda, \tag{2.35}$$

where $\bar{C}$ is the mean random speed given by (1.16).

Chapman finds that for the special case of Maxwellian molecules the coefficients of the series (2.27) are given by

$$\beta_{-1} = \beta_0 = \gamma_0 = 1; \quad \beta_r = \gamma_r = 0, \quad (r>0). \tag{2.36}$$

As expected, in this case the expansion includes the terms up to the third order only in the molecular velocities. For the general case, however, including that of the hard sphere molecules, the infinity of terms β_r, γ_r in the expansion representation are required. In the following table are given the results of the successive approximations obtained for the β_r and γ_r coefficients for hard spheres ($s = \infty$):

Approximation	1st	2nd	3rd	4th
β_0	1	1.3409	1.5202	1.6230
β_1	-	-0.3182	-0.6521	-0.9432
β_2	-	-	0.1567	0.4328
β_3	-	-	-	-0.0875
$\Sigma\beta_r$	1	1.02273	1.02482	1.02513
γ_0	1	1.2228	1.3094	1.3663
γ_1	-	-0.2079	-0.3688	-0.5263
γ_2	-	-	0.0754	0.2218
γ_3	-	-	-	0.0457
$\Sigma\gamma_r$	1	1.01485	1.01588	1.01607

The table shows that the approximations to the values of the individual coefficients converge by no means quickly, but the sums $\Sigma\beta_r$ and $\Sigma\gamma_r$ rapidly tend to their limiting values.

The general equations of motion of a gas whose state is slightly non-uniform may be found by substituting in the conservation equations of section (1.4) for such quantities as $\rho\overline{C_x^2}$, $\rho\overline{C_xC_y}$, ..., which are calculated on the basis of our new distribution function. This distribution yields the pressure system (1.30) and the thermal conductivity terms (2.34), and leads to the Navier-Stokes equations (Vincenti and Kruger, 1965, p. 392). These equations, when combined with the equation (1.28) of state and the relationship (2.32) of the viscosity coefficient with the temperature, make a determinate system.

The first approximation to the expansion representation (2.27) for the case of hard sphere molecules can be determined by making use of the appropriate data presented in this section. Provided that the correct $\mu^{(1)}$ is used, the result, $\Phi^{(1)}$, is exact for Maxwellian molecules and is, in fact, valid for all the molecular models investigated by Chapman and Enskog. It may be written in the form

$$\Phi^{(1)} = -\frac{\mu^{(1)}}{P}\left[\frac{3}{2}(c^2-\frac{5}{2})\vec{C}.\frac{\partial \log T}{\partial \vec{r}} + 2\,\vec{c}\overset{o}{}\vec{c} : \frac{\partial \vec{U}}{\partial \vec{r}}\right], \tag{2.37}$$

and it also leads to the Navier-Stokes equations, predicting a Prandtl number of 2/3. It is the function $\Phi^{(1)}$ that Chapman used in the analysis of his first paper.

The conclusion to be drawn from Chapman's two papers is that for a simple gas the first term of the expansion (2.27) affords, macroscopically, approximate values that are slightly different from those obtained by using Φ itself.

2.4 The Bhatnagar-Gross-Krook Equation

The Boltzmann equation (1.4) may be written in the form

$$df/dt = G(f) - f\,L(f). \tag{2.38}$$

The symbols G(f) and L(f) represent nonlinear integral operators giving, respectively, the number of molecules gained and lost per unit volume and unit time at $(\vec{V},\vec{r},t)$ where the distribution function is f. The complex form of these operators has led in recent years to the introduction into the kinetic theory of various model equations as replacements for Boltzmann's equation. The basic idea behind this approach is that a detailed specification of the molecular collision processes is much too fine for many purposes, and that a simpler representation of them may well be adequate and useful. We discuss here one such model which will prove to have a special relation to the scheme proposed in Chapter 4 for generating models of the Boltzmann equation.

Bhatnagar-Gross-Krook (1954) proposed that eq. (2.38) be replaced by the following model equation:

$$df/dt = An(F-f), \tag{2.39}$$

where F is a locally Maxwellian function with n, $\vec{U}$ and T being the simple moments of f, that is, number density, flow velocity and temperature, respectively. The factor A is a free parameter which is allowed to be a function of n, $\vec{U}$ and T but not of the random velocity. As a consequence, when the model (2.39) is multiplied by a function Ψ_i representing a summational invariant and then integrated, the r.h.s. vanishes

$$\int \Psi_i\,(F-f)d\vec{V} = 0, \tag{2.40}$$

and the l.h.s. yields the same conservation equations of motion as those obtained in section (1.4). The H-theorem mentioned in section (1.3) also applies to the B.G.K. model; it is noted that in this case

$$\frac{dH}{dt} = \int(\log f + 1)\,\frac{df}{dt}\,d\vec{V} = An\int(F-f)\log f\,d\vec{V},$$

and since, by (1.10), the quantity logF itself is a summational invariant, we have

$$\int(F-f)\log f\,d\vec{V} = \int(F-f)\log(f/F)d\vec{V} \leqslant 0. \tag{2.41}$$

The precise relationship between the Boltzmann collision integral and the B.G.K. collision model is not easily established. It may be pointed out that for Maxwellian molecules the loss term, $L(f) = \int f_1 \Omega b db\, d\epsilon\, d\vec{V}_1$, is just proportional to the number density, since the integrand is then independent of the relative velocity. The constant of proportionality is represented by A, noting that a cut-off in the extent of the force field must be applied in order to make the integral finite. A further integration of fL(f) over all velocities will yield An^2. If the loss term is now calculated for a gas of hard spheres in equilibrium and the result is equated to An^2, that is the number of collisions is matched, we determine on this basis that

$$A = \bar{C}/n\lambda, \tag{2.42}$$

where the mean free path λ and the mean random speed $\bar{C}$ are given by (1.17) and (1.16), respectively.

The relation between the model and the exact gain terms is more difficult to elucidate. The requirement that the collision integral should vanish when f is Maxwellian suggests that the gain term is equal to AnF. The assumption behind this may be considered equivalent to the approximation that after a collision the molecules are instantaneously accommodated to the local Maxwellian distribution.

The B.G.K. model is still a nonlinear integro-differential equation and, although it is simpler than the Boltzmann equation, its solution in most cases is still a matter of considerable difficulty. However, some of its implications can be inspected by applying to it a Chapman-Enskog type of analysis. When the model is nondimensionalized through multiplying eq. (2.39) by l/u, where u and l are some reference speed and characteristic length respectively, we get

$$df/dt = (F-f)/\alpha\ ; \quad \alpha = u/Anl. \tag{2.43}$$

If $u \sim \bar{C}$, α is proportional to the ratio of the mean free path to the characteristic length; this ratio is the Knudsen number K_n. If $u \sim U$, then $\alpha \sim MK_n$ where M is the Mach number. Hence, for most situations encountered in gas dynamics at ordinary densities the parameter α will be very small, and when $\alpha = 0$, $f = F$. In the Chapman-Enskog procedure, f is expanded in powers of a small quantity α_o, some typical value of α:

$$f = f^{(o)} + \alpha_o f^{(1)} + \alpha_o^2 f^{(2)} + \dots \qquad (2.44)$$

By substituting this representation in the B.G.K. model and equating coefficients, we obtain

$$f^{(o)} = F; \; f^{(n)} = -\frac{\alpha}{\alpha_o}\frac{df^{(n-1)}}{dt}, \quad n \geq 1. \qquad (2.45)$$

When the zeroth-order solution is introduced in the conservation equations of section (1.4), the Euler equations are obtained which, in turn, are used to calculate $df^{(o)}/dt$. This is precisely the quantity d_oF/dt, given by eq. (2.7). Hence, to the first order, the solution is

$$f^{(o)} + \alpha_o f^{(1)} = F\left[1 - \frac{1}{An}\left\{(c^2 - 5/2)\vec{c}.\frac{\partial \log T}{\partial \vec{r}} + 2\overset{\circ}{\overrightarrow{c\,c}} : \frac{\partial \vec{U}}{\partial \vec{r}}\right\}\right], \qquad (2.46)$$

which is very similar to the Chapman-Enskog truncated solution (2.37) of the full Boltzmann equation. If eq. (2.46) is used to work out $\rho\overline{C_x^2}$ and $\rho\overline{C_x C^2}/2$, we get

$$\rho\overline{C_x^2} = P + \frac{mRT}{A}\left(\frac{2}{3}\frac{\partial . \vec{U}}{\partial \vec{r}} - 2\frac{\partial U_x}{\partial x}\right) \; ; \; \tfrac{1}{2}\rho\overline{C_x C^2} = -\frac{5}{2}\frac{mR^2T}{A}\frac{\partial T}{\partial x}. \qquad (2.47)$$

By comparison with the corresponding equations of hydrodynamics, we make the identifications

$$\mu = \frac{mRT}{A} \; ; \; k = \frac{5}{2}\frac{mR^2T}{A}, \qquad (2.48)$$

and the Stokesian relation is automatically satisfied. Hence, the Prandtl number for the B.G.K. model is $Pr = \mu\, c_p/k = 1$ whereas, by section (2.3), the correct value for monatomic gases is very nearly $Pr = 2/3$. The parameter A is a function of the temperature only and may be determined for any gas from its viscosity, at the same time the dependence of k on the temperature is established.

The B.G.K. model has been used extensively in recent years in the study of various problems in rarefied gas dynamics such as couette flow, freely expanding jets, shock structure and many others. Its popularity is perhaps to some extent an indication to the success of its predictions. There have also been many variants and extensions to this model, for a survey of these and their applications see Guiraud (1967).

3. TRANSFORMATION OF THE COMPLETE BOLTZMANN EQUATION

The approach we shall adopt in Chapter 4 for describing a state of a gas in non-equilibrium will be one of approximating the collision term of the Boltzmann equation on the basis of an assumed distribution function. This proposed treatment entails the evaluation of the complete collision term and, in our case, would involve lengthy calculations to an extent that the practicability of the method of evaluation becomes questionable. However, the task can be facilitated substantially if the final velocities appearing in the collision term are substituted for using the encounter equations, prior to the assignment of an expression to the distribution function. In this way, the collision term is obtained as a function of the initial velocities, and the geometry of the encounter, alone. The required transformation of Boltzmann's equation is considered in the present chapter; it will lead to a collision term which will prove to be, in practice, much simpler than the original form, and more suitable for the approximation scheme we shall employ.

Consider the two alternative forms of Boltzmann's equation given by (1.45) and (2.38),

$$\frac{df}{dt} = \int (f'f_1'-ff_1)\ \tau d\vec{k}\ d\vec{V}_1 = G(f) - fL(f) \tag{3.1}$$

where, it is tacitly assumed, the gain and loss terms can actually be separated. Introduce the representation $f = F(1+\Phi)$, with F being a Maxwellian distribution, and substitute in G and L,

$$G = \int FF_1\ (1+\Phi'+\Phi_1'+\Phi'\Phi_1')\ \tau d\vec{k}\ d\vec{V}_1 \tag{3.2a}$$

$$L = \int F_1\ (1+\Phi_1)\ \tau d\vec{k}\ d\vec{V}_1. \tag{3.2b}$$

Our aim is to eliminate the explicit dependence of the collision term on the final molecular velocities by making use of the equations of binary encounters. The necessary transformation was first devised by Hilbert (1912) for rigid elastic spheres and small Φ (i.e. $\Phi'\Phi_1'$ is negligible). Chapman and Cowling (1960, p. 129), and subsequently Waldmann (1958, p. 366) employing a different approach, extended the transformation to include molecules whose interaction is always repulsive and, it appears, to other forms of interaction as well. Pidduck (1915), in his treatment of the motion of ions in gases, also made this extension to the transformation.

Here, we relax the assumption that Φ is small and require the transformation of all parts of eq. (3.2). We shall follow the treatment of Chapman and Cowling which makes use of the geometrical aspects of molecular encounters, the insight thus gained will prove to be very useful for evaluating collision integrals. Initially, we consider molecules whose potential is repulsive and later specialize the results to hard sphere molecules.

Define the dimensionless velocities

$$\vec{c} = \beta^{\frac{1}{2}}\vec{C}, \quad \vec{v} = \beta^{\frac{1}{2}}\vec{V}, \quad u = \beta^{\frac{1}{2}}\vec{U}, \quad \vec{g} = \beta^{\frac{1}{2}}\vec{\Omega}, \quad \beta = 1/2RT. \qquad (3.3)$$

Let M and N be any functions of $\vec{V},\vec{r},t$ and consider the integral

$$I = \beta^{-3/2}\int FF_1\, M'N_1'\, \tau(g,\psi)\, d\vec{k}\, d\vec{c}_1 \qquad (3.4)$$

which represents the various parts of (3.2a). By (1.40), the initial and final molecular velocities are related by

$$\vec{c}\,' = \vec{c} + (\vec{g}.\vec{k})\vec{k}, \quad \vec{c}_1' = \vec{c}_1 - (\vec{g}.\vec{k})\vec{k}, \quad \vec{g} = \vec{c}_1 - \vec{c}, \qquad (3.5)$$

where $\vec{k}$ is a unit vector in the direction of the apse-line making an angle ψ with $\vec{g}$. Figure 4 exhibits the geometry involved.

Introduce the relative velocity

$$\vec{R} = \vec{c}\,' - \vec{c} = (\vec{g}.\vec{k})\vec{k}$$

in the direction of $\vec{k}$, having the magnitude $R = g\cos\psi$ and a volume element

$$d\vec{R} = d\vec{c}\,' = \cos^3\psi\, g^2\, dg d\vec{k},$$

with $d\vec{k}$ being an element of solid angle. Further, let $\vec{n}$ be a unit vector in the direction of $\vec{g}$, then

$$d\vec{k}\, d\vec{c}_1 = d\vec{k}\, d\vec{g} = g^2 dg\, d\vec{k}\, d\vec{n} = \sec^3\psi\, d\vec{n}\, d\vec{c}\,'. \qquad (3.6)$$

Equation (3.4) may take the form

$$I = \beta^{-3/2}\int F'F_1'\, M'N_1'\, \tau(R\sec\psi,\, \psi)\, \sec^3\psi\, d\vec{n}\, d\vec{c}\,'. \qquad (3.7)$$

Next, we seek expressions for $\vec{c}_1'$ and $c_1'^2$:

$$\vec{c}_1' = \vec{c} + \vec{g} - \vec{R} = \vec{c} + g\vec{n} - R\vec{k} = \vec{c} + R\sec\psi(\vec{n} - \{\vec{n}.\vec{k}\}\,\vec{k});$$

the modulus of the bracketed quantity is equal to $\sin\psi$, hence

$$\vec{c}_1' = \vec{c} + R\,\mathrm{tg}\psi\, \vec{k}_1, \qquad (3.8)$$

where $\vec{k}_1$ is a unit vector perpendicular to $\vec{k}$ and lies in the $(\vec{R},\vec{g})$ plane. Squaring (3.8), noting that $\vec{R}.\vec{k}_1 = 0$, we have

$$c_1'^2 = c^2 + R^2\mathrm{tg}^2\psi + 2R\,\mathrm{tg}\psi\, \vec{c}\,'.\vec{k}_1.$$

Let θ be the angle between $\vec{c}'$ and $\vec{R}$ and define $\vec{j}$ to be a unit vector perpendicular to $\vec{R}$ in the $(\vec{c}',\vec{R})$ plane, then

$$R\vec{c}'.\vec{k}_1 = R(c'\cos\theta\ \vec{k} + c'\sin\theta\ \vec{j}).\vec{k}_1 = |\vec{R}\wedge\vec{c}'|\ \vec{j}.\vec{k}_1 = |\vec{c}\wedge\vec{c}'|\ \cos\epsilon_1,$$

where ϵ_1 is the angle between the $(\vec{c}',\vec{R})$ and $(\vec{R},\vec{g})$ planes. Hence

$$c_1'^2 = c^2 + R^2 tg^2\psi + 2\,|\vec{c}\wedge\vec{c}'|\ tg\psi\ \cos\epsilon_1. \qquad (3.9)$$

The orientation of $\vec{n}$ about $\vec{R}$ is now given by ψ and ϵ_1, so

$$d\vec{n} = \sin\psi\ d\psi\ d\epsilon_1. \qquad (3.10)$$

Finally, the positive scalar $\tau(g,\psi)$, given by (1.44), is expressed as

$$\tau(g,\psi) = 4\beta^{-1/2} g\ \cos\psi\ \tau_1(g,\psi),\ \tau_1(g,\psi) = b\left|\frac{\partial b}{\partial\psi}\right|/2\sin 2\psi, \qquad (3.11)$$

with b being the encounter parameter and τ_1 a function termed the collision cross section. For hard sphere molecules (see (1.47)) with diameter σ, we have

$$b = \sigma\ \sin\psi,\ \ \tau_1 = \sigma^2/4. \qquad (3.12)$$

Making use of eqs. (3.8) to (3.11), eq. (3.7) takes the form

$$I = 4\beta^{-2}\int FF'M'd\vec{c}'\int N(\vec{c}+Rtg\psi\ \vec{k}_1)R\tau_1(R\sec\psi,\psi)\exp(-R^2tg^2\psi-2|\vec{c}\wedge\vec{c}'|\,tg\psi\ \cos\epsilon_1)$$

$$.\sec^3\psi\ \sin\psi d\psi d\epsilon_1. \qquad (3.13)$$

The inner integral is taken over the range of values of ψ between 0 and $(\pi-\delta)/2$, say, and of ϵ_1 between 0 and 2π. That is, a cut-off is being introduced, since I is a separate integral; however, if the complete collision term is evaluated simultaneously such a cut-off is, in principle, unnecessary. The orientation of the unit vector $\vec{k}_1$ about $\vec{R}$ depends on ϵ_1 only since the two vectors are perpendicular to each other.

The transformation of eq. (3.4) could have been obtained by expressing $\vec{c}_1$ and $\vec{c}'$ in terms of $\vec{c}_1'$. In this case a relative velocity

$$\vec{R}_1 = \vec{c}_1' - \vec{c} = \vec{g} - (\vec{g}.\vec{k})\vec{k} \qquad (3.14)$$

is introduced, having the magnitude $R_1 = g\ \sin\psi$ and the direction of $\vec{k}_1$, so that

$$d\vec{R}_1 = d\vec{c}_1' = \sin^3\psi\ g^2dg\ d\vec{k}_1.$$

The unit vector $\vec{k}_1$ is perpendicular to $\vec{k}$, and $(\vec{k}_1,\vec{k},\vec{g})$ lie in the same plane. If the orientation of $\vec{k}$ about $\vec{g}$ is given by the angle ψ and ϵ, then $\vec{k}_1$ about $\vec{g}$ is specified by $\pi/2-\psi$ and $\epsilon+\pi$, thus

$$d\vec{k} = \sin\psi d\psi d\epsilon,\ \ d\vec{k}_1 = \cos\psi d\psi d\epsilon.$$

The corresponding relation to (3.6) may be verified to be

$$d\vec{k}\, d\vec{c}_1 = \operatorname{cosec}^3\psi\ \operatorname{tg}\psi\ d\vec{n}\, d\vec{c}_1',$$

and eq. (3.4) becomes

$$I = \beta^{-3/2}\int F'F_1'\, M'N_1'\ \tau(R_1\operatorname{cosec}\psi,\psi)\operatorname{cosec}^3\psi\ \operatorname{tg}\psi\ d\vec{n}\, d\vec{c}_1'. \qquad (3.15)$$

Next, expressions for $\vec{c}\,'$ and $\vec{c}\,'^2$ are sought. In this case we have

$$\vec{c}\,' = \vec{c} + \vec{g} - \vec{R}_1 = \vec{c} + R_1\operatorname{ctg}\psi\vec{k} \qquad (3.16)$$

which is similar to (3.8). Now let θ_1 be the angle between $\vec{c}_1'$ and $\vec{R}_1$, and ϵ_2 be the angle between the $(\vec{c}_1',\vec{R}_1)$ and $(\vec{R}_1,\vec{g})$ planes; by squaring (3.16) and proceeding as before we get

$$c'^2 = c^2 + R_1^2\operatorname{ctg}^2\psi + 2|\vec{c}\wedge\vec{c}_1'|\operatorname{ctg}\psi\ \cos\epsilon_2. \qquad (3.17)$$

In this case, where $\vec{R}_1$ is taken as axis, $d\vec{n} = \cos\psi d\psi d\epsilon_2$. The scalar $\tau(g,\psi)$ appears in the form

$$\tau(R_1\operatorname{cosec}\psi,\psi) = 4\beta^{-1/2}R_1\ \operatorname{ctg}\psi\ \tau_1(R_1\operatorname{cosec}\psi,\psi). \quad (3.18)$$

By introducing all these relations in (3.15) and, in order to arrive at a result similar to (3.13), substituting $\psi_1 = \pi/2-\psi$, we have

$$I = 4\beta^{-2}\int FF_1'N_1'd\vec{c}_1'\int M(\vec{c}+R_1\operatorname{tg}\psi_1\ \vec{k})R_1\tau_1(R_1\sec\psi_1,\pi/2-\psi_1)\exp(-R_1^2\operatorname{tg}^2\psi_1-2|\vec{c}\wedge\vec{c}_1'|$$

$$.\operatorname{tg}\psi_1\ \cos\epsilon_2)\ \sec^3\psi_1\ \sin\psi_1\ d\psi_1\ d\epsilon_2. \qquad (3.19)$$

Here ψ_1 varies between $\delta/2$ and $\pi/2$ and the unit vector $\vec{k}$ is, in this event, a function of ϵ_2 only.

Define in the plane $(\vec{R},\vec{g},\vec{R}_1)$ a unit vector $\vec{n}_1$ perpendicular to $\vec{g}$, and denote by ϵ the angle between the $(\vec{c}_1,\vec{g})$ and the $(\vec{R},\vec{g},\vec{R}_1)$ planes. Inspection of (3.13) and (3.19) reveals that the symbols $(\psi,\epsilon_1,\vec{c}\,',\vec{R},\vec{k}_1)$ and $(\psi_1,\epsilon_2,\vec{c}_1',\vec{R}_1,\vec{k})$ may be replaced by $(\psi,\epsilon,\vec{c}_1,\vec{g},\vec{n}_1)$, since their respective meanings are identical and the value of the integral is not altered. Thus, the two expressions for I may take the form

$$I = 4\pi^{-3/2}n\beta^{-\frac{1}{2}}F\int M_1\exp(-c_1^2)d\vec{c}_1\int g\ \tau_1(g\sec\psi,\psi)\exp(-g^2\operatorname{tg}^2\psi)\sec^3\psi\sin\psi d\psi$$

$$.\int N(\vec{c}+g\operatorname{tg}\psi\vec{n}_1)\ \exp(-2|\vec{c}\wedge\vec{c}_1|\ \operatorname{tg}\psi\ \cos\epsilon)\ d\epsilon \qquad (3.20a)$$

$$= 4\pi^{-3/2}n\beta^{-\frac{1}{2}}F\int N_1\exp(-c_1^2)d\vec{c}_1\int g\ \tau_1(g\ \sec\psi,\pi/2-\psi)\exp(-g^2\operatorname{tg}^2\psi)\sec^3\psi\sin\psi d\psi$$

$$.\int M(\vec{c}+g\ \operatorname{tg}\psi\vec{n}_1)\exp(-2|\vec{c}\wedge\vec{c}_1|\ \operatorname{tg}\psi\cos\epsilon)\ d\epsilon. \qquad (3.20b)$$

The transformed relations for the various parts of the gain term (3.2a) can be obtained from (3.20) by assigning suitable values to M and N. For instance, when $M = \Phi$ and $N = 1$, eq. (3.20) yields the expression for the part involving Φ'. The loss term may also be made explicit by introducing in (3.2b) the expressions for $\vec{dk}$ and τ using (1.43) and (3.11).

The determination of the collision cross section requires the specification of the type of encounter between the molecules. The problem, at this stage, is restricted to hard sphere molecules, for which τ_1 is simply a constant equal to $\sigma^2/4$. Using this and the results of the transformation we find that the gain and loss terms can be expressed as follows:

$$L(\Phi) = (\lambda\beta^{\frac{1}{2}})^{-1}\left[K_o(\vec{c}) + \int_{-\infty}^{\infty} \Phi_1 K_1(\vec{c},\vec{c}_1)\exp(-c_1^2)d\vec{c}_1\right] = (K_o+\overline{\Phi K_1})/\lambda\beta^{\frac{1}{2}} \tag{3.21}$$

$$G(\Phi) = (\lambda\beta^{\frac{1}{2}})^{-1}\ F\left[K_o(\vec{c}) + \int_{-\infty}^{\infty}\Phi_1\{K_2(\vec{c},\vec{c}_1)+K_4(\Phi,\vec{c},\vec{c}_1)\}\exp(-c_1^2)d\vec{c}_1\right]$$

$$= F(K_o + \overline{\Phi K_2} + \overline{\Phi K_4})/\lambda\beta^{\frac{1}{2}}. \tag{3.22}$$

Referring to the original equation (3.2) for L and G, we verify that K_o relates to that part of the integral which involves unity, while $\overline{\Phi K_1}$, $\overline{\Phi K_2}$ and $\overline{\Phi K_4}$ relate to Φ_1, $\Phi'+\Phi_1'$ and $\Phi'\Phi_1'$ respectively. The K's are various average weighting functions which account for the molecular model, and for hard sphere molecules are given by the following expressions:

$$K_o(\vec{c}) = \int_{-\infty}^{\infty} K_1(\vec{c},\vec{c}_1)\exp(-c_1^2)d\vec{c}_1 \tag{3.23a}$$

$$= \tfrac{1}{2}\int_{-\infty}^{\infty} K_2(\vec{c},\vec{c}_1)\exp(-c_1^2)d\vec{c}_1, \tag{3.23b}$$

$$K_1(\vec{c},\vec{c}_1) = 2^{-\frac{1}{2}}\pi^{-5/2}g\int_0^{\pi/2}\sin\psi\cos\psi\, d\psi\int_0^{2\pi} d\epsilon, \tag{3.24}$$

$$K_2(\vec{c},\vec{c}_1) = 2^{\frac{1}{2}}\pi^{-5/2}g\int_0^{\pi/2} \exp(-g^2 tg^2\psi)\sec^3\psi\sin\psi\, d\psi$$

$$.\int_0^{2\pi}\exp(-2|\vec{c}\wedge\vec{c}_1|\ tg\psi\ \cos\epsilon)\ d\epsilon, \tag{3.25}$$

$$K_4(\Phi,\vec{c},\vec{c}_1) = 2^{-\frac{1}{2}}\pi^{-5/2}g\int_0^{\pi/2}\exp(-g^2 tg^2\psi)\sec^3\psi\sin\psi\, d\psi$$

$$.\int_0^{2\pi}\Phi(\vec{c}+g tg\psi\vec{n}_1)\ \exp(-2|\vec{c}\wedge\vec{c}_1|\ tg\psi\cos\epsilon)\ d\epsilon. \tag{3.26}$$

Two expressions are obtained for K_o since it occurs both in L and G. The unit vector $\vec{n}_1$ is perpendicular to $\vec{g}$, and λ is the mean free path. The integrations in the expression of K_o, K_1 and K_2 can be performed analytically, thus yielding:

$$K_o(c) = (2\pi)^{-\frac{1}{2}}\left[\exp(-c^2) + (2c+c^{-1})\int_0^c \exp(-x^2)\ dx\right], \qquad (3.27)$$

$$K_1(\vec{c},\vec{c}_1) = 2^{-\frac{1}{2}}\pi^{-3/2}g, \qquad (3.28)$$

$$K_2(\vec{c},\vec{c}_1) = 2^{\frac{1}{2}}\pi^{-3/2}g^{-1}\exp(|\vec{c}\wedge\vec{c}_1|/g)^2. \qquad (3.29)$$

The relation for K_4 remains unchanged since it depends on Φ which is unknown. The second expression for K_o, (3.23b), which depends on K_2, is most easily verified by noting that $d\vec{g} = d\vec{c}_1$ and introducing as variables the polar angles defining $\vec{g}$ when $\vec{c}$ is taken as axis.

It is observed from eq. (3.27) that K_o is a monotonically increasing function and is proportional to c for large values of the peculiar speed. Furthermore, it is of order unity when c is of order unity. Meyer (1899, Appendix III) suggested an approximate expression for K_o:

$$K_o(c) \simeq \left(\frac{2}{\pi} + \frac{c^2}{2}\right)^{\frac{1}{2}}. \qquad (3.30)$$

This formula agrees remarkably well with the exact expression, both for small and large values of c, while for the middle values of c a regular overestimation occurs. Nevertheless, the errors are in all cases less than $2\frac{1}{2}$ per cent.

Finally, using eq. (3.27) for K_o, we note the following mean values taken with a Maxwellian distribution (symbolized by curly brackets):

$$n\{\overline{K_o}\} = \int K_o F\ d\vec{C} = \frac{2}{\sqrt{\pi}}n \qquad (3.31a)$$

$$n\{\overline{C_x K_o}\} = n\{\overline{C_y K_o}\} = n\{\overline{C_z K_o}\} = 0 \qquad (3.31b)$$

$$n\{\overline{C^2 K_o}\} = \int C^2 K_o F\ d\vec{C} = \frac{7}{4}\,\frac{2}{\sqrt{\pi}}\,\frac{n}{\beta} \qquad (3.31c)$$

$$n\{\overline{C_x^2 K_o}\} = \frac{1}{3}\,n\,\{\overline{C^2 K_o}\}. \qquad (3.31d)$$

These mean values will be used in Chapter 4.

4. A TREATMENT OF A NON-EQUILIBRIUM STATE

The problem we shall investigate later is that of the steady state normal shock wave. The object of the present chapter is to develop a kinetic theory description which contains a phenomenon of this nature.

In order to specify clearly what the required kinetic description is supposed to provide, the analysis is initiated by an examination of the physical features of the shock problem, and by their interpretation on the basis of the kinetic concepts presented in the previous chapters. The method of replacing the Boltzmann equation by a model equation is then proposed as a promising means for achieving this description. The main body of the present chapter is concerned with the actual derivation of such a model and, when obtained, the investigation of its capabilities.

4.1 The Problem and Proposed Method of Solution

On the basis of Chapman-Enskog solution of the Boltzmann equation, exemplified by the result (2.37), the definition of a gas state in near-equilibrium implies that the following dimensionless quantities are restricted:

$$\beta^{-\frac{1}{2}}\,\frac{\mu}{p}\left|\frac{\partial \log T}{\partial r_\alpha}\right| \ll 1\;;\qquad \frac{\mu}{p}\left|\frac{\partial U_\alpha}{\partial r_\beta}\right| \ll 1.$$

Accordingly, we regard as a non-equilibrium state one for which these parameters are not necessarily very small, and that their second and higher order products and derivatives need not necessarily be negligible. In section (4.3) an interpretation of the dimensionless parameters is given as representing some local Knudsen numbers based on the rates at which the macroscopic quantities vary.

The shock problem is the case of a one-dimensional steady flow in which a transition occurs from one equilibrium state at $-\infty$ to another equilibrium state at $+\infty$, the two states being related by the Rankine-Hugoniot conditions. The transition takes place over a layer whose thickness is of the order of a few mean free paths, across which the macroscopic variables of the flow undergo a sharp change. This sudden change of state is accompanied by viscous effects and heat conduction. The free stream Mach number is the one single parameter which characterizes the problem, and is usually used as a measure of the strength of the shock. For a strong shock, the two end states are (thermodynamically) far apart and the changes across the transition layer are great. The flow in the shock layer is, therefore, highly non-uniform and its state can depart from equilibrium so much so that the Navier-Stokes description of the gas is no longer applicable. Indeed, Liepmann et al (1962) demonstrated, on the basis of the Navier-Stokes theory, that for strong shocks the parameters $(\mu/P)dU/dx$ and $(\mu/P)d\log T/dx(\beta^{-\frac{1}{2}})$ attain, notably upstream, values far in excess of the limits imposed by the assumptions of the theory. Although these non-equilibrium effects may be related to the nature of the gas being locally rarefied, the problem as a whole has no characteristic length with which a universal Knudsen number can be associated. These effects are dependent, therefore, only on the Mach number typical of the case. At the present, there does not exist a general and reliable solution to the normal shock problem.

It is accepted in current literature that the Boltzmann equation is fully capable of describing the shock structure in a monatomic gas for any shock strength. However, its highly nonlinear and complex collision term is the source of great difficulty in the treatment of most flow problems. An alternative kinetic formulation, that appears promising, for obtaining a description of a gas state in non-equilibrium is that of a model equation replacing the Boltzmann equation, and, specifically, one which approximates the gain term G and the loss term L of eq. (2.38). On the basis of the B.G.K. model, itself a special form of (2.38), the actual distribution f can be represented in a Taylor series-type expansion involving the Maxwellian function F and its high order derivatives (Liepmann et al, p. 1320). This representation arises from an integration by parts of the integral equation form of the B.G.K. model. The first order derivative of F multiplied by a small quantity μ/P, eq. (2.7), has already been shown to depend on the Chapman-Enskog parameters which have been used to indicate departure from equilibrium. Liepmann et al deduce, in fact, that the Chapman-Enskog-type expansion is contained in the integral equation formulation. In summary, the main reasons for choosing the approach of devising a model equation, and in particular one having eq. (2.38) as its basic form, are as follows:

i) It is simpler to handle than the Boltzmann equation.

ii) Its solutions are not limited to those of a small perturbation type.

iii) The form of its collision term can be made to imitate the specific form of Boltzmann's collision term.

iv) Most of the techniques used in the analysis of the Boltzmann equation can be applied to it.

v) It has scope for application to flow problems of more than one type.

For the model equation it is most desirable to solve problems by the integral equation method. This approach is exact and it avoids the difficulties associated with the treatment of the model's l.h.s. term.

More generally, a formal scheme of generating model equations may be envisaged. In such a scheme the Boltzmann eq. (2.38) is replaced by a succession of relationships, or models, having the form

$$\frac{df^{(n+1)}}{dt} = G(f^{(n)}) - f^{(n+1)}L(f^{(n)}), \quad n \geqslant 0 \tag{4.1}$$

whereby the collision term is approximated at each level from the information of the previous level. Then by rearranging (4.1) as a pure integral equation, the (n+1) iteration to the distribution function is expressed by a relation of the form

$$f^{(n+1)} = D(f^{(n)}), \tag{4.2}$$

where D is a functional representation. The problem, as such, reduces to one of choosing an initial distribution function and investigating the convergence of the iterative solutions. The difficulties arising from a scheme such as this are as follows:

i) The convergence of the iterations to a unique solution (which corresponds to the Boltzmann equation) must be established. (The problem of existence and uniqueness of the solution of the Boltzmann equation in general is still unresolved in kinetic theory (Grad 1958)).

ii) The analytical integration of more than one iteration is usually impracticable.

iii) Hence, the 'adequate' choice of the initial solution becomes crucial.

iv) Elaborate numerical computations are usually necessary.

As a consequence, one has to strike a compromise between the crude description of a simple model and the presumed accuracy of a formal and complex scheme.

Of the other methods of approach, on the other hand, the pursuit of higher approximations in the Chapman-Enskog procedure is not likely to substantially extend the range of applicability of the Navier-Stokes equations. Wang Chang (1948), taking into account the third order terms in the distribution function, shows that for shock wave thickness this theory yields series in powers of (M-1) which converge very slowly and is, therefore, only applicable for Mach numbers which are only slightly bigger than one. At any rate, it was indicated earlier that these higher approximations are actually contained in a model equation such as the B.G.K. model. In the alternative method of assuming an orthogonal expansion of the distribution function in terms of the molecular velocity, the form of the solution is prescribed in practice when a finite sum of polynomials is considered. At low densities a large number of the polynomials is needed in order to obtain a good approximation. Furthermore, in the integral equation resulting from a model having the basic form of eq. (2.38), there always appears in the integrand the quantity $\exp(-a/x)/x$ which is non-analytic at $x=a=o$. If this behaviour is in accord with the Boltzmann equation, the question arises as to the suitability of the expansion methods to account for this feature accurately.

In view of the foregoing, it is decided to follow the approach of replacing the Boltzmann equation by a single model equation that will approximate the gain and loss terms of eq. (2.38) on the basis of an assumed distribution function. In order to facilitate the choice of the initial distribution, the representation $f=F(1+\Phi)$ is introduced in G and L resulting in eq. (3.2). Here F is a locally Maxwellian distribution and Φ is a deviation function which is not necessarily a small quantity. The introduction of Φ into the problem is made in order to separate in the collision term those quantities which are affected by departure from equilibrium from those which are not. While no restrictions are imposed on the magnitude of Φ, the use of the local Maxwellian distribution (rather than a particular distribution such as the free stream absolute Maxwellian, for example) will certainly help to restrict the variations of Φ. The nature of the quantities to be approximated in (3.2) is further simplified by an application of the transformation of Chapter 3. The Boltzmann loss and gain terms may thus be expressed by eqs. (3.21) and (3.22) in which there appears the deviation function, and other average weighting functions depending on the molecular model. At this stage, the formulation is specialised to a gas composed of hard sphere molecules for which the subsequent mathematics will prove to be tractable, and which does not present the problem of applying a cut-off in the force field. The weighting functions have been determined in Chapter 3 on this basis, and the problem at present is to choose an expression for Φ which is the sole remaining unknown in eqs. (3.21) and (3.22). In the remainder of this chapter two such choices are made and the resulting models are determined and investigated.

4.2 Exploratory Analysis

The present section is concerned with the investigation of a preliminary case of a model equation which results from a crude approximation to Boltzmann's collision term. An inspection of eqs. (3.21) and (3.22) immediately suggests that an approximation to the loss and gain terms may be obtained by taking the deviation function $\Phi \equiv 0$. This simplifies the Boltzmann equation significantly and results in the following model:

$$\frac{df}{dt} = \frac{K_o(c)}{\lambda\beta^{\frac{1}{2}}} \quad (F-f), \tag{4.3}$$

where K_o is given by (3.27) for hard sphere molecules. On the other hand, by eqs. (2.39) and (2.42), the B.G.K. model has the form

$$\frac{df}{dt} = An\ (F-f), \quad A = \bar{\bar{C}}/n\lambda. \tag{4.4}$$

It is noted that these two model equations are very similar. In particular, if K_o is approximated by its mean Maxwellian value, $2/\sqrt{\pi}$, (see eq. (3.31a)) the two models become identical since

$$\frac{2/\sqrt{\pi}}{\lambda\beta^{\frac{1}{2}}} = \frac{2}{\lambda}\ (2RT/\pi)^{\frac{1}{2}} = \frac{\bar{\bar{C}}}{\lambda},$$

in accordance with (1.16). The B.G.K. model is therefore related to the Boltzmann equation and can be derived from it by the introduction of few simplifying assumptions. The essence of the approximation behind (4.3) and (4.4) is that the distribution function in the Boltzmann gain and loss terms is replaced by a local Maxwellian distribution. Specifically, f_1, f' and f_1' are replaced by F_1, F', F_1', respectively.

The quantity $K_o/\lambda\beta^{\frac{1}{2}}$ signifies the average number of collisions per unit time per molecule of speed V, with molecules of other classes. It is called the collision frequency for a molecule having the speed V. The presence of K_o in eq. (4.3) implies that the rate of change in the number of molecules of a certain class depends on the collision frequency of this class, rather than on an overall average frequency as suggested by eq. (4.4). Thus, the rate at which molecular properties are exchanged by collisions is not the same in both models. In a gas which has no mass motion and subject to no external forces, the B.G.K. Model is characterized by a single relaxation time. That is, all of the velocity moments decay to their respective equilibrium values at the same rate, and the equation describing this decay is the same for all. However, it was found earlier by Maxwell that for Maxwellian molecules the rates of decay of the stress system and heat flow moments are different (Maxwell, Collected Papers, 2, 681; Jeans, 1952, p.233).

The Maxwellian distribution, F, which appears in eq. (4.3) contains five constants. The values of these constants are prescribed by the conservation requirements which the model equation must satisfy. Specifically, it is necessary that

$$\int \psi_i \; K_o(c) \; (F-f) \quad d\vec{V} = 0, \tag{4.5}$$

in which ψ_i represents the collisional invariants 1, $\vec{V}$ and V^2. This indicates that the five constants in F can no longer be identified with the lowest moments of f, such as in the case of the B.G.K. model where K_o is approximated by a constant. By denoting the basic parameters which F contains by n^*, $\vec{U}^*$ and T^*, eq. (4.5) together with (3.31) yield

$$n^* = \frac{\overline{nK_o}}{2/\sqrt{\pi}}, \quad \frac{7}{2}RT^* + U^{*2} = \overline{V^2K_o}/\overline{K_o}, \tag{4.6a}$$

$$U_x^* = \overline{V_xK_o}/\overline{K_o}, \quad U_y^* = \overline{V_yK_o}/\overline{K_o}, \quad U_z^* = \overline{V_zK_o}/\overline{K_o}. \tag{4.6b}$$

The mean values in eq. (4.6) are, as usual, taken with respect to the distribution f. The quantities n^*, $\vec{U}^*$ and T^* arise here as new moments of f, and their meanings are different from those associated with the usual n, $\vec{U}$ and T. Nevertheless, by use of the integral equation method, the application of the model equation (4.3) to the shock problem is feasible. Initial solutions of n^*, U_x^* and T^* are introduced in the integral expression for f, then, by making use of the definitions in eq. (4.6), a new set of solutions n^*, U_x^* and T^* is generated. By continuing this process of iteration, and provided that convergence is achievable, the last iteration to the distribution function can be used to obtain the profiles of n, U_x and T across a plane shock wave.

Further, the H-theorem mentioned in section (1.3) is applicable to the model equation (4.3); for by eqs. (1.5), (4.3) and (4.5), and for a gas whose state depends on time alone, we have

$$\frac{dH}{dt} = \int (1+\log f)\,\frac{df}{dt}\,d\vec{V} = \frac{1}{\lambda\beta^{\frac{1}{2}}}\int K_o(F-f)\log f\,d\vec{V}.$$

By eq. (1.10), the quantity log F depends on a constant, on $\vec{V}$ and on V^2, and is therefore itself a summational invariant. Thus, using (4.5), we can write the inequality

$$\int K_o(F-f)\log f\,d\vec{V} = \int (K_oF-K_of)\log(K_of/K_oF)d\vec{V} \leqslant 0, \tag{4.7}$$

which manifests the irreversible nature of our model. In conclusion, by making the model satisfy the conservation requirements, the H-theorem is automatically made valid for it too.

We have seen that the presence of K_o in eq. (4.3) affects the collision frequency and necessitates the introduction of new constants in F. In order to see a bit further how this model differs from the B.G.K. model, we apply to it the Chapman-Enskog procedure which was used in the analysis of the latter model in section (2.4). For the sake of clarity of the notation, it is convenient to rewrite (4.3) in the form

$$\frac{df}{dt} = \left[\frac{K_o}{\lambda\beta^{\frac{1}{2}}}\right]^{*}(F^{*}-f),\quad F^{*} = n^{*}(\beta^{*}/\pi)^{\frac{3}{2}}\exp(-\beta^{*}\{\vec{V}-\vec{U}^{*}\}^2), \tag{4.8}$$

in order to indicate explicitly that the constants in F^{*} are so chosen that (4.8) satisfies the conservation requirements and yields the conservation equations of section (1.4). The notation $[K_o/\lambda\beta^{\frac{1}{2}}]^{*}$ signifies that this expression contains λ^{*}, $\sqrt{\beta^{*}}$ and K_o of c^{*}; furthermore, the entire term is labelled by a star since it originated from an integration over F_1^{*} (see Chapter 3). Following the analysis in section (2.4), eqs. (2.43) to (2.46), in the course of which the Chapman-Enskog method was applied to the B.G.K. model, we expand the distribution f of eq. (4.8) in powers of a small parameter. By evaluating the coefficients of the first two terms, the truncated solution is simply

$$f = F^{*}(1+\Phi^{*}), \tag{4.9a}$$

$$\Phi^{*} = -\left[\frac{\lambda\beta^{\frac{1}{2}}}{K_o}\left\{(c^2-5/2)\,\vec{c}.\frac{\partial\log T}{\partial\vec{r}} + 2\overset{o}{\vec{c}\,\vec{c}} : \frac{\partial\vec{U}}{\partial\vec{r}}\right\}\right]^{*}. \tag{4.9b}$$

Again, the star label denotes that all the symbols inside the brackets refer to the quasi-equilibrium state described by F^*. The quantity $[\lambda\beta^{\frac{1}{2}}]^*$ is presumed to be of first order, meaning that $\Phi^* \ll 1$, and any result of a calculation in which f of (4.9) is used, will be correct to within the same order of approximation. The problem is to determine the stress and heat flow moments resulting from the solution (4.9).

Initially, n, $\vec{U}$ and T must be related to n^*, $\vec{U}^*$ and T^*. We note

$$n = \int f \, d\vec{V} = \int F^*(1+\Phi^*) \, d\vec{V} = \int F^* \, d\vec{V} = n^*, \qquad (4.10)$$

so that the number density is the same as n^*.

Next, determine the mean speed U_x:

$$nU_x = \int V_x f \, d\vec{V} = \int (U_x^* + C_x^*) f \, d\vec{V} = nU_x^* + \int C_x^* \, F^* \Phi^* d\vec{V}.$$

Substituting for Φ^* from (4.9b) and integrating, we obtain

$$U_x = U_x^* - \frac{8A_o}{3\sqrt{\pi}} R \left[\lambda\beta^{\frac{1}{2}} \frac{\partial T}{\partial x} \right]^*, \qquad (4.11a)$$

likewise

$$U_y = U_y^* - \frac{8A_o}{3\sqrt{\pi}} R \left[\lambda\beta^{\frac{1}{2}} \frac{\partial T}{\partial y} \right]^*, \qquad (4.11b)$$

$$U_z = U_z^* - \frac{8A_o}{3\sqrt{\pi}} R \left[\lambda\beta^{\frac{1}{2}} \frac{\partial T}{\partial z} \right]^*, \qquad (4.11c)$$

where A_o is a pure number given by

$$A_o = \int_o^\infty \frac{x^4}{K_o(x)} \left(x^2 - \frac{5}{2}\right) \exp(-x^2) dx. \qquad (4.12)$$

That is, $\vec{U}$ differs from $\vec{U}^*$ but $(\vec{U}-\vec{U}^*)$ is a quantity of first order. It is seen from (4.12) that if K_o is regarded as a constant, the value of A_o would be zero and $\vec{U}^* = \vec{U}$. This is the case of the B.G.K. model.

Finally, the calculation of the kinetic temperature,

$$3nRT = n\overline{C^2} = \int C^2 f d\vec{V} = \int (C^{*2} - \{\vec{U}-\vec{U}^*\}^2) f d\vec{V} = 3n^* RT^*, \qquad (4.13)$$

shows that, to first order, T is the same as the quasi-equilibrium temperature.

Consequently, the hydrostatic pressure remains unaltered, $P = P^*$.

Having related n, $\vec{U}$ and T to the basic quantities labelled by a star, we are now in a position to determine the normal pressure component $\rho\overline{C_x^2}$. To first order, we may write

$$n\overline{C_x^2} = \int C_x^2 \ f \ d\vec{V} = \int C_x^{*2} \ f \ d\vec{V} = n^* RT^* + \int C_x^{*2} \ F^* \Phi^* d\vec{V}.$$

Substituting for Φ^* and integrating, we obtain

$$\rho\overline{C_x^2} = \left[P + \frac{8A_1}{15\sqrt{\pi}} \rho\lambda\beta^{-\frac{1}{2}} \left(\frac{2}{3} \frac{\partial . \vec{U}}{\partial \vec{r}} - 2 \frac{\partial U_x}{\partial x} \right) \right]^*, \quad A_1 = \int_0^\infty \frac{x^6}{K_0(x)} \exp(-x^2) dx, \qquad (4.14)$$

and A_1 is a pure number. The star superscript on the r.h.s. of (4.14) can be omitted altogether since, by (4.11a), the error in so doing is of an order higher than the first. Hence, by comparison with eq. (1.30), a coefficient of viscosity can be defined as follows:

$$\mu = \frac{8A_1}{15\sqrt{\pi}} \rho\lambda\beta^{-\frac{1}{2}}. \qquad (4.15)$$

The determination of the rest of the stress components merely reproduces eq. (1.30), but with μ always given by the relation (4.15).

Turning next to the heat flow moments we find, to within the order of our approximation, that

$$n\overline{C_x C^2} = \int C_x C^2 \ f \ d\vec{V} = 5(U_x^* - U_x) \ nRT + \int C_x^* C^{*2} F^* \Phi^* d\vec{V}.$$

Carrying out the integration and substituting for $(U_x^* - U_x)$ using (4.11a), we get

$$\tfrac{1}{2}\rho\overline{C_x C^2} = - \left(\frac{4}{3} A_2 - \frac{10}{3} A_0 \right) \frac{R}{\sqrt{\pi}} \rho\lambda\beta^{-\frac{1}{2}} \frac{\partial T}{\partial x} \qquad (4.16)$$

where, again, the star label has been omitted, and A_2 is a pure number,

$$A_2 = \int_0^\infty \frac{x^6}{K_0(x)} \left(x^2 - \frac{5}{2} \right) \exp(-x^2) \ dx. \qquad (4.17)$$

Likewise, we can derive the expressions for two other heat flow components. Equation (4.16) allows the definition of a coefficient of thermal conductivity k,

$$k = \left(\frac{4}{3} A_2 - \frac{10}{3} A_0 \right) \frac{R}{\sqrt{\pi}} \rho\lambda\beta^{-\frac{1}{2}} = \mu c_p \left(A_2 - \frac{5}{2} A_0 \right) / A_1, \qquad (4.18)$$

where μ has been introduced from (4.15) and $c_p = 5R/2$. By substituting in (4.18) for A_o, A_1 and A_2, an expression for the reciprocal of the Prandtl number can be obtained,

$$1/\mathrm{Pr} = k/\mu c_p = \left[\int_0^\infty \frac{x^4}{K_o(x)}\,(x^4-5x^2+\tfrac{25}{4})\exp(-x^2)dx\right] \Big/ \left[\int_0^\infty \frac{x^6}{K_o(x)}\,\exp(-x^2)dx\right] \quad (4.19)$$

wherein K_o is given by (3.27). Tait (Scientific Papers, 2, 158) considered integrals of the form

$$C_r = \int_0^\infty \left[4x^{r+4}\exp(-x^2)/\{x\,\exp(-x^2)+(2x^2+1)\int_0^x \exp(-y^2)dy\}\right]dx. \quad (4.20)$$

By making use of this notation, eq. (4.19) takes the form

$$1/\mathrm{Pr} = (C_5 - 5C_3 + \tfrac{25}{4}C_1)/C_3. \quad (4.21)$$

Tait (p. 178) performed the evaluation of C_1, C_3 and C_5 by means of quadrature, and assigned to them the values 0.838, 1.852 and 5.849, respectively. On this basis, we get

$$1/\mathrm{Pr} = k/\mu c_p = 0.986 = 1/1.014, \quad (4.22)$$

whereas for the B.G.K. model $\mathrm{Pr} = 1$, and the Boltzmann equation value for monatomic gases in the near-equilibrium state is very nearly $\mathrm{Pr} = 2/3$.

It is seen that the introduction of the new moments n^*, $\vec{U}^*$ and T^* into eq. (4.3) has presented no difficulty in investigating the near-equilibrium solution. The analysis shows that for a small deviation from equilibrium the B.G.K. model approximates eq. (4.3) well. This strengthens the expectation that, in general, the predictions of the two models should be in good qualitative agreement, since their collision terms are very similar. On the other hand, the inclusion in eq. (4.3) of a variable collision frequency has not given a Prandtl number any closer to the exact value. The ratio of heat conductivity to viscosity is still not given correctly by eq. (4.3). But, it is also recalled, that by replacing ff_1 by FF_1 in our model equation, first order terms have been neglected which otherwise would have contributed to the first approximation of a Chapman-Enskog type of analysis. The conclusion, therefore, must be that both models are too simple to provide an adequate representation of the Boltzmann equation. In order to derive a more sophisticated model, we have to resort again to eqs. (3.21) and (3.22), assigning this time some (suitable) expression to the deviation function, Φ, instead of the value zero used in the present section. In so doing, the specific form of the Boltzmann collision term will be represented more correctly than hitherto. A plan such as this will be followed in the next section.

Finally, it must be remarked that Tait has actually arrived at eqs. (4.11), (4.14) and (4.16) which he obtained by means of the so-called methods of the free path. Thus, the results of his analysis fit within the ambit of a kinetic description that is governed by the model eq. (4.3). However, these early methods of elementary kinetic theory must be treated with caution since they lack rigour and generality. As such, they must be distinguished from the systematic methods of analysis that led to the rigorous kinetic theory of Boltzmann's equation and its equilibrium solution, and gave us the exact results of Chapman and Enskog.

4.3 Derivation of a Model Equation

Our scheme for acquiring models of the Boltzmann equation is to approximate its loss and gain terms, given conveniently in terms of a deviation function, Φ, by eqs. (3.21) and (3.22). Once a choice is made for Φ, the collision term becomes definite and a model equation is obtained. In the case of the B.G.K. model (and the exploratory model of section (4.2)), Φ is taken to be zero. The choice of a more realistic expression for Φ, while problematic, would be expected to result in a better representation of the Boltzmann equation. In order to make a choice such as this, let us examine the analysis by means of which the Boltzmann equation was initially derived in section (1.2). In the course of that analysis we looked at the probability that a single molecule of a given class experiences an encounter, within time dt, with molecules of another specified class contained in a slant cylinder. In the derivation of Boltzmann's equation this number is based on the actual distribution function, which is f. In the case of the B.G.K. and the exploratory models, a (local) Maxwellian distribution is ascribed to the molecules in the cylinder and their number is calculated accordingly. In addition, the gain term, due to the inverse collisions, is calculated on the assumption that both classes of molecules involved are governed by a Maxwellian distribution. The next logical approximation to the collision term would seem to be to consider, instead of the Maxwellian, a distribution function that can describe a state of a gas slightly departing from equilibrium. This level of approximation to f is afforded by the Chapman-Enskog distribution and leads to the Navier-Stokes equations. Its deviation function, Φ, is given by the infinite series (2.27) and accounts, to some degree, for the viscous and heat flow effects involved in the molecular collision processes. The choice of this distribution function is appealing, all the more so because it stems from the kinetic theory and yields the reliable Navier-Stokes equations; equations which are proving useful even beyond the expected range of their applicability. This does not, a priori, conclusively mean that a model equation based on this distribution would be more accurate than the previous models. It does, however, place the approach on logical basis to warrant the investigation of this avenue.

What is then the feasibility of making use of the distribution function leading to the Navier-Stokes equations to calculate collision integrals? Clearly, the handling of the entire infinite series is impracticable, even if the series' coefficients are available. But, it was pointed out in section (2.3), that a good approximation to this series representation, particularly at the macroscopic level, is provided by its truncated form, eq. (2.37). This, in standard tensor notation, can be expressed as

$$\Phi = -\frac{\mu}{P}\left[\frac{3}{2}\left(c^2-\frac{5}{2}\right)\frac{c_\alpha}{\sqrt{\beta}}\,\frac{\partial \log T}{\partial r_\alpha} + 2\left(c_\alpha c_\beta - \delta_{\alpha\beta}c^2/3\right)\frac{\partial U_\alpha}{\partial r_\beta}\right], \qquad (4.23)$$

with summation being carried over the subscripts $\alpha, \beta = x,y,z$; and δ is the Kronecker delta. In this, the dependence of the coefficient of viscosity, μ, on the temperature is considered to be known for various molecular models from the Chapman-Enskog solution; for hard sphere molecules it is given by (2.21). Equation (4.23) is exact for Maxwellian molecules, but for other molecular models it contains the first term only of the series (2.27) in the molecular speed. When eq. (4.23) is used to determine the collision integrals of (3.21) and (3.22), which involve velocity integrations alone, the result, that is G and L, will include the same spatial gradients as in (4.23) but each will be multiplied by some weighting function which depends on the molecular random speed only. These weighting functions, like $K_o(c)$ of eq. (4.3), affects, according to the speed of the molecule, the contribution of the spatial gradients to G and L, or, in other words, to the collision frequency. However, the effect of using the entire series (2.27), instead of (4.23), is only to alter in the previous result the form of these weighting functions; the space functions remain unchanged. We can expect, therefore, at least a qualitative agreement between the results of the two approaches.

It is convenient to introduce the following space-dependent parameters:

$$t_\alpha = \left[\frac{3}{2} \frac{\mu}{P\beta^{\frac{1}{2}}} \frac{\partial \log T}{\partial r_\alpha} \right]^{-1} = \left[3 \frac{\mu}{P} \frac{\partial \sqrt{2RT}}{\partial r_\alpha} \right]^{-1}, \qquad (4.24a)$$

$$t_{\alpha\beta} = \left[2 \frac{\mu}{P} \frac{\partial U_\alpha}{\partial r_\beta} \right]^{-1}. \qquad (4.24b)$$

Equation (4.23) may then be expressed more concisely as follows:

$$\Phi = - \left[(c^2 - 5/2) c_\alpha / t_\alpha + (c_\alpha c_\beta - \frac{1}{3} \delta_{\alpha\beta} \, c^2)/t_{\alpha\beta} \right]. \qquad (4.25)$$

By eq. (2.35), μ/P is proportional to the mean collision time; and $\partial U_\alpha/\partial r_\beta$ is proportional to the inverse of a time increment during which a component of the mass velocity undergoes a unit change; likewise, the characteristic time of the most probable speed is inversely proportional to $\partial\sqrt{2RT}/\partial r_\alpha$. Thus t_α and $t_{\alpha\beta}$ represent ratios of two times or, alternatively, the inverse of some local Knudsen numbers associated with the rate at which the macroscopic quantities vary.

Having chosen the Navier-Stokes truncated distribution function for the purpose of approximating the Boltzmann collision term, the question arises as to how do we proceed to calculate the loss and gain terms. The direct method of integration is to calculate the original expressions for G and L, as given by eq. (3.2). This requires first the substitution for Φ_1, Φ', Φ_1' and $\Phi'\Phi_1'$ using eq. (4.25) for Φ; then the expression of the final molecular velocities in terms of the initial velocities and the geometry of the collision through use of eqs. (1.55) and (1.56). Finally, by adopting the hard sphere molecular model the resulting equations are rendered integrable. However, this approach to the determination of G and L not only involves very lengthy and tedious calculations but must also be repeated in full whenever a new expression for Φ is chosen. We are, thus, led to search for an alternative method of integration. An approach, which proved to be tractable, is to make use of Hilbert's transformation of the linearized

Boltzmann collision term (Chapman and Cowling, p. 129). To this end, however, it is necessary to extend the transformation to include the non-linear part involving $\Phi'\Phi_1'$, which is by far the most difficult term to calculate. The required extension to the transformation is presented in Chapter 3, and the resulting expressions for L and G are given, respectively, by (3.21) and (3.22). The chief simplification which ensues is that the integration of the product $\Phi'\Phi_1'$ is replaced by an integration of a quantity $\Phi_1 K_4(\Phi)$ which does not involve the final molecular velocities. Thus, the next step in this approach is to introduce Φ, as given by eq. (4.25), in the transformed expressions of L and G and perform the necessary integrations. This has been done, and the details of the method of integration are given in Appendix 2.

By eq. (3.1) the model equation we have been seeking to determine has the basic form

$$\frac{df}{dt} = G(\Phi) - fL(\Phi) \ . \tag{4.26}$$

From eqs. (3.21) and (3.22), L and G are expressible by

$$L = \frac{1}{\lambda\beta^{\frac{1}{2}}}\left[K_o(c) + \overline{\Phi K_1}\right] , \tag{4.27a}$$

$$G = \frac{F}{\lambda\beta^{\frac{1}{2}}}\left[K_o(c) + \overline{\Phi K_2} + \overline{\Phi K_4}\right] \tag{4.27b}$$

wherein K_o is given by (3.27), and $\overline{\Phi K_1}$, $\overline{\Phi K_2}$ and $\overline{\Phi K_4}$ are determined in Appendix 2 on the basis of eq. (4.25). We find that

$$\overline{\Phi K_1} = K_{11}(c)\ c_\alpha/t_\alpha + K_{12}(c)\ (c_\alpha c_\beta - \tfrac{1}{3}\delta_{\alpha\beta}\, c^2)/t_{\alpha\beta}, \tag{4.28}$$

where K_{11} and K_{12} are given by (A2.10) and (A2.11) respectively; and

$$\overline{\Phi K_2} = K_{21}(c)\ c_\alpha/t_\alpha + K_{22}(c)\ (c_\alpha c_\beta - \tfrac{1}{3}\delta_{\alpha\beta} c^2)/t_{\alpha\beta}, \tag{4.29}$$

where K_{21} and K_{22} are given by (A2.17) and (A2.18) respectively; and finally

$$\begin{aligned}\overline{\Phi K_4} = {} & K_{40}(c)c_\alpha c_\beta/t_\alpha t_\beta + K_{41}(c)/t_\alpha t_\alpha + K_{42}(c)c_\alpha c_\beta c_\gamma c_\delta/t_{\alpha\beta}t_{\gamma\delta} + K_{43}(c)/t_{\alpha\alpha}t_{\beta\beta} \\ & + K_{44}(c)\left(\frac{1}{t_{\alpha\beta}} + \frac{1}{t_{\beta\alpha}}\right)\left(\frac{1}{t_{\alpha\beta}} + \frac{1}{t_{\beta\alpha}}\right) + K_{45}(c)c_\alpha c_\beta/t_{\alpha\beta}t_{\gamma\gamma} + K_{46}(c)c_\alpha c_\beta\left(\frac{1}{t_{\alpha\gamma}} + \frac{1}{t_{\gamma\alpha}}\right)\left(\frac{1}{t_{\beta\gamma}} + \frac{1}{t_{\gamma\beta}}\right) \\ & + K_{47}(c)c_\alpha/t_\alpha t_{\beta\beta} + K_{48}(c)\ \frac{c_\alpha}{t_\beta}\left(\frac{1}{t_{\alpha\beta}} + \frac{1}{t_{\beta\alpha}}\right) + K_{49}(c)c_\alpha c_\beta c_\gamma/t_{\alpha\beta}t_\gamma, \quad \alpha,\beta,\gamma,\delta = x,y,z,\end{aligned} \tag{4.30}$$

where the functions K_{40} to K_{49} are given by (A2.52) to (A2.61), respectively.

The expressions for $\overline{\Phi K_1}$ and $\overline{\Phi K_2}$ and $\overline{\Phi K_4}$ arise as sums of terms involving the original Navier-Stokes stress and heat flow components, but with each term multiplied by some function K. The K's are average weighting functions that depend on a single variable, c, the dimensionless random speed. The effective contribution of the stress and heat terms is thus directly influenced by the specific speed of the molecule, or class of molecules, whose number density the model equation is describing. The model is characterized by two variable collision frequencies, L and G/F, which depend in the present case on the viscous and thermal conductivity effects, in addition to the basic inertia effect that can be regarded to be represented by K_o. The present model thus emerges as an extension to the exploratory model, much in the sense that the Navier-Stokes equations are an extension to Euler equations, but the description here is at the microscopic level. The additional parameters, $1/t_{\alpha}$ and $1/t_{\alpha\beta}$, are usually small but become of importance as the state of the gas departs from equilibrium or as the gas becomes locally rarefied in the sense defined earlier.

The behaviour of the functions K's in terms of c must next be inspected. These functions have been computed and their plots are given in Figures 5 and 6. The values of the K's at $c = 0$ are determined by first expressing the error and the exponential functions in terms of power series in c, and then seeking the required limits as c tends to zero. It is noted that at this limit all the K's are bounded, although an inspection of their analytical expressions does not suggest this at first. Further, as $c \rightarrow \infty$, all the K's included in the gain term become unbounded, but since G also contains the exponential function F, the decay of these K's is assured. As to the loss term, L, it involves K_o, K_{11} and K_{12}; as $c \rightarrow \infty$, K_o becomes unbounded while K_{11} and K_{12} decay to zero, as shown in Fig. 6. Thus the K's in $\overline{\Phi K_1}$ are bounded at both ends of the range of variation of c and, in fact, assume their largest absolute value at $c = 0$. More significant for us here, however, is the behaviour of all the functions of c which appear in any one term of G and L. We call this the effective contribution of the weighting function of the particular term. As examples, the effective contributions of K_{40} and K_{11} may be verified to be, respectively, $\exp(-c^2)c^2K_{40}$ and cK_{11}. The orientation of $\vec{c}$ is not accounted for in this representation, but it may be exemplified by a numerical factor varying between 0 and ±1. The effective contributions of the weighting functions appearing in G and $\overline{\Phi K_1}$ are plotted on Figures 7 and 8. The plots show that all the functions involved are bounded throughout the domain of variation of c. It is noted with regard to G that the effective contributions of the K's contained in the nonlinear term $\overline{\Phi K_4}$ are suppressed most heavily, and those of the linear term $\overline{\Phi K_2}$ less so, while K_o is suppressed least. Clearly, when $1/t_\alpha$ and $1/t_{\alpha\beta}$ are sufficiently small, the quantities $\overline{\Phi K_2}$ and $\overline{\Phi K_4}$ can be neglected altogether. Regarding the loss term, we compare K_o (Fig. 5, curve 0) with the effective contributions of K_{11} and K_{12} (Fig. 7, curves 3 and 4). The function K_o is about 0.8 when $c = 0$, and becomes of order unity when c is of order unity, then increases linearly beyond bounds as $c \to \infty$. In sharp contrast, the effective contributions of K_{11} and K_{12} are always bounded and are, at most, a few per cent of K_o in the vicinity of $c = 1$. This means that, for moderately small $1/t_\alpha$ and $1/t_{\alpha\beta}$, the quantity $\overline{\Phi K_1}$ is always small in comparison with K_o. This result is of great significance and will be discussed more fully later in this section.

It is desirable to verify, by some alternative means, the form obtained for the model equation and the calculations associated with it. The direct method mentioned earlier for the evaluation of the model's gain and loss terms has, in fact, been employed initially to derive the one-dimensional form (in space) of the model. The agreement obtained with the results of the present section is a verification of the validity of the transformation of Chapter 3 for a gas composed of hard sphere molecules. The results of this section can be further inspected, rather conveniently, as follows: If the Navier-Stokes distribution function is introduced in the r.h.s. of Boltzmann's equation, with the full quadratic expression $(f'f_1'-ff_1)$, the result is a collision term which satisfies the conservation requirements, since all four distributions are the same. In the notation of the present section, this signifies that

$$\int \psi_i \left[F(K_o + \overline{\Phi K_2} + \overline{\Phi K_4}) - F(1+\Phi)\,(K_o + \overline{\Phi K_1}) \right] d\vec{V} = 0, \qquad (4.31)$$

where Φ is given by (4.25) and ψ_i is the usual summational invariant. By substituting for the various quantities appearing in (4.31) from the results derived earlier, and performing the necessary integrations, these conditions are found to be satisfied.

The model equation must next be made to satisfy the conservation requirements. Following section (4.2), we require that

$$\int \psi_i \left[F(K_o + \overline{\Phi K_2} + \overline{\Phi K_4}) - (K_o + \overline{\Phi K_1})\, f \right] d\vec{V} = 0. \tag{4.32}$$

These conditions provide us with the five parameters which F must contain, and simultaneously insure that the usual equations of conservation of mass, momentum and energy of section (1.4) are obtained. When the known quantities in the integrand of (4.32) are substituted for, and the necessary operations are carried out, the following results are obtained for the one-dimensional case depending on x alone:

$$\int_{-\infty}^{\infty} \left[K_o + \overline{\Phi K_1} \right]^* f\, d\vec{V} = \frac{2}{\sqrt{\pi}} \left[n\left(1 - \frac{1}{180}\frac{1}{t_{xx}^2} - \frac{1}{64}\frac{1}{t_x^2}\right) \right]^* \tag{4.33a}$$

$$\int_{-\infty}^{\infty} V_x \left[K_o + \overline{\Phi K_1} \right]^* f\, d\vec{V} = \frac{2}{\sqrt{\pi}} \left[nU_x \left(1 - \frac{1}{180}\frac{1}{t_{xx}^2} - \frac{1}{64}\frac{1}{t_x^2} - \frac{5}{24}\frac{1}{u_x t_x} + \frac{1}{120}\frac{1}{u_x}\frac{1}{t_x t_{xx}}\right) \right]^* \tag{4.33b}$$

$$\int_{-\infty}^{\infty} V^2 \left[K_o + \overline{\Phi K_1} \right]^* f d\vec{V} = \frac{2}{\sqrt{\pi}} \left[\frac{n}{\beta} \left(u_x^2 \{1 - \frac{1}{180}\frac{1}{t_{xx}^2} - \frac{1}{64}\frac{1}{t_x^2}\} + u_x \{- \frac{5}{12}\frac{1}{t_x} + \frac{1}{60}\frac{1}{t_x t_{xx}}\} + \right.\right.$$
$$\left.\left. + \{\frac{7}{4} - \frac{11}{720}\frac{1}{t_{xx}^2} + \frac{1}{768}\frac{1}{t_x^2}\} \right) \right]^* . \tag{4.33c}$$

The star label is added, as in section (4.2), to indicate that all the functions inside the brackets refer to some quasi-equilibrium state whose distribution function is denoted by F^*. The dimensionless mass flow speed u_x is defined by eq. (3.3). It may be ascertained that the definitions (4.33) are a generalization of the definitions (4.6) which have arisen in connection with the exploratory model of section (4.2). However, the system of equations (4.33) is, in the present case, a complex one since n^*, U_x^* and T^* are no longer directly related to the moments of the distribution f. None-the-less, the situation remains unaltered in that there are three unknowns and three equations, and in principle it is possible to express n^*, U_x^* and T^* directly in terms of some moments of f. It is thus feasible to apply the model equation to the shock problem using an iterative method of solution. For this purpose one may envisage the following procedure. Initially, the system of equations (4.33) is simplified by making the quantities 1, C^*_x, C^{*2} appear in the integrands on the l.h.s. instead of 1, V_x, V^2, where $\vec{C}^* = \vec{V}-\vec{U}^*$; and then substituting for $\overline{\Phi K_1}$ using eq. (4.28). Three equations will result having the variables n^*, $1/t^*_x$ and $1/t^*_{xx}$ on the r.h.s., while the l.h.s. will involve $1/t^*_x$, $1/t^*_{xx}$ and some mean values of K_o, K_{11} and K_{12} taken with respect to f. First, n^*, U^*_x, T^*, $1/t^*_x$ and $1/t^*_{xx}$ are prescribed from an assumed solution and are introduced in the model equation. Its solution yields an approximation to f, which is then used to determine a new set of solutions to n^*, $1/t^*_x$ and $1/t^*_{xx}$ from the three equations which define them. Finally, by using eq. (4.24), T^* and U^*_x may also be found. The new five starred quantities can then serve to determine a new f, and the process is repeated.

The state whose variables have been labelled by a star requires some elucidation. In the opening discussion of the present section the Navier-Stokes distribution is chosen for the purpose of approximating Boltzmann's collision term. The parameters n^*, $\vec{U}^*$ and T^* of this distribution are presumably meant to be the actual state variables n, $\vec{U}$ and T. It turns out, however, that they are not; their precise meaning is dictated by the conservation laws. Thus, all we have done at the outset in choosing the Navier-Stokes distribution is to specify its form, but not its real significance. As such, the chosen distribution merely refers to some hypothetical state with variables n^*, $\vec{U}^*$ and T^*; consequently, F^* is not the local Maxwellian F that contains the actual state variables. It seems that the model equation recognizes two distinct states, not necessarily both thermodynamic. The first is one governed by a distribution $F^*(1+\Phi^*)$, interpreted in such a way that the model has a summational invariant and a second state governed by f. At equilibrium, by what amounts to letting the collision time approach zero, f and F^* become identical and equal to a uniform Maxwellian distribution. At near-equilibrium conditions, it can be shown, using the Chapman-Enskog expansion method, that n and T degenerate to n^* and T^* and that $\vec{U}$ becomes equal to $\vec{U}^*$, except for a quantity of first order. However, when the state of the gas is removed from equilibrium, the starred quantities can be quite different from the corresponding unstarred variables. But in general, the powerful constraints imposed on our model by the conservation requirements are necessary, since they insure that it is physically meaningful. We may expect, therefore, that the emergence of the starred quantities in the model helps to enhance its validity. It may be relevant to report here that Grad (1963) has shown that the Hilbert and Chapman-Enskog expansions are asymptotic to a special class of solutions of the Boltzmann equation for a small mean free path. Moreover, he finds that these expansions can be made asymptotic to very general solutions by reinterpreting the variables that enter these expansions. Grad concludes that in this way the scope of the Euler, Navier-Stokes equations, etc., is greatly extended.

Inspection of the model equation shows that for a gas whose state depends on time alone, the quantities $\overline{\Phi K_1}$, $\overline{\Phi K_2}$ and $\overline{\Phi K_4}$ vanish, in view of the spatial derivatives they contain. Under these conditions, the present model reduces to the exploratory model and, consequently, satisfies the H-theorem. The applicability of this theorem to the latter model has been demonstrated in section (4.2).

The question of the Prandtl number characterizing the model equation near the equilibrium state can perhaps be discussed without the need to resort to an analysis similar to that presented in section (4.2). The Boltzmann collision term involves four distributions which are all identical in their basic form. In the near-equilibrium case, the solution is the full Navier-Stokes distribution function and leads to the exact Prandtl number for the specific molecular model adopted. However, if the truncated solution (4.23) is used to substitute for f in the Boltzmann equation, and then the pressure tensor and heat flux are worked out, the correct Prandtl number value, Pr = 2/3, arises automatically. Under the same conditions, the model equation yields for f a solution similar to the Navier-Stokes truncated distribution, but with different functions of the molecular speed preceding the spatial gradients. In this case the four distributions contained in the model's collision term are not all the same as the Navier-Stokes distribution; clearly, the correct value of the Prandtl number cannot be expected. Suppose, however, that our method of approximating the Boltzmann equation is continued by a process of iteration, and that the process is convergent, then the ultimate model obtainable will be the Boltzmann equation itself, leading to the correct Prandtl number value. Hence, all that can be hoped for from the present model is a value nearer to the correct one than that of the B.G.K. model, say. An attempt has been made, following the analysis of section (4.2), to evaluate the Prandtl number of the present model, but its determination requires the computation of numerous integrals. The indication, however, is that the value is less than unity (roughly 0.8).

It is pertinent next to review the properties which the model equation has in common with the Boltzmann equation. Firstly, it has the same structure, that is, it involves space and time derivatives on its l.h.s. and a collision term on its r.h.s. Secondly, during collisions it conserves the number of molecules, the momentum they carry and their kinetic energy, and yields the usual set of conservation equations. Thirdly, at equilibrium its collision term reduces to $K_oF - K_of = 0$, thus admitting the Maxwellian solution as the only possible type. Fourthly, for a state of a gas which depends on time alone, the model reduces to the exploratory model and as such it satisfies the H-theorem, i.e. its nature is irreversible and dissipative. Fifthly, it exhibits, like the Boltzmann equation, an infinite number of relaxation times. Sixthly, for near-equilibrium conditions the model yields a distribution function which is very similar to the truncated Navier-Stokes distribution of the full Boltzmann equation; it also implies a Stokesian gas. Seventhly, in the derivation of the model a strong analytical use is made of the specific form of Boltzmann's collision term in order to faithfully imitate its exact structure (this is the essential feature of this model). However, like the Boltzmann equation too, the model is still a nonlinear integro-differential equation of a very complicated and awkward type to handle, in general. In conclusion, the model equation exhibits all the elementary qualitative features of the Boltzmann equation, and has a structure which has been based on it.

Although our model equation arises as an extension to the B.G.K. model, the following question must be raised relating to its mathematical basis: Does the model we have derived truly approximate the Boltzmann equation, and under what conditions? In order to answer this we must investigate the convergence of the iteration scheme in general. A scheme such as this consists of first solving for the distribution function which arises from our model equation, and using it to generate a new model, then repeating this process indefinitely. The scheme would be convergent if, for a given, and sufficient set of boundary and initial conditions, there exists an ultimate distribution which, once obtained, remains unchanged by further iterations. This solution if obtainable, would then correspond to the exact Boltzmann equation for the conditions used. This, in fact, is the general problem of existence and uniqueness of a solution of the Boltzmann equation itself, and is as yet unresolved. The existence methods available for special cases, however, are all iterative and are based on a reduction of the Boltzmann equation to an integral equation, though the precise form depending on the estimates to be made in the particular case. Of the initial functions used to initiate the iterations are some bound Maxwellians, bound functions that satisfy some conditions, and in some cases the existence methods used are very general insofar as restrictions on the initial functions are concerned. However, there are other and more serious considerations; for instance, the existence proof for a problem such as that of the shock wave structure is particularly difficult since it involves the full quadratic Boltzmann equation, it is spatially inhomogeneous and the physical space is unbounded. For a survey of the existence theory and of recent contributions to it, see Grad (1958) and Guiraud (1967). All this, however, is of little relevance to us since, even if convergence can be proved, no knowledge can be gained of how good a representation of the Boltzmann equation our model is. The lack of an existence proof should not prevent us from attempting to use devices, which are reasonably acceptable on some grounds, for the study of a particular problem. As far as the existence theory is concerned, the B.G.K. model, for example, seems to be as intractable as the Boltzmann equation, although the model is used frequently.

None-the-less, by an inspection of the specific results of the model we can still gain considerable insight into its expected validity. Consider the basic equation of the model, eq. (4.26), and solve for f regarding G and L to be function of $\vec{V},\vec{r},t$. The solution is determined by formally integrating eq. (4.26) which, in the absence of external forces, yields

$$f(\vec{V},\vec{r},t) = f(\vec{V},\vec{r}-\vec{V}(t-t_o),t_o)\exp\left[-\int_{t_o}^{t} L(\vec{V},\vec{r}-\vec{V}(t-s),s)\,ds\right] + \\ + \int_{t_o}^{t} \exp\left[-\int_{\tau}^{t} L(\vec{V},\vec{r}-\vec{V}(t-s),s)\,ds\right] G(\vec{V},\vec{r}-\vec{V}(t-\tau),\tau)\,d\tau \qquad (4.34)$$

in which τ and s are variables of integration and the integrals are line integrals; the boundary, or initial, condition is assumed to be known at the time t_o. For further remarks about (4.34) see Grad (1958, Chapter III). For our model, L is given by (4.27a) as the sum of K_o and $\overline{\Phi K_1}$. Clearly, it is imperative that L, for any molecular velocity and at any point in the physical space, should never become negative (or vanish). This means that the distribution function is negative, in which event the exponential function in eq. (4.34) will be divergent. The function K_o is monotonically increasing with c, and has a minimum value of about 0.8 when $c = 0$, while $\overline{\Phi K_1}$ contains the weighting functions K_{11} and K_{12} whose effective contributions are always finite and are comparatively very much smaller (maximum values are less than 0.08 and 0.06, respectively, at $c \simeq 1.5$, fig. 7). The result that $\overline{\Phi K_1}$ involves finite functions of c, unlike all other weighting functions, is of great importance since it ensures that, by appropriately choosing $1/t_\alpha$ and $1/t_{\alpha\beta}$, L can never become negative. In fact, even when $1/t_\alpha$ and $1/t_{\alpha\beta}$ are of order unity, L does not even approach the value of zero. It is interesting to note from Figures 7 and 8 that the effective contributions of the weighting functions contained in $\overline{\Phi K_2}$ and $\overline{\Phi K_4}$ enjoy a similar damping effect which enables $1/t_\alpha$ and $1/t_{\alpha\beta}$ to be of order unity before the effect of $\overline{\Phi K_2}$ and $\overline{\Phi K_4}$ is felt significantly on G. This result is rather interesting since, having made use of the Navier-Stokes solution for which $1/t_\alpha$ and $1/t_{\alpha\beta}$ should not become much in excess of 0.2, we note from the results of our model that this restriction has been eased significantly, perhaps by one order of magnitude. This result is not really curious, for having obtained G and L as the outcome of certain integrations, a degree of smoothing or coarse-graining with respect to the velocity variables has been introduced. In fact a transition from microscopic to macroscopic variables always requires some kind of smoothing. It may be that we have an argument here for approximating the Boltzmann equation at the microscopic level (e.g. as we have done) rather than at the macroscopic level. Furthermore, it will be shown later that the application of the model to the shock problem yields for $1/t_x$ and $1/t_{xx}$ values which are smaller than those obtained from the solution of the Navier-Stokes equations. All this seems to indicate that the range of validity of the model is not very narrow.

It may be argued, on the basis of the present model, that the B.G.K. model can provide an improvement on the Navier-Stokes description as long as $1/t_\alpha$ and $1/t_{\alpha\beta}$ are such that $\overline{\Phi K_1}$, $\overline{\Phi K_2}$ and $\overline{\Phi K_4}$ in our model do not markedly affect L and G.

The question now must be asked as to whether we have achieved our objective of determining a description of a state of a gas in non-equilibrium. The indication is that the equation we have arrived at reproduces all the known features of the Boltzmann equation. Further, it is well-behaved, even for values of $1/t_{\alpha}$ and $1/t_{\alpha\beta}$ of order unity. It is, therefore, concluded that our model can provide a description of a gas whose state is removed from equilibrium. Whether, however, this description is in accordance with the Boltzmann equation, we do not know; but for slight non-equilibrium, we expect it to be so.

The rest of the present work will be concerned with the application of the model equation to the problem of the normal shock wave.

5. APPLICATION OF PROPOSED METHOD TO THE SHOCK WAVE PROBLEM

The present Chapter is concerned with the application of the model equation derived in section (4.3) to the problem of the normal shock wave. The assumption which underlies the resulting equations is that it is possible to replace the collision frequency of the loss term by a set of average frequencies characterizing the specific macroscopic quantities of the shock and obtained by satisfying the conservation requirements. The Chapter is concluded by preliminary remarks regarding the numerical solution of the shock equations undertaken in Chapter 6.

5.1 The One-Dimensional Model Equation

For a one-dimensional flow of a gas in steady state and in the absence of external forces, the model equation (4.26) reduces to

$$V_x\, df/dx = G^*(\vec{V},x) - f\, L^*(\vec{V},x). \tag{5.1}$$

The quantities G and L are superscripted by a star in order to indicate that they depend on the variables n^*, U^*, T^* and their derivatives which are so defined that eq. (5.1) satisfies the conservation requirements. As in section (4.3), we have the notation

$$G(\vec{V},x) = F(K_o+\overline{\Phi K_2}+\overline{\Phi K_4})/\lambda\beta^{\frac{1}{2}};\quad L(\vec{V},x) = (K_o+\overline{\Phi K_1})/\lambda\beta^{\frac{1}{2}}, \tag{5.2}$$

where at the present

$$F = \frac{n(x)}{\{2\pi RT(x)\}^{3/2}}\exp\left[-\{(V_x-U(x))^2+V_y^2+V_z^2\}/2RT(x)\right] = n(x)\{\beta(x)/\pi\}^{3/2}\exp(-c^2). \tag{5.3}$$

The weighting function $K_o(c)$ is given by (3.27), and from eq. (4.28) we have

$$\overline{\Phi K_1} = K_{11}(c)\; c_x/t_x + K_{12}(c)\;(c_x^2 - c^2/3)/t_{xx}; \tag{5.4a}$$

similarly, by eq. (4.29), we obtain

$$\overline{\Phi K_2} = K_{21}(c)\; c_x/t_x + K_{22}(c)\;(c_x^2-c^2/3)/t_{xx}; \tag{5.4b}$$

and lastly, eq. (4.30) simplifies to the expression

$$\overline{\Phi K_4} = (K_{40}c_x^2+K_{41})/t_x^2 + (K_{42}c_x^4 + c_x^2\{K_{45}+4K_{46}\} + K_{43} + 4K_{44})/t_{xx}^2 + $$
$$+ (c_x\{K_{47} + 2K_{48}\} + K_{49}c_x^3)/t_x t_{xx}. \tag{5.4c}$$

The functions K's are given in Appendix 2, and by eqs. (4.24) we also have

$$1/t_x = 3\,\frac{\mu}{P}\,\frac{d\sqrt{2RT}}{dx};\quad 1/t_{xx} = 2\,\frac{\mu}{P}\,\frac{dU}{dx}. \tag{5.5}$$

The starred variables are defined in terms of moments of f by eq. (4.33) which, in addition to (5.5), make five equations relating the five quantities n^*, U^*, T^*, $1/t_x^*$ and $1/t_{xx}^*$.

The integral equation arising from eq. (5.1) is readily obtained from the general solution (4.34) of the model equation. The one-dimensional solution has the form

$$f(\vec{V},x) = f(\vec{V},x_o)\exp\left[-\frac{1}{V_x}\int_{x_o}^{x} L^*(\vec{V},x')dx'\right] + \int_{x_o}^{x}\exp\left[-\frac{1}{V_x}\int_{x'}^{x} L^*(\vec{V},x'')dx''\right]\frac{G^*(\vec{V},x')}{V_x}dx', \tag{5.6}$$

where $f(\vec{V},x_o)$ is the boundary or initial condition at $x = x_o$, and the time differential in the original equation is replaced by dx/V_x. Equation (5.6) states that the number of particles at point x, having velocity $\vec{V}$, is made up of a decaying contribution of those which started out at $x = x_o$, and a second contribution due to those gained in the process of moving from x_o to x. The exponential factor inside the integral measures the probability of this gain.

The model equation (5.1) results in a set of conservation equations of motion which govern the behaviour of the actual state variables and are obtainable from the original equations (1.22,23,24). Thus, for a gas which depends on x alone,

$$d(nU)/dx = 0 \tag{5.7a}$$

$$nUdU/dx + d(n\overline{C_x^2})/dx = 0, \tag{5.7b}$$

$$nUd\overline{C^2}/dx + 2n\overline{C_x^2}\,dU/dx + d(n\overline{C_xC^2})/dx = 0, \tag{5.7c}$$

where the moments are taken with respect to the solution, f, of eq. (5.1).

5.2 Boundary Conditions

Consider a plane shock wave moving into a uniform gas, and fix the coordinate system at the centre of the shock. In this frame of reference the shock wave is at rest. Let the state parameters upstream ($x = -\infty$) be n_1, U_1 and T_1, and downstream ($x = \infty$) be n_2, U_2 and T_2; the flow velocity is everywhere in the direction of the positive x - axis. The gas is in thermodynamic equilibrium at both ends of the physical space, and the boundary conditions are

$$f(\vec{V},-\infty) = F_1 = n_1(\beta_1/\pi)^{3/2}\exp\left[-\beta_1(\vec{V}-\vec{U}_1)^2\right];\ \beta_1 = 1/2RT_1, \tag{5.8a}$$

$$f(\vec{V},+\infty) = F_2 = n_2(\beta_2/\pi)^{3/2}\exp\left[-\beta_2(\vec{V}-\vec{U}_2)^2\right];\ \beta_2 = 1/2RT_2, \tag{5.8b}$$

so that the parameters of the two end states are governed by the Rankine-Hugoniot relations. These relations express the conservation of mass, momentum and energy through the shock wave, and result from eqs. (5.7) and (5.8),

$$n_1U_1 = n_2U_2, \tag{5.9a}$$

$$n_1U_1^2 + n_1RT_1 = n_2U_2^2 + n_2RT_2, \tag{5.9b}$$

$$U_1^2 + 5RT_1 = U_2^2 + 5RT_2. \tag{5.9c}$$

In order to introduce the boundary conditions (5.8) in the integral equation (5.6) for f, it is necessary to define the distribution function as f_- in the half space $V_x < 0$, and as f_+ in the half space $V_x > 0$. The distributions f_- and f_+ incorporate respectively the boundary conditions F_2 and F_1. Thus, eq. (5.6) reduces to the form

$$f(V_x>0,V_y,V_z,x) = f_+ = \int_{-\infty}^{x}\frac{G^*(\vec{V},x')}{V_x}\exp\left[-\frac{1}{V_x}\int_{x'}^{x}L^*(\vec{V},x'')dx''\right]dx', \tag{5.10a}$$

$$f(V_x<0,V_y,V_z,x) = f_- = \int_{+\infty}^{x}\frac{G^*(\vec{V},x')}{V_x}\exp\left[-\frac{1}{V_x}\int_{x'}^{x}L^*(\vec{V},x'')dx''\right]dx' \tag{5.10b}$$

where the complementary function in (5.6) containing the boundary condition has been omitted as the boundaries are at infinity. The boundary conditions are implicit in eq. (5.10) since, far away from the shock $F \to F_{1,2}$, $L \to K_o$ and $G \to F_{1,2}K_o$, the equation yields

$$\lim_{x\to-\infty} f_\pm = F_1;\quad \lim_{x\to\infty} f_\pm = F_2, \tag{5.11}$$

so that the distribution is Maxwellian at both ends, $x = \pm\infty$. The separate definition of the distribution function in the two ranges of the velocity space ensures that, for $L > 0$, the exponential function is always well-behaved.

For the shock problem, one is primarily interested in the behaviour across the shock of the lowest moments of the distribution function. By observing the definitions in eq. (5.10), it is found that the local number density, flow velocity and temperature are given in the present case as follows:

$$n(x) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{0} f_- \, dV_x + \int_{0}^{\infty} f_+ \, dV_x \right] dV_y \, dV_z, \tag{5.12a}$$

$$n(x)U(x) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{0} V_x f_- \, dV_x + \int_{0}^{\infty} V_x f_+ \, dV_x \right] dV_y \, dV_z, \tag{5.12b}$$

$$3Rn(x)T(x)+n(x)U^2(x) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{0} V^2 f_- \, dV_x + \int_{0}^{\infty} V^2 f_+ \, dV_x \right] dV_y \, dV_z. \tag{5.12c}$$

At the boundaries, through use of eq. (5.11), the system (5.12) reproduces the corresponding constant parameters. Similarly, if a set of solutions n = constant, U = constant and T = constant is introduced in eq. (5.12), the integration of the system merely reproduces these solutions.

The Rankine-Hugoniot relations (5.9) may be expressed in terms of the upstream Mach number, M_1. Manipulation of these relations results in the following shock constants:

$$n_2/n_1 = U_1/U_2 = 4M_1^2/(M_1^2+3), \tag{5.13a}$$

$$T_2/T_1 = (5M_1^4+14M_1^2-3)/16M_1^2, \tag{5.13b}$$

$$M_1^2 = U_1^2/\tfrac{5}{3}RT_1, \tag{5.13c}$$

where M_1 must satisfy the inequality $M_1 \geqslant 1$. Thus, the shock problem is characterized by a single dimensionless parameter - the upstream Mach number, M_1. Our aim is to determine from eqs. (5.12) the solutions $n(x)$, $U(x)$ and $T(x)$ across the shock wave for a given set of boundary conditions on the assumption that these solutions exist and are differentiable.

5.3 Analysis of Conservation Requirements

The expression (5.10) for the distribution f involves three basic unknowns, n^*, U^* and T^*, which themselves are related to some moments of f functions of x alone. (The velocity-dependent functions in (5.10) are prescribed once and for all by the initial choice of the Navier-Stokes distribution as basis for approximating Boltzmann's collision term). Equally, the system of integral equations for n, U and T, which results from using (5.10) to substitute for f in (5.12), depends on n^*, U^* and T^*; the system of equations which defines the starred variables is given by (4.33). Thus, in seeking a solution for (5.12) the auxiliary system given by (4.33) must be treated simultaneously. In section (4.3) a method of solution is proposed whereby the system of equations (4.33) is solved by a process of iterations initiated by the use of an assumed set of solutions for n^*, U^*, T^*, $1/t_x^*$ and $1/t_{xx}^*$. Any new set of solutions obtained from the iterative process may subsequently be used in (5.12) to determine an approximation for n, U and T.

The iteration scheme we intend to use is a numerical one, in view of which it is necessary at this stage to examine the computational task involved in applying the proposed method of solution. When the expression (5.10) for f is introduced in (5.12) and (4.33), there results equations involving a fivefold integration of which three are w.r.t. V_x, V_y, V_z and a further two are w.r.t. x' and x''. Thus, in order to calculate one iteration for n, U and T five such integrations must be numerically performed for each quantity at each point of the physical space. Each additional iteration necessitates not only the solution once of the auxiliary system (4.33), which means repeating the fivefold integration, but also the actual determination of the five starred quantities. This last step involves the solution of three simultaneous algebraic equations for n^*, $1/t_x^*$ and $1/t_{xx}^*$ and two separate integrations arising from (5.5) to finally obtain U^* and T^*. The main difficulty, however, would seem to lie in the actual fivefold integration common to both systems of equations, (5.12) and (4.33). Consequently, prior to undertaking a task such as this, it is necessary to verify by some other means the validity of the model equation as a true representation of Boltzmann's equation. The situation would be radically different if the two integrations w.r.t. V_y and V_z can be performed analytically before computations are started. Inspection of eq. (5.10) shows that the exponential function in the integrand contains L which is $K_o + \overline{\Phi K_1}$ of (3.27) and (5.4a). Clearly, with such complicated functions of velocity appearing in the exponent, there is little or no hope of a direct evaluation of the required double integration. Let us, therefore, consider the possibility of approximating $K_o + \overline{\Phi K_1}$. It is demonstrated in section (4.2) that the B.G.K. model can be obtained from the exploratory model by replacing K_o in the latter by its mean value (i.e. matching the number of collisions in both models) without, however, altering the situation fundamentally, at least when the departure from equilibrium is small. It is considered, therefore, that the approximation of $K_o + \overline{\Phi K_1}$ by some mean value chosen on similar physical grounds may well retain the essential features of the model and, simultaneously, provide the simplification required. But the quantity L cannot be approximated arbitrarily, since a model equation must always satisfy the conservation requirements if it is to be physically meaningful. These requirements provide, in fact, the proper means for determining an approximation for L.

By using eq. (5.10) to substitute for f in the system of equations (5.12), the quantity $L(\vec{V},x)$ will appear in the exponential function of the integrand. It is proposed to replace $L(\vec{V},x)$ in the resulting equations (5.12a), (5.12b) and (5.12c) by $L_o(x)$, $L_1(x)$ and $L_2(x)$, respectively, where these L's are functions independent of the molecular velocity. The new functions are determined as follows: The model equation (5.1) must satisfy the conservation requirements, thus

$$\int \psi_i \left[G^*(\vec{V},x) - L^*(\vec{V},x) f \right] d\vec{V} = 0; \ i = 0,1,2 \tag{5.14}$$

where $\psi_o=1$, $\psi_1=V_x$ and $\psi_2=V^2$. Likewise, the new functions must be subjected to the conditions

$$\int \psi_i \left[G^*(\vec{V},x) - L_i(x) f \right] d\vec{V} = 0. \tag{5.15}$$

From the two relations we determine

$$L_i(x) = \left[\int \psi_i \ L^*(\vec{V},x) f d\vec{V} \right] / \int \psi_i f d\vec{V}. \tag{5.16}$$

The numerator of eq. (5.16) has previously been calculated and is given by eq. (4.33), while the denominator simply yields the lowest moments of f. Furthermore, we may choose to identify n^*, U^* and T^* with n, U and T respectively, on which basis we readily establish:

$$L_i(x) = l_i(x)/\lambda(x)\sqrt{\beta(x)}; \quad i=0,1,2 \tag{5.17}$$

where

$$l_o(x) = \frac{2}{\sqrt{\pi}} \left[1-1/180t_{xx}^2 - 1/64t_x^2 \right], \tag{5.18a}$$

$$l_1(x) = \frac{2}{\sqrt{\pi}}\left[(-5/24 + 1/120t_{xx})/ut_x\right] + l_o(x), \qquad (5.18b)$$

$$l_2(x) = \left[\frac{2}{\sqrt{\pi}}\left(\frac{7}{4} - \frac{11}{720}\,\frac{1}{t^2_{xx}} + \frac{1}{768}\,\frac{1}{t^2_x}\right) + u^2[2\,l_1(x) - l_o(x)]\right]\Big/\left(\frac{3}{2} + u^2\right), \qquad (5.18c)$$

and u is a dimensionless macroscopic speed defined by eq. (3.3). In this way, the model equation (5.1) is replaced by

$$V_x\,\frac{df}{dx} = G(\vec{V},x) - f\,L_i(x)\;. \qquad (5.19)$$

When $i = 0$, the equation conserves the number of molecules and will be used to determine $n(x)$; when $i = 1$, it conserves their momentum and will be used to find $n(x)U(x)$; and when $i = 2$, the equation conserves the energy and will be used to determine $3RnT + nU^2$. In conclusion, three model equations are obtained for the three lowest moments of f, with each model, however, having an approximate, but suitably chosen, collision frequency.

The approximation of $L(\vec{V},x)$ has far-reaching implications. Firstly, the problem as a whole has been rid of the presence of the starred quantities and, as a consequence, a system of pure (but still coupled) integral equations will result for $n(x)$, $U(x)$ and $T(x)$. Secondly, with L_o, L_1 and L_2 depending on x alone, the integrations in (5.12) w.r.t. V_y and V_z may now be performed analytically, thus facilitating subsequent numerical work. Thirdly, $L_i(x)$ are so chosen as to satisfy the conservation requirements. Fourthly, in contrast with the B.G.K. model where both collision frequencies, G/F and L, are approximated and set equal to one value for all moments, in our case <u>only</u> L is approximated, and different expressions are assigned to it for the different moments required.

5.4 Derivation of Expressions for the Macroscopic Quantities

When the modified model equation (5.19) is solved for f and subjected to the boundary conditions of section (5.2), the result will be given by (5.10) but with $L_i(x)$ replacing $L(\vec{V},x)$. This solution, with the appropriate $L_i(x)$, should next be introduced in the system (5.12). However, it is convenient to consider at this stage those integrations w.r.t. V_y and V_z which would result from so doing. The double integrals in question have the form

$$J_i(V_x,x) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(V_y^2 + V_z^2)^i\,G(\vec{V},x)\,dV_y\,dV_z;\; i = 0,1. \qquad (5.20)$$

The integral for $i = 0$ arises in eqs. (5.12a) and (5.12b), and that for $i = 1$ arises in connection with (5.12c) which contains $V^2=V_x^2+V_y^2+V_z^2$. The function G and all the quantities it includes are given in section (5.1). The integrations in eq. (5.20) are considered in Appendix 3, and yield the following results:

$$J_i(V_x,x) = \pi^{-\frac{1}{2}} j_i(V_x,x)\ n(x)/\lambda(x)\ \beta^i(x); \quad i = 0,1 \tag{5.21}$$

where

$$j_o(V_x,x) = k_o(c_x)+k_1(c_x)/t_{xx}+k_2(c_x)/t_x+k_3(c_x)/t_{xx}^2+k_4(c_x)/t_x^2+k_5(c_x)/t_x t_{xx} \tag{5.22a}$$

$$j_1(V_x,x)=\kappa_o(c_x)+\kappa_1(c_x)/t_{xx}+\kappa_2(c_x)/t_x+\kappa_3(c_x)/t_{xx}^2+\kappa_4(c_x)/t_x^2+\kappa_5(c_x)/t_x t_{xx}. \tag{5.22b}$$

The k's and the κ's are weighting functions which depend on the dimensionless component c_x of the random velocity, and are given in Appendix 3.

The stage is finally set to write down the full set of equations which result from introducing eq. (5.10), with the appropriate $L_i(x)$, into the system (5.12). In the following we drop the subscript x in V_x, C_x, and U_x and in their dimensionless symbols, v_x, c_x and u_x, and use simply V,C,U,v,c and u, respectively. We get

$$n(x) = \left[\int_{-\infty}^{x}\int_{0}^{\infty} dvdx' + \int_{x}^{\infty}\int_{0}^{-\infty} dvdx'\right] \frac{n(x')\pi^{-\frac{1}{2}}}{\lambda(x')\ v}$$

$$\cdot\ j_o(v,x')\ \exp\{-h_o(x,x')/v\}, \tag{5.23a}$$

$$n(x)\ U(x) = \left[\int_{-\infty}^{x}\int_{0}^{\infty} dvdx' + \int_{x}^{\infty}\int_{0}^{-\infty} dvdx'\right] \frac{n(x')\pi^{-\frac{1}{2}}}{\lambda(x')\sqrt{\beta(x')}}$$

$$\cdot\ j_o(v,x')\exp\{-h_1(x,x')/v\}, \tag{5.23b}$$

$$3Rn(x)T(x)+n(x)U^2(x) = \left[\int_{-\infty}^{x}\int_{0}^{\infty} dvdx' + \int_{x}^{\infty}\int_{0}^{-\infty} dvdx'\right] \frac{n(x')\pi^{-\frac{1}{2}}}{\lambda(x')\beta(x')}$$

$$\cdot\{vj_o(v,x')+j_1(v,x')/v\}\exp\{-h_2(x,x')/v\}, \tag{5.23c}$$

where

$$h_i(x,x') = \sqrt{\beta(x')} \int_{x'}^{x} L_i(x'')dx''. \tag{5.24}$$

The functions $L_i(x)$ are given by eqs. (5.17) and $j_o(v,x)$ and $j_1(v,x)$ have the expressions (5.22). The system (5.23) of the coupled integral equations constitutes the fundamental set of relations governing the behaviour of the flow quantities $n(x)$, $U(x)$ and $T(x)$ across a normal shock wave.

The functions which characterize the present description of the shock structure are j_o, j_1, l_o, l_1 and l_2, and the quantities which enter these functions must next be investigated. All these functions depend on the two parameters $1/t_{xx}$ and $1/t_x$ but, in addition, j_o and j_1 involve the weighting functions k's and κ's which depend on the molecular speed c alone. The analytical expressions for the weighting functions are given in Appendix 3, and are plotted on Figures 9 and 10. Essentially, their behaviour is similar to that of the effective contribution of the weighting functions of the model equation itself. Figure 9 shows that k_o has the largest weighting effect, and that k_1 and k_2 weight $1/t_{xx}$ and $1/t_x$ less so, while k_3, k_4 and k_5 weight $1/t_{xx}^2$, $1/t_x^2$ and $1/t_x t_{xx}$ further less. The functions κ's behave in a similar fashion. For the exploratory model of section (4.2) $1/t_x = 1/t_{xx} = 0$, hence by (5.22), $j_o = k_o$ and $j_1 = \kappa_o$. For the B.G.K. model, on the other hand, it may be verified that its j_o and j_1 are equal and can be represented by the function $(2/\sqrt{\pi})\exp\{-c^2\}$. This function is plotted on Figs. 9 and 10 so that comparison can be made with the curves of k_o and κ_o of eqs. (A3.11) and (A3.30). It is interesting to note that this simple function is in good general agreement with both k_o and κ_o, although a significant and regular underestimation of the latter function does occur. (In fact, a B.G.K. model which matches the energy exchanged by collisions in a gas in equilibrium, yields $j_1 = (7/6)(2/\sqrt{\pi})\exp\{-c^2\}$). Thus, insofar as our model equation is concerned, and even for a small departure from equilibrium, the B.G.K. model predicts the number density more accurately than it does so with the temperature.

The stage is reached where it is necessary for us to have some knowledge of the variations in $1/t_{xx}$ and $1/t_x$ across a normal shock wave. For weak shocks, where the Navier-Stokes treatment is applicable, these parameters are of the order of 0.1 or less. As shocks become stronger, the parameters increase in magnitude and the validity of the Navier-Stokes description becomes increasingly questionable. Even so, estimates of

$1/t_{xx}$ and $1/t_x$ based on this theory provide useful means both for investigating our equations for the shock wave and for assessing the range of applicability of the Navier-Stokes equations. On Figures 11 and 12 plots based on these equations are shown giving the variations across the shock in the two parameters. The plots are made for upstream Mach numbers $M_1 = 1.5$, 3.0, 5.0 and 10.0, Prandtl number $Pr = 2/3$ and for an argon gas for which μ is proportional to T raised to the power 0.816. The ordinate on Fig. 11 represents the absolute magnitude of $1/t_{xx} = (2\mu/P)dU/dx$ and that on Fig. 12 represents $1/t_x = (3\mu/P)d\sqrt{2RT}/dx$. The dimensionless physical coordinate x/Λ_1 is measured on the abscissa, where Λ_1 is the mean free path far upstream and is obtained from eq. (2.35) by taking $0.499 \simeq 1/2$. Thus

$$\Lambda_1 = 2\mu_1/\rho_1\overline{C}_1 = (5\pi/6)^{\frac{1}{2}}M_1\mu_1/\rho_1 U_1. \tag{5.25}$$

Figures 11 and 12 show that the curves in general reach a maximum on the upstream side of the shock layer, the value of which depends on the Mach number. As the Mach number increases the maximum value increases too and its position moves further upstream. It is noted that the increase with the Mach number in $1/t_x$ is sharper than that in $1/t_{xx}$. For $M_1 = 1.5$ both parameters have a maximum value between 0.10 and 0.15; for $M_1 = 10.0$, $1/t_x \simeq 4.0$ at $x/\Lambda_1 = -2.75$ and $|1/t_{xx}| \simeq 1.5$ at $x/\Lambda_1 = -1.5$. Clearly with these parameters attaining large values such as these in certain regions of the shock layer, the Navier-Stokes description can no longer be considered valid in these cases. It is in such regions that all the terms in our model equation come into play and contribute significantly. It would also appear that the predictions of the B.G.K. model should be in agreement with those of our model, except in the regions where $1/t_x$ and $1/t_{xx}$ are large enough for the additional terms to make an appreciable contribution. In fact, because of the nature of the integral equations for the shock quantities, the effect of the additional terms is felt away from the low density region, but to a lesser degree.

Having obtained some indication to the behaviour of $1/t_{xx}$ and $1/t_x$ across the shock, we must inquire about the variations in the functions $l_o(x)$, $l_1(x)$ and $l_2(x)$ which appear in h_o, h_1 and h_2, respectively. On Figures 13 and 14 curves of the Navier-Stokes values for $(\sqrt{\pi}/2)l_o(x)$ and $(\sqrt{\pi}/2)l_2(x)$, eqs. (5.18), are plotted for the four Mach number cases considered earlier. The plots are continuous throughout the physical space, have a minimum value at the upstream side of the shock layer and, in general, reflect the variations in $1/t_{xx}$ and $1/t_x$. For the B.G.K. model the quantities $(\sqrt{\pi}/2)l_o$ and $(\sqrt{\pi}/2)l_2$ are constants independent of Mach number and equal to unity. Figures 13 and 14 indicate that for relatively low Mach numbers, less than 3.5 say, the values of the two parameters deviate little from unity, but for a Mach number 10.0 the quantities $(\sqrt{\pi}/2)l_o(x)$ and $(\sqrt{\pi}/2)l_2(x)$ assume minimum values as low as 0.75 and 0.45, respectively. On this basis the B.G.K. approximation at high Mach numbers and in the low density region of the shock is suspect.

With the nature of the important quantities appearing in the integrands of eqs. (5.23) crudely explored, next we discuss the practical aspects of solving this system of equations. The method we shall use is one of numerical iterations, for the initiation of which a first guess at the solutions of n, U, T, $1/t_{xx}$ and $1/t_x$ will be required. These solutions are then introduced in the integrands of (5.23) and new approximations for n, U and T are generated; the corresponding quantities $1/t_{xx}$ and $1/t_x$ are then obtained from eq. (5.5). The process may thus be repeated. The calculations must be made for a given set of constants which will characterize the solutions. Four upstream Mach number cases will be investigated; these are $M_1 = 1.5$, 3.0, 5.0 and 10.0. Also, the usual specific heat ratio for a monatomic gas, $\gamma = 5/3$, will be used together with the correct Prandtl number, $Pr = 2/3$. Finally, the monatomic gas Argon will be chosen as the gas medium, for which μ depends on T with an index 0.816. Thus, the task reduces to one of deciding on the initial solutions for the shock profiles. Although use has been made of the Navier-Stokes distribution function to derive the model equation, the solutions of the Navier-Stokes equations for the shock profiles need not necessarily be used for the initiation of the iterative scheme proposed to solve (5.23). However, it is most desirable to do so since the Navier-Stokes solution is known to be valid for weak shocks. In this way, not only a rapid convergence of the iterations can be hoped for, but more so the prerequisite, that our model equation should yield for weak shocks solutions that are in agreement with the Navier-Stokes solutions, can be verified. However, this means that the Navier-Stokes equations themselves must first be solved for the shock problem for all the cases required.

Strictly speaking, our model equation is applicable only to a gas composed of hard sphere molecules; the features of the molecular model have been made use of in the determination of the collision integrals. However, there is a strong motivation to apply the model to a realistic gas. Firstly, its predictions must be verifiable by experiment and, secondly, shock structures are known to be very sensitive to the viscosity-temperature relationship of the gas, which makes the relation $\mu \sim T^{\frac{1}{2}}$ unsuitable, even as an approximation, for most gases. The gas Argon has been used frequently in investigations of the shock problem both of analytical and experimental natures. For these reasons we, too, shall use this gas in the numerical solution of our shock equations. For this purpose, the mean free path λ will be expressed in terms of μ, using eq. (5.25), and then the viscosity-temperature relationship for Argon will be used to substitute for μ wherever it occurs in the equations. Thus, insofar as our equations are concerned μ will be related to T with an index 0.816 instead of 1/2. Let us investigate the significance of this substitution. Suppose that the exploratory model appropriate for Argon is required. The molecules of this gas can be represented, in a certain range of the temperature, as point centres of force inversely varying with distance raised to the power $s = 7.35$. The form of Boltzmann's equation appropriate to a case such as this is given by eq. (1.51). Before the collision term of this equation can be separated into a gain and a loss term, and then approximated, a cut-off in the force field must be effected. Thus, an exploratory model, similar to eq. (4.3), may result, having a collision frequency which depends on μ for Argon, on a finite numerical factor representing the particular cut-off and on a weighting function somewhat similar to K_o, eq. (3.27). When this exploratory model and the one for hard spheres are applied to the shock problem, simplified as explained in section (5.3) and then integrated in the velocity space, the ultimate results of both models would differ by a numerical factor alone. However, it should be possible to match these results since the model for Argon involves a free parameter. Thus, the significance of replacing in eq. (4.3) μ for hard spheres by μ for Argon, would appear to be to impose a cut-off in a certain prescribed manner. The B.G.K. model itself has been used in the study of the shock structure in Argon. For weak shocks, its predictions were found to reproduce the Navier-Stokes solutions for an Argon gas (Liepmann et al, 1962).

Chapter 6 will be concerned with the numerical solution of the system of equations (5.23) for the macroscopic shock quantities. The iterative scheme will be based on the solution of the Navier-Stokes equations for the normal shock wave.

6. NUMERICAL METHOD OF SOLUTION OF THE SHOCK WAVE EQUATIONS

The application of the B.G.K. model to the shock structure problem results in a set of integral equations which is similar to the system (5.23) but with $l_i = 2/\sqrt{\pi}$ and $j_i = (2/\sqrt{\pi})\exp(-c^2)$. Numerically exact solutions for this case have been obtained by two different approaches with satisfactory agreement between results.

In the first approach, due to Anderson (1965a) and Anderson and Macombre (1965), use is made of the single collision frequency $\nu(x)$ of the B.G.K. model to define a new independent variable $\tau = \int_0^x \nu(x'')dx''$. The macroscopic variables are represented by truncated Chebyshev polynomial expansions and the integral operators are replaced by Gaussian quadrature formulae. The resulting finite set of nonlinear transcendental equations for the Chebyshev expansion coefficients is solved by iteration. The initial i~~n~~terates are chosen as hyperbolic tangent profiles. The solutions obtained as functions of τ are universal in the sense that they are independent of any particular prescription of the collision frequency. The transformation from τ to x can be determined by quadrature once a law of force between molecules is specified. This method of iteration converges rapidly and the use of the τ variable proves to be most convenient and simplifies the numerical problem considerably. However in the case of eqs. (5.23) where different collision frequencies appear in the individual expressions a fundamental variable cannot be used. The presence of $1/t_x$ and $1/t_{xx}$ in the equations complicates the problem further in that universal solutions, in the sense defined above, are no longer possible. The chief difficulty in defining more than one 'universal' variable would seem to be the determination, at each stage of the iteration, of the relationship between the independent variables. Whilst a development of the method could prove successful for some cases in overcoming this problem (Anderson 1965b, p. 31), one can still expect a drastic (one to two orders of magnitude) increase in computing time.

The second approach, initially employed by Liepmann et al (1962) and later developed by Chahine and Narasimha (1965), is to compute the B.G.K. shock profiles by a successive substitution iteration scheme carried out on $n(x)$, $U(x)$ and $T(x)$ and initiated by the Navier-Stokes profiles. Here, all integrations are carried out step-by-step in subintervals using Gaussian quadrature. This somewhat laborious procedure converges rather slowly and, because a particular molecular model has to be chosen a priori, the computation time (averaging 2-3 minutes for each value of x on the IBM 7090/4) is significantly longer than in the previous case. However, the basic successive substitution iteration method is, in this case, essentially a straightforward one and can certainly be applied to solve the system (5.23) numerically. The attitude adopted here is that the numerical solution is sought in order to verify the validity of our equations and the assumptions on which they are based, rather than to obtain exact numerical solutions. With this view in mind and by making use of a high speed computer, Chahine's approach is expected to be adequate for our purposes. This can be elaborated upon as required in the light of the results it yields. The numerical procedures employed here are parallel to Chahine's and the discussion is, therefore, abbreviated and confined to differences arising from the particular form of the present equations. In order to expedite the convergence of the numerical iterative scheme, the law of conservation of mass is enforced at all points in the physical space and eq. (5.23b) simply becomes $n(x)U(x) =$ constant. As a consequence, the variables of the problem are reduced to two, namely $n(x)$ and $T(x)$, and are determined by (5.23a) and (5.23c). The reasoning behind this is that the mode of convergence of an iteration process for solving the problem will depend on the number of unknowns, but the same solution will result if the process is self-consistent.

In Appendix 4, a computational analogue to eqs. (5.23a) and (5.23c) is derived by imposing that far upstream beyond a point ξ_1 and far downstream beyond a point ξ_2, the parameters of the flow assume their respective Rankine-Hugoniot values. The resulting equations (A4.4) and (A4.5) are solved iteratively by a procedure the essence of which can be described very briefly. Initial solutions for $n(x)$, $U(x)$, $T(x)$, $dU(x)/dx$ and $dT(x)/dx$ are prescribed and introduced into the equations to yield a new $n(x)$, $U(x)$ and $T(x)$. Then by employing a numerical differentiation procedure, the corresponding $dU(x)/dx$ and $dT(x)/dx$ are also determined. In turn, the new solutions are used to generate the next step in the iterative scheme. The computations made in connection with the present work are based on tabulated solutions of the Navier-Stokes shock equations for upstream Mach numbers $M_1 = 1.5$, 3.0, 5.0 and 10.0, $Pr = 2/3$ and for an argon gas. These initial solutions were communicated by Chahine and were computed by solving the one-dimensional Navier-Stokes equations for a monatomic gas in steady flow according to the saddle-point singularity methods suggested by Gilbarg and Paolucci (1953), Grad (1952) and Sherman (1955).

By prescribing an initial solution and subsequently using an interpolation formula, values of the integrands of (A4.4) and (A4.5) become known at any given point (v,x) in the phase space. The remaining numerical problem is essentially one of integration. Since the equations involve a threefold integration with very large ranges, the accuracy of the calculations can be enhanced by dividing each range into small subintervals. The efficacy of the numerical method then largely depends upon the number, the size and the distribution of these subintervals. Initially, Chahine (1963a) performed the computations on the basis of a uniform subdivision of the velocity domain of integration (1963b). Later, however, Chahine and Narasimha (1963) noted that the factor

$$\exp-\{(v-u)^2 + h(x,x')/v\}$$

which occurs in their equations tends to zero as v approaches either end point of the path of integration, thus concluding that only the immediate vicinity of the saddle point is of significance. By investigating the extrema of the exponent, they were able to derive approximate expressions for the saddle point; these are given in Appendix 4. Details about the variable subinterval lengths they selected later for their more accurate computations are to be found in Chahine (1965). The results of the saddle point analysis are certainly applicable to the present shock equations for the low Mach number cases since, then, $j_o = k_o$ and $j_1 = \kappa_o$. The exponential-like behaviour of k_o and κ_o has already been discussed (see Figs. 9 and 10). For the high Mach number cases the use of the saddle point results may be justified on the grounds that the contributions of the weighting functions $k_1, \ldots, k_5, \kappa_1, \ldots, \kappa_5$, always occur in the vicinity of the contributions of k_o and κ_o. Further, the behaviour of l_o and l_2, which ultimately enter the saddle point expression, has been shown to reflect the variations in $1/t_x$ and $1/t_{xx}$ across the shock (see Figs. 11 to 14). For the stronger shocks, therefore, it should only be necessary to extend the region of the finer subintervals about the saddle point.

The procedure of the computation is the same as that outlined by Chahine and will not be repeated here. A Gaussian quadrature formula is applied in each of the integration subintervals. For interpolation purposes a third order polynomial is used in view of the monotonic nature of the shock profiles. For extrapolation, the flow parameters are set equal to their respective upstream values for $x < \xi_1$ and downstream values for $x > \xi_2$. The derivative of the interpolation formula is conveniently employed for the purpose of differentiation. As Chahine (1965) points out, computational errors accumulate as x moves downstream and profiles thicken as the Mach number increases. Therefore, in computing several iterations it is necessary to determine the decay of the profiles. Lyubarskii (1961) showed that for the B.G.K. model n(x), U(x) and T(x) approach their limits with increasing $|x|$ as $\exp-\{C|x|^{3/2}\}$. This rate of decay may equally be applicable to our model equation since, away from the shock layer, it essentially reduces to the B.G.K. model.

Details of the computer programme are presented in Appendix 4 and include information about the programme structure, the function of its various components and a list of principal symbols used. The computations were programmed on an I.C.T. Atlas Computer, which has a multiplication time of 5 μsec, and the results obtained are presented in Chapter 7.

7. RESULTS AND CONCLUSIONS

Within the numerical method used to solve the present shock equations, the computer programme has been written in some generality insofar as input data are concerned. These data are represented by a set of constants and need only be specified when actual computations are to be carried out. Of the data to be given are the initial shock profiles, the upstream Mach number, the index of viscosity dependence on temperature, the number of iterations to be computed and so forth. In addition, one must specify certain constant factors relating to the fineness of the integration subintervals. The values of these constants are primarily dictated by the accuracy required. After the computer programme has been duly compiled, sample computations were carried out for the case $M_1 = 1.5$. The values chosen for the constant factors were roughly the same as those used by Chahine (1965). The Navier-Stokes data were specified at 204 points (as compared with the 1001 points used by Chahine). The computing time required to evaluate the number density and temperature at the one point $x/\Lambda_1 = 4.5$ was 55 minutes and, it was estimated, some 40000 integrations were performed. It was then apparent that a drastic reduction in computing time had to be effected. In view of this, computations were repeated specifying the initial data at 52 points only and curtailing the number of subintervals by an order of magnitude. On this basis, the computing time was about 7 minutes and the values obtained for n and T were smaller than the previous values by only 0.03% and 0.05% respectively. These slight differences were due not only to less accurate integration but also to accumulation of round-off and truncation errors. The new computing time still imposed severe limitations on the evaluation of several iterations, since at each stage sufficiently accurate profiles must be computed to generate the next iteration. However, it was argued in Chapter 6 that Chahine's saddle point results might equally be used in the computation of strong shock profiles provided that the regions of fine subintervals are extended. For this reason it was decided not to reduce the accuracy of the numerical method any further. Subsequently, it turned out that the computing time varied from one point to another. On the average it was about 2 minutes for points away from the transition layer whereas at its centre, where the various integrals made comparable contributions, the computing time was about 9 minutes per point.

Computations were made for the four cases $M_1 = 1.5$, 3.0, 5.0 and 10.0 and one iteration to the macroscopic variables was evaluated at respectively 13, 16, 16 and 19 values of x/Λ_1. The number of points at which input data were specified varied from 52 to 57 and the values of the constant factors used were the same for all Mach number cases. The results obtained for n, U and T are shown in Figs. 16 to 27 and some of their important features and implications are discussed below. It should be noted that values of the speed U were calculated by using the mass conservation equation after the number density profile has been computed.

i) At $M_1 = 1.5$ the iteration is in very close agreement with the Navier-Stokes profile. The maximum relative deviation, occuring at $x/\Lambda_1 \approx -2.0$, is about 0.5% for n and U and 1% for T. Thus, for weak shocks, the Navier-Stokes solution with $Pr = 2/3$ is in fact very close to the present kinetic solution.

ii) At $M_1 = 3.0$ the iteration deviates from the Navier-Stokes on the upstream side and, to a lesser degree, on the downstream side.

iii) At $M_1 = 5.0$ and 10.0 the iteration shows progressively larger deviations upstream, the shock thickens and a long precursor develops as predicted by the B.G.K. model. Furthermore, the iteration exhibits the development of a kink in n and U profiles and a pronounced departure in the temperature profile from Navier-Stokes. In general, the deviations downstream are smaller than predicted by the B.G.K. model.

iv) The changes in the local total enthalpy across the shock (see Fig. 28) increase with Mach number and are more pronounced than either of those predicted by Navier-Stokes and B.G.K. model. Thus at high Mach numbers the flow departs from a locally adiabatic motion.

In attempting to discuss these results it should be borne in mind that only one iteration to the solution has been obtained and that the model equation has not been duly solved. Insofar as the present formulation is concerned, the agreement at low Mach numbers between the results of the computation and Navier-Stokes solution has significant implications as well as conceptual importance:

i) At least for low Mach numbers, the model equation provides a true representation of Boltzmann's equation. As such, the method and assumptions on which the derivation of the model is based are justified.

ii) The computer programme, the computational methods used and the accuracy of the numerical techniques may be considered to be essentially satisfactory.

iii) The approximation of the model's loss term by suitable mean values <u>without</u> also approximating the gain term G, appears to be justified. This result is important since it gives confidence in the validity of this approximation for strong shocks when contributions of the terms in $1/t_x$ and $1/t_{xx}$ become significant.

iv) The results indicate that in deriving a model equation for hard sphere molecules and then applying it to Argon, the error so incurred is negligible.

v) The weak shock results demonstrate that the Prandtl number of the model is effectively $2/3$. This value is also yielded by the Boltzmann equation at this limit.

vi) As a consequence of (iii) and the manner in which the B.G.K. model arises from the present formulation, the application of the exploratory model to the shock problem may be expected to yield profiles which agree with the predictions of the B.G.K. model. Hence, if the solution of the present model differs from the B.G.K. solution, it will do so because of the additional terms it includes.

In spite of the close agreement with the Navier-Stokes solution for weak shocks some deviation does occur. In general, the computed profile overestimates the Navier-Stokes solution upstream and underestimates it downstream. Thus, there is a certain regularity in the deviation. The reason for this does not appear to lie in the Prandtl number effect since, if the model has a value sensibly larger than $2/3$, the trend of the deviation from Navier-Stokes would then be in reverse to that obtained (Chahine 1963a, Fig. 10). Neither does the accuracy of the computations seem to be the cause for the discrepancy. However, the regularity of the deviation and its intensification at high Mach numbers do point to the terms linear in $1/t_{xx}$ and $1/t_x$ entering the functions j_0 and j_1 as being the likely cause for the deviation. Indeed, the relevant weighting functions, k_1, k_2, κ_1, κ_2 (Figs. 9 and 10), make relatively important contributions and the linear terms are, in fact, the ones responsible for bringing the Prandtl number value to the vicinity of 2/3. In the absence of more accurate computations it is not possible to state whether from the viewpoint of the present model the Navier-Stokes solution is or is not in some slight error at $M_1 = 1.5$. This question here is of little or no importance anyway.

What is more relevant, however, is the apparently complete agreement at $M_1 = 1.5$ between the numerically exact solution of the B.G.K. model and the Navier-Stokes profile with Pr = 1. This agreement is in all the three, density, velocity and temperature profiles. As far as the present formulation is concerned, this result is somewhat unexpected since it has been shown earlier that the temperature as predicted by the B.G.K. model is quantitatively not correct even for weak shocks. In fact, the Navier-Stokes equations with Pr = 1 do not arise from the Boltzmann equation; the Chapman-Enskog solution of this equation has been shown to yield the Navier-Stokes equations with a Prandtl number value very nearly equal to 2/3. What is then the kinetic basis for the Navier-Stokes equations with Pr = 1? These equations arise, in fact, from the distribution function (2.46) which is the first order approximation in Chapman-Enskog series solution of the B.G.K. model itself. This then explains the reason for the complete agreement at the low Mach number and confirms the validity of Chapman-Enskog method to the B.G.K. model. Thus, in conclusion, the numerical results for weak shocks of both the B.G.K. model and the present model appear to justify the argument, given towards the end of section (4.2), that the exploratory model is too simple a representation of the Boltzmann equation.

At the higher Mach numbers, some light may be shed on the results of the present iteration by examining the Navier-Stokes predictions of the variations across the shock in the parameters $1/t_{xx}$ and $1/t_x$. Figure 11 shows that $1/t_{xx}$ can assume, particularly upstream, values much larger than about 0.3 (corresponding to $M_1 < 2.0$) which value is usually considered as a reasonable limit for the convergence of Chapman-Enskog series. Furthermore, the changes in the parameter $1/t_x$, shown in Fig. 12, are even greater and values nearly equal to 4.0 are attained. One can expect therefore deviations which become larger, particularly upstream, as the shock strength increases. This observation is in accord with the results obtained.

It is important, however, to see how the deviations are brought about by the shock equations themselves. Following the argument of Liepmann et al (1962, 1964), we may remark that the shock equations (5.23) crucially depend on the magnitude of the so-called sampling distance $V_x/L_i = V_x\lambda\beta^{\frac{1}{2}}/l_i$ appearing in the exponent. This distance represents a kind of free path at velocity V_x and depends on the entire loss term. In general, the velocities V_x which contribute most to the first few moments may be expected to be of order U. Downstream, the Mach number is of order unity, the parameters $1/t_{xx}$ and $1/t_x$ are small (i.e. l_i is large) and hence the sampling distance here is proportional to the mean free path. Under these circumstances, it can be shown (Liepmann et al) that the distribution function (5.10) may be expanded in series the first two terms of which giving the Navier-Stokes equations. On this basis also, the deviation of our iteration noticed downstream at high Mach numbers could possibly be due to the higher order terms of these series (which are largely influenced by the first three terms of j_0 and j_1, eq. (5.22)). For strong shocks the situation upstream is quite different Here, the Mach number, $1/t_{xx}$ and $1/t_x$ are large and the sampling distance is large too. The previous expansion is no longer possible but since a larger part of the input is now weighted, larger deviations from the Navier-Stokes profile may be expected. In fact, if the computed profiles are made use of to plot the relative deviation from the Navier-Stokes solution (e.g. $(n-n_{NS})/n_{NS}$, $(T-T_{NS})/T_{NS}$) versus distance, x/Λ_1, the behaviour of the resulting curves is found to be similar to that of l_i

(Figs. 13, 14). In other words, through their influence on the sampling distance, the input changes in $1/t_{xx}$ and $1/t_x$ provide some measure of the resulting relative deviation in the flow quantities.

It is recalled that the quantity l_o enters the number density equation and l_2 enters the temperature equation. Figures 13 and 14 show that l_2 is generally smaller than l_o and, hence, the sampling distance in the temperature equation is usually larger than the sampling distance in the number density equation. As a consequence, deviations occuring in the temperature profile are larger than those in number density and velocity profiles.

The results obtained for the high Mach number cases may be considered to be in broad general agreement with the B.G.K. solution. However, at $M_1 = 5.0$ and 10.0 a kink develops in the density and velocity profiles. The question first arises whether the present model has been solved numerically exactly. Clearly in cases of strong shocks a single iteration cannot be expected to produce very accurate results and, indeed, the computed profile is quite different from the initial profile. At $M_1 = 10.0$, for example, the values of n and U at $x/\Lambda_1 = -1.0$ deviate from the corresponding Navier-Stokes values by some 15% whereas the temperature, at points - 1.0, - 1.5, - 2.0, departs by 62%, 84% and 116% respectively. Also at $M_1 = 10.0$, the new values of $1/t_{xx}$ and $1/t_x$ at $x/\Lambda_1 = -2.0$ are estimated to be - 1.3 and 2.0 as compared with Navier-Stokes respective values of - 1.5 and 3.0. In fact, an inspection of the new profiles indicates that the changes in $1/t_{xx}$ and $1/t_x$ are generally less pronounced than those given by Navier-Stokes equations. Their new plots, while still showing a maximum, will be flatter, thicker and less peaky. Thus, if the present results are used to generate a new iteration the sampling distances upstream will generally be smaller than those used previously and new and somewhat less pronounced deviations can be expected. This means that, as far as the internal consistency of the model is concerned, the values of $1/t_{xx}$ and $1/t_x$ predicted upstream by the Navier-Stokes solution are too large. In computing the present iteration this caused the sampling distance to also become too large which in turn resulted in exaggerated corrections in this region. It may thus be concluded that on the upstream side of the shock all of our profiles are somewhat overestimated. The observed kink merely loosely marks the limit where the Navier-Stokes values of $1/t_{xx}$ and $1/t_x$ become more consistent with the description of the model. The absence of a kink in the temperature profile appears to be of no particular consequence. It should be added that the corrections required to smooth out the n and U profiles and make the kink disappear are at most 1% to 2% only. On the other hand, if the present results are used to generate a new iteration, the indication is that the profiles will be modified on the upstream side. The conclusion must be, therefore, that at this stage we cannot consider the kink as a real physical phenomenon implied by our model equation.

The energy equation (5.7c) may be rewritten in the form

$$m(H-H_1) = U\tau - q \; ; \; m = \rho_1 U_1 ,$$

where H is the total enthalpy, τ the viscous stress and q the heat flux. The relative deviation in the total enthalpy, H/H_1-1, calculated on the basis of the first iteration is plotted in Fig. 28 together with corresponding Navier-Stokes variation. The plots show that Navier-Stokes total enthalpy remains constant to within a few per cent whereas the present iteration predicts a progressively larger deviation with increases in Mach number. At $M_1 = 10.0$, the maximum relative deviation is nearly 15% while the corresponding value of the B.G.K. model is under 6% and the Navier-Stokes, Pr = 1, value is - 5% (Liepmann et al, 1964). Thus, our first iteration generally predicts $(-q) > (-U\tau)$, exhibits a larger degree of non-equilibrium than does the B.G.K. model and displays the inadequacy at high Mach numbers of the Navier-Stokes description of the viscous and heat conduction effects.

Other remarks can be made in connection with the first iteration but in the absence of more accurate computations such remarks merely serve as conjectures. However, one aspect of the results is worth mentioning here. The iteration shows that for strong shocks the parameters $1/t_{xx}$ and $1/t_x$ do not increase as fast as the Navier-Stokes equations predict. It is possible that the higher iterations will confirm this trend and that, more generally, the model equation will yield for these parameters certain limiting values. If this proves to be the case, the range of validity of the model will be wider than envisaged initially and its predictions will be in sharp contrast with those of Navier-Stokes. For according to this latter theory the parameter $1/t_{xx}$ tends to the limiting value 2.25 whereas $1/t_x$ increases beyond bounds as $M_1 \to \infty$ (Liepmann et al, 1962). This behaviour certainly demonstrates the failure of the Navier-Stokes description in such cases.

In conclusion, the shock structure in a monatomic gas is contained in the present formulation. For weak shocks it provides a description which duly agrees with that of Boltzmann's equation, while for strong shocks further iterations are required to solve the model equation. The presence of the kink in the density and velocity profiles does not permit the customary definition of a maximum slope thickness, though at $M_1 = 1.5, 3.0$ the maximum density slope thickness is in complete agreement with results of existing measurements. It is considered that the computation of further iterations is necessary and worthwhile, a task which may entail refining the present computer programme or the use of a more suitable numerical method in order to curtail sufficiently the computing time. Only when more accurate numerical results are available can conclusions be drawn regarding the structure of strong shocks in the present model and the behaviour of its distribution function within the shock.

The essence of the present method of approach has been to obtain an approximation to the distribution function. It is believed that for the whole range of Mach numbers the model equation derived provides a better representation of the Boltzmann equation than does the B.G.K. model.

REFERENCES

Anderson, D.G., (1965a). Numerical Solutions of the Krook Kinetic Equation. Technical Report No. 15, Engineering Sciences Laboratory, Harvard University.

Anderson, D.G., (1965b). On the Steady Krook Kinetic Equation. Technical Report No. 20, Engineering Sciences Laboratory, Harvard University.

Anderson, D.G. and Macomber, H.K., (1965). Numerical Experiments in Kinetic Theory. In 'Rarefied Gas Dynamics' (J.H. de Leeuw, ed.), Vol. I, p. 96. Academic Press.

Becker, R., (1922). 'Stosswelle und Detonation'. Z. Physik., 321 - 362, Bd. 8, (English Translation - NACA TM 505, NACA TM 506).

Bhatnagar, P.L., Gross, E.P. and Krook, M., (1954). A Model for the Collision Processes in Gases, I., Small Amplitude Processes in Charged and Neutral One-Component Systems. Phys. Rev., Vol. 94, No. 3, 511-525.

Burnett, D., (1935, 1936). The Distribution of Velocities in a Slightly Non-Uniform Gas, Proc. London Math. Soc., Vol. 39, 385. Also, the Distribution of Molecular Velocities and the Mean Motion in a Non-Uniform Gas. Proc. London Math. Soc., Vol. 40, 382.

Camac, M., (1965). Argon Shock Structure. In 'Rarefied Gas Dynamics' (J.H. de Leeuw, ed.), Vol. I, p. 240, Academic Press.

Chahine, M.T., (1963a). The Structure of Strong Shock Waves in the Krook Collision Model. In 'Rarefied Gas Dynamics' (J.A. Laurmann, ed.), Vol. I, p. 260, Academic Press. Also Technical Report No. 32 - 327, Jet Propulsion Laboratory, California Institute of Technology.

Chahine, M.T., (1963b). Numerical Techniques for the Solution of the Complete B.G.K. Kinetic Equation for Plane Shock Wave. Technical Report No. 32 - 421, Jet Propulsion Laboratory, California Institute of Technology.

Chahine, M.T., (1965). Numerical Solution of the Complete Krook-Boltzmann Equation for Strong Shock Waves. In 'Methods in Computational Physics' (B. Alder et al, eds.), Vol. 4, p. 83, Academic Press.

Chahine, M.T. and Narasimha, R., (1963). Evaluation of the Integral $\int_0^\infty V^n \exp[-(V-u)^2-x/V]dV$. Technical Report No. 32 - 459, Jet Propulsion Laboratory, California Institute of Technology.

Chahine, M.T. and Narasimha, R., (1965). Exact Numerical Solution of the Complete B.G.K. Equation for Strong Shock Waves. In 'Rarefied Gas Dynamics' (J.H. de Leeuw, ed.), Vol. I, p. 140, Academic Press.

Chapman, S., (1912). The Kinetic Theory of a Gas Constituted of Spherically Symmetrical Molecules. Phil. Trans. Roy. Soc., A , 211, 433.

Chapman, S., (1916). On the Law of Distribution of Molecular Velocities, and on the Theory of Viscosity and Thermal Conduction, in a Non-Uniform Simple Monatomic Gas. Phil. Trans. Roy. Soc., A, 216, 279.

Chapman, S. and Cowling, T.G., (1960). 'The Mathematical Theory of Non-Uniform Gases'. Cambridge Univ. Press.

Gilbarg, D. and Paolucci, D., (1953). The Structure of Shock Waves in the Continuum Theory of Fluids. Jour. Rational Mech. and Analysis, Vol. 2, No. 4, 617 - 642.

Glansdorff, P., (1961). The Thickness of Shock Waves by the Two-Fluid Theory Extended to Rarefied Gases. In 'Rarefied Gas Dynamics' (L. Talbot ed.), p. 475, Academic Press.

Grad, H., (1949). On the Kinetic Theory of Rarefied Gases. Comm. Pure and Applied Math., Vol. 2, p. 331.

Grad, H., (1952). The Profile of a Steady Plane Shock Wave. Comm. Pure and Applied Math., Vol. 5, p. 257.

Grad, H., (1958). Principles of the Kinetic Theory of Gases. In 'Handbuch der Physik' (S. Flugg, ed.), Vol. 12, p. 205, Springer, Berlin.

Grad, H., (1963). Asymptotic Theory of the Boltzmann Equation. Phys. Fluids, Vol. 6, No. 2, 147.

Guiraud, J.P., (1967). Kinetic Theory and Rarefied Gas Dynamics. In 'Rarefied Gas Dynamics' (C.L. Brundin, ed.), Vol. 1, p. 289, Academic Press.

Hugoniot, H., (1889). Journal de l'Ecole Polytechnique, 58, 1.

Jeans, J.H., (1952). 'An Introduction to the Kinetic Theory of Gases'. Cambridge Univ. Press.

Liepmann, H.W., Narasimha, R. and Chahine, M.T., (1962). Structure of a Plane Shock Layer. Phys. Fluids, Vol. 5, No. 11, 1313 - 1324.

Liepmann, H.W., Narasimha, R. and Chahine, M.T., (1964). Theoretical and Experimental Aspects of the Shock Structure Problem. Proc. of 11th International Conference Applied Mechanics, Munich, p. 973, Springer-Verlag, Berlin.

Lyubarskii, G. Ya, (1961). On the Kinetic Theory of Shock Waves. Soviet Phys. JETP 13, (4), 740 - 745.

Maxwell, J.C., (1867-9). Collected Works, 2, p. 26 and p. 681. Cambridge Univ. Press (1890).

Meyer, O.E., (1899). 'The Kinetic Theory of Gases'. Longmans Green and Co., London.

Mineur, H., (1952). 'Techniques de Calcul Numerique'. Librairie Polytechnique Ch. Beranger, Paris et Liege.

Morduchow, M. and Libby, P.A., (1949). On a Complete Solution of the One-Dimensional Flow Equations of a Viscous, Heat-Conducting, Compressible Gas. Jour. Aero. Sc., Vol. 16, p. 674.

Mott-Smith, H.M., (1951). The Solution of the Boltzmann Equation for a Shock Wave. Phys. Rev., Ser. 2, Vol. 82, No. 6, 885-892.

Muckenfuss, C., (1960). Bimodal Model for Shock Wave Structure. Phys. Fluids, Vol. 3, No. 2, 320-321.

Pennington, R.H., (1965). 'Introductory Computer Methods and Numerical Analysis'. The Macmillan Co., New York; Collier-Macmillan Ltd., London.

Pidduck, F.B., (1916). The Kinetic Theory of the Motions of Ions in Gases. Proc. Lond. Math. Soc., 15, p. 89.

Radin, S.H. and Mintzer, D., (1966). Orthogonal Polynomial Solution of the Boltzmann Equation for a Strong Shock Wave. Phys. Fluids, Vol. 9, No. 9, 1621 - 1633.

Rankine, W.J. Macquorn, (1870). On the Thermodynamic Theory of Waves of Finite Longitudinal Disturbance. Phil. Trans. Roy. Soc. (London), Vol. 160, Pt. 2, 277 - 288.

Rayleigh, Lord, (1910). Aerial Plane Waves of Finite Amplitude. Proc. Roy. Soc. (London), Ser. A, Vol. 84, No. 570, 247-284.

Russell, D., (1965). Electron-Beam Measurements of Shock-Wave Thickness. In 'Rarefied Gas Dynamics' (J.H. de Leeuw, ed.), Vol. I, p. 265, Academic Press.

Sherman, F.S.,(1955). A Low-Density Wind Tunnel Study of Shock-Wave Structure and Relaxation Phenomena in Gases, NACA TN 3298.

Sherman, F.S. and Talbot, L., (1960). Experiments Versus Kinetic Theory for Rarefied Gases. In 'Rarefied Gas Dynamics' (F.M. Devienne, ed.), p. 161, Pergammon Press.

Tait, P.G., (1886-8). Scientific Papers, 2, p. 124. Cambridge Univ. Press (1900).

Talbot, L. and Sherman, F.S., (1959), Structure of Weak Shock Waves in a Monatomic Gas. NASA Memo 12-14-58W.

Taylor, G.I., (1910). The Conditions Necessary for Discontinuous Motion in Gases. Proc. Roy. Soc. (London), Ser. A, Vol. 84, No. 571, 371-377.

Thomas, L.H., (1944). Note on Becker's Theory of the Shock Front. Jour. Chem. Phys., Vol. 12, No. 11, 449-453.

Vincenti, W.G. and Kruger, C.H., (1965). 'Introduction to Physical Gas Dynamics'. J. Wiley and Sons.

Waldmann, L., (1958). Transporterscheinungen in Gasen von Mittlerem Druck. In 'Handbuch der Physik' (S. Flugg, ed.), Vol. 12, p. 295, Springer, Berlin.

Wang Chang, C.S., (1948). On the Theory of the Thickness of Weak Shock Waves. Rep. UMH-3-F, Dept. Eng. Res., Univ. of Mich. (Also CM-503, Appl. Phys. Lab., Johns Hopkins Univ., Md.).

Ziering, S., Ek, F. and Koch, P., (1961). Two-Fluid Model for the Structure of Neutral Shock Waves. Allied Research Associates Inc., Boston, Mass., Document No. ARA-933.

Zollar, K., (1951). 'Fur Struktur des Verdichtungsstosses'. Z. Physik., Bd. 130, Heft 1, 1-38.

APPENDIX 1. MATHEMATICAL AIDS

1) $$\int_{c_1-c}^{c_1+c} x^2 dx = \frac{2}{3}c(3c_1^2+c^2), \qquad c_1 > c > 0.$$
$$= \frac{2}{3}c_1(3c^2+c_1^2), \qquad c > c_1 > 0.$$

2) $$\int_{c_1-c}^{c_1+c} x^4 dx = \frac{2}{5}c(5c_1^4+10c_1^2c^2+c^4), \qquad c_1 > c > 0.$$
$$= \frac{2}{5}c_1(5c^4+10c_1^2c^2+c_1^4), \qquad c > c_1 > 0.$$

3) $$\int_{c_1-c}^{c_1+c} x^6 dx = \frac{2}{7}c(7c_1^6+35c_1^4c^2+21c_1^2c^4+c^6), \qquad c_1 > c > 0.$$
$$= \frac{2}{7}c_1(7c^6+35c_1^2c^4+21c_1^4c^2+c_1^6), \qquad c > c_1 > 0.$$

4) $$\int x\, e^{-ax^2}dx = -\frac{e^{-ax^2}}{2a} ;$$ 5) $$\int x^3e^{-ax^2}dx = -\frac{e^{-ax^2}}{2a}(x^2+\frac{1}{a});$$

6) $$\int x^5e^{-ax^2}dx = -\frac{e^{-ax^2}}{2a}(x^4+\frac{2}{a}x^2+\frac{2.1}{a^2});$$

7) $$\int x^7e^{-ax^2}dx = -\frac{e^{-ax^2}}{2a}(x^6+\frac{3}{a}x^4+\frac{3.2}{a^2}x^2+\frac{3.2.1}{a^3});$$

8) $$\int x^9e^{-ax^2}dx = -\frac{e^{-ax^2}}{2a}(x^8+\frac{4}{a}x^6+\frac{4.3}{a^2}x^4+\frac{4.3.2}{a^3}x^2+\frac{4.3.2.1}{a^4});$$

9) $$\int x^{2n+1}e^{-ax^2}dx = -e^{-ax^2}\frac{n!}{2a^{n+1}}\sum_{0}^{n}\frac{(ax^2)^{\nu}}{\nu!}, \qquad n = 0,1, \ldots$$

10) $$\int x^2e^{-ax^2}dx = -\frac{e^{-ax^2}}{2a}x + \frac{1}{2a}\int e^{-ax^2}dx;$$

11) $$\int x^4e^{-ax^2}dx = -\frac{e^{-ax^2}}{2a}(x^3+\frac{3}{2a}x) + \frac{3.1}{2^2a^2}\int e^{-ax^2}dx;$$

12) $$\int x^6e^{-ax^2}dx = -\frac{e^{-ax^2}}{2a}(x^5+\frac{5}{2a}x^3+\frac{5.3}{2^2a^2}x) + \frac{5.3.1}{2^3a^3}\int e^{-ax^2}dx;$$

13) $$\int x^8 e^{-ax^2}dx = -\frac{e^{-ax^2}}{2a}\left(x^7+\frac{7}{2a}x^5+\frac{7.5}{2^2a^2}x^3+\frac{7.5.3}{2^3a^3}x\right)+\frac{7.5.3.1}{2^4a^4}\int e^{-ax^2}dx;$$

14) $$\int x^{2n}e^{-ax^2}dx = -e^{-ax^2}\frac{x^{-1}}{2a^{n+1}}\frac{(2n)!}{2^{2n}n!}\sum_1^n\frac{2^{2\nu}\nu!}{(2\nu)!}(ax^2)^\nu+\frac{(2n)!}{2^{2n}n!.a^n}\int e^{-ax^2}dx,$$

$n = 0, 1, \ldots,$

15) $$\int_{-x}^{x} y\int_{-y}^{\infty} e^{-z^2}dzdy = e^{-x^2}\frac{x}{2} + \left(x^2-\frac{1}{2}\right)\int_0^x e^{-y^2}dy\ ;$$

16) $$\int_{-x}^{x} y^3\int_{-y}^{\infty} e^{-z^2}dzdy = \frac{1}{4}e^{-x^2}\left(x^3+\frac{3}{2}x\right) + \left(\frac{x^4}{2}-\frac{3}{8}\right)\int_0^x e^{-y^2}dy\ ;$$

17) $$\int_{-x}^{x} y^5\int_{-y}^{\infty} e^{-z^2}dzdy = \frac{1}{6}e^{-x^2}\left(x^5+\frac{5}{2}x^3+\frac{15}{4}x\right) + \left(\frac{x^6}{3}-\frac{15}{24}\right)\int_0^x e^{-y^2}dy.$$

18) $$\int_x^\infty \frac{e^{-2y^2}}{y^3}dy = e^{-2x^2}\frac{1}{2x^2} - 2\int_x^\infty\frac{e^{-2y^2}}{y}dy\ ;$$

19) $$\int_x^\infty \frac{e^{-2y^2}}{y^5}dy = e^{-2x^2}\left(\frac{1}{4x^4}-\frac{1}{2x^2}\right)+\frac{2^2}{2!}\int_x^\infty\frac{e^{-2y^2}}{y}dy;$$

20) $$\int_x^\infty \frac{e^{-2y^2}}{y^7}dy = e^{-2x^2}\left(\frac{1}{6x^6}-\frac{1}{6x^4}+\frac{1}{3x^2}\right) - \frac{2^3}{3!}\int_x^\infty\frac{e^{-2y^2}}{y}dy;$$

21) $$\int_x^\infty \frac{e^{-2y^2}}{y^9}dy = e^{-2x^2}\left(\frac{1}{8x^8}-\frac{1}{12x^6}+\frac{1}{12x^4}-\frac{1}{6x^2}\right)+\frac{2^4}{4!}\int_x^\infty\frac{e^{-2y^2}}{y}dy.$$

22) $$\int_x^\infty e^{-y^2}\int_0^y e^{-z^2}dzdy = \frac{1}{2}\left[\frac{\pi}{4} - \left(\int_0^x e^{-y^2}dy\right)^2\right];$$

23) $$\int_x^\infty y^2e^{-y^2}\int_0^y e^{-z^2}dzdy = \frac{1}{2^2}\left[\frac{\pi}{4} - \left(\int_0^x e^{-y^2}dy\right)^2\right] + x\frac{e^{-x^2}}{2}\int_0^x e^{-y^2}dy+\frac{1}{8}e^{-2x^2};$$

24) $$\int_x^\infty y^4e^{-y^2}\int_0^y e^{-z^2}dzdy = \frac{3.1}{2^3}\left[\frac{\pi}{4}-\left(\int_0^x e^{-y^2}dy\right)^2\right]+\left(x^3+\frac{3}{2}x\right)\frac{e^{-x^2}}{2}\int_0^x e^{-y^2}dy$$

$$+\frac{1}{8}e^{-2x^2}\left(x^2+\frac{4}{2}\right);$$

25) $$\int_x^\infty y^6 e^{-y^2}\int_0^y e^{-z^2}dz\,dy = \frac{5\cdot 3\cdot 1}{2^4}\left[\frac{\pi}{4}-\Big(\int_0^x e^{-y^2}dy\Big)^2\right]$$
$$+\Big(x^5+\frac{5}{2}x^3+\frac{5\cdot 3}{2^2}x\Big)\frac{e^{-x^2}}{2}\int_0^x e^{-y^2}dy + \frac{1}{8}e^{-2x^2}\Big(x^4+\frac{7}{2}x^2+\frac{22}{4}\Big);$$

26) $$\int_x^\infty y^8 e^{-y^2}\int_0^y e^{-z^2}dz\,dy = \frac{7\cdot 5\cdot 3\cdot 1}{2^5}\left[\frac{\pi}{4}-\Big(\int_0^x e^{-y^2}dy\Big)^2\right]+\Big(x^7+\frac{7}{2}x^5+\frac{7\cdot 5}{2^2}x^3+\frac{7\cdot 5\cdot 3}{2^3}x\Big).$$
$$\cdot\ \frac{e^{-x^2}}{2}\int_0^x e^{-y^2}dy+\frac{1}{8}e^{-2x^2}\Big(x^6+\frac{10}{2}x^4+\frac{55}{4}x^2+\frac{160}{8}\Big);$$

27) $$\int_x^\infty y^{10} e^{-y^2}\int_0^y e^{-z^2}dz\,dy = \frac{9\cdot 7\cdot 5\cdot 3\cdot 1}{2^6}\left[\frac{\pi}{4}-\Big(\int_0^x e^{-y^2}dy\Big)^2\right]+\Big(x^9+\frac{9}{2}x^7+\frac{9\cdot 7}{2^2}x^5+\frac{9\cdot 7\cdot 5}{2^3}x^3+$$
$$+\frac{9\cdot 7\cdot 5\cdot 3}{2^4}x\Big)\ \frac{e^{-x^2}}{2}\int_0^x e^{-y^2}dy+\frac{1}{8}e^{-2x^2}\Big(x^8+\frac{13}{2}x^6+\frac{102}{4}x^4+\frac{519}{8}x^2+\frac{1464}{16}\Big).$$

28) $$\int_x^\infty \frac{e^{-y^2}}{y^2}\int_0^y e^{-z^2}dz\,dy = \int_x^\infty \frac{e^{-2y^2}}{y}dy - \left[\frac{\pi}{4}-\Big(\int_0^x e^{-y^2}dy\Big)^2\right] + \frac{1}{x}e^{-x^2}\int_0^x e^{-y^2}dy;$$

29) $$\int_x^\infty \frac{e^{-y^2}}{y^4}\int_0^y e^{-z^2}dz\,dy = -\frac{4}{3}\int_x^\infty \frac{e^{-2y^2}}{y}dy+\frac{2}{3\cdot 1}\left[\frac{\pi}{4}-\Big(\int_0^x e^{-y^2}dy\Big)^2\right] +$$
$$+\ \frac{1}{6x^2}e^{-2x^2}+\Big(\frac{1}{3x^3}-\frac{2}{3x}\Big)e^{-x^2}\int_0^x e^{-y^2}dy;$$

30) $$\int_x^\infty \frac{e^{-y^2}}{y^6}\int_0^y e^{-z^2}dz\,dy = \frac{14}{15}\int_x^\infty \frac{e^{-2y^2}}{y}dy-\frac{2^2}{5\cdot 3\cdot 1}\left[\frac{\pi}{4}-\Big(\int_0^x e^{-y^2}dy\Big)^2\right] +$$
$$\Big(\frac{1}{20x^4}-\frac{1}{6x^2}\Big)e^{-2x^2} + \Big(\frac{1}{5x^5}-\frac{2}{15x^3}+\frac{4}{15x}\Big)e^{-x^2}\int_0^x e^{-y^2}dy;$$

31) $$\int_x^\infty \frac{e^{-y^2}}{y^8}\int_0^y e^{-z^2}dz\,dy = \frac{-16}{35}\int_x^\infty \frac{e^{-2y^2}}{y}dy + \frac{2^3}{7\cdot 5\cdot 3\cdot 1}\left[\frac{\pi}{4}-\Big(\int_0^x e^{-y^2}dy\Big)^2\right] +$$
$$+\ \Big(\frac{1}{42x^6}-\frac{4}{105x^4}+\frac{2}{21x^2}\Big)e^{-2x^2}+\Big(\frac{1}{7x^7}-\frac{2}{35x^5}+\frac{4}{105x^3}-\frac{8}{105x}\Big)e^{-x^2}\int_0^x e^{-y^2}dy.$$

32) $$\int_x^\infty ye^{-y^2}\int_0^y e^{-z^2}dzdy = \frac{e^{-x^2}}{2}\int_0^x e^{-y^2}dy + \frac{1}{2}\int_x^\infty e^{-2y^2}dy;$$

33) $$\int_x^\infty y^3e^{-y^2}\int_0^y e^{-z^2}dzdy = (x^2+1)\frac{e^{-x^2}}{2}\int_0^x e^{-y^2}dy + \frac{e^{-2x^2}}{8}x + \frac{5}{8}\int_x^\infty e^{-2y^2}dy;$$

34) $$\int_x^\infty y^5e^{-y^2}\int_0^y e^{-z^2}dzdy = (x^4+2x^2+2\cdot 1)\frac{e^{-x^2}}{2}\int_0^x e^{-y^2}dy +$$
$$+ \frac{e^{-2x^2}}{8}(x^3+\frac{11}{4}x) + \frac{43}{32}\int_x^\infty e^{-2y^2}dy;$$

35) $$\int_x^\infty y^7e^{-y^2}\int_0^y e^{-z^2}dzdy = (x^6+3x^4+3\cdot 2x^2+3\cdot 2\cdot 1)\frac{e^{-x^2}}{2}\int_0^x e^{-y^2}dy +$$
$$+ \frac{e^{-2x^2}}{8}(x^5+\frac{17}{4}x^3+\frac{147}{16}x) + \frac{531}{128}\int_x^\infty e^{-2y^2}dy;$$

36) $$\int_x^\infty y^9e^{-y^2}\int_0^y e^{-z^2}dzdy = (x^8+4x^6+4\cdot 3x^4+4\cdot 3\cdot 2x^2+4\cdot 3\cdot 2\cdot 1)\ \frac{e^{-x^2}}{2}\int_0^x e^{-y^2}dy +$$
$$+ \frac{e^{-2x^2}}{8}(x^7+\frac{23}{4}x^5+\frac{307}{16}x^3+\frac{2457}{64}x) + \frac{8601}{512}\int_x^\infty e^{-2y^2}dy.$$

APPENDIX 2. INTEGRATIONS RELATING TO THE MODEL EQUATION

The loss and gain terms of Boltzmann's equation have been transformed in Chapter 3 and, for hard sphere molecules, are given by eqs. (3.21) and (3.22). These two equations contain, basically, a single unknown - the deviation function from Maxwellian, Φ. In section (4.3) an approximation to Φ has been chosen, as follows:

$$\Phi(\vec{c}) = -\{(c^2-\tfrac{5}{2})\, c_\alpha/t_\alpha + (c_\alpha c_\beta - \tfrac{1}{3}\delta_{\alpha\beta}c^2)/t_{\alpha\beta}\} \qquad \text{(A2.1)}$$

wherein standard tensor notation is being used, summing up over α, β = x, y, z; and δ is the Kronecker delta. The present Appendix is devoted to the determination of the three quantities $\overline{\Phi K_1}$, $\overline{\Phi K_2}$ and $\overline{\Phi K_4}$, which appear in (3.21) and (3.22), on the basis of the expression (A2.1) for Φ.

A. Determination of $\overline{\Phi K_1}$

By eq. (3.21) we require to determine the quantity

$$\overline{\Phi K_1} = \int_{-\infty}^{\infty} \Phi_1\, K_1(\vec{c},\vec{c}_1)\, \exp(-c_1^2)\, d\vec{c}_1$$

$$= -2^{-\frac{1}{2}}\pi^{-3/2}\int_{-\infty}^{\infty}\{(c_1^2-5/2)c_{1\alpha}/t_\alpha + (c_{1\alpha}c_{1\beta}-\tfrac{1}{3}\delta_{\alpha\beta}c_1^2)/t_{\alpha\beta}\}g\, \exp(-c_1^2)\, d\vec{c}_1, \qquad \text{(A2.2)}$$

in which Φ and K_1 have been substituted for from (A2.1) and (3.28), respectively. The presence of g, where $\vec{g} = \vec{c}_1 - \vec{c}$, in the integrand of (A2.2) necessitates the introduction of new variables of integration. Following the transformation presented at the end of section (1.5), we consider coordinate axes $\tilde{c}_{1\alpha}$ chosen in such a way that $\tilde{c}_{1_z}$ lies in the direction of $\vec{c}$. We may then write

$$c_{1\alpha} = \tilde{c}_{1_x}\xi_\alpha + \tilde{c}_{1_y}\eta_\alpha + \tilde{c}_{1_z}\zeta_\alpha, \qquad \text{(A2.3)}$$

where ξ_α, η_α, ζ_α are the direction cosines of the transformation, and are given by eq. (1.54), but with Ω and its components being correspondingly replaced by c and its components. Clearly, the Jacobian of the transformation is unity. Further, as in eq. (1.53), the velocity $\vec{c}_1$ may be expressed in terms of polar coordinates c_1, θ_1, ϕ_1 about $\vec{c}$ as axis. Thus,

$$\vec{c}_1 = (\tilde{c}_{1_x},\tilde{c}_{1_y},\tilde{c}_{1_z}) = (c_1\sin\theta_1\cos\phi_1, c_1\sin\theta_1\, \sin\phi_1, c_1\cos\theta_1); \qquad \text{(A2.4)}$$

and, in addition, we have

$$g^2 = c_1^2 + c^2 - 2cc_1\cos\theta_1, \qquad \text{(A2.5)}$$

so that the relative speed g does not involve ϕ_1. Furthermore, the direction cosines satisfy the relations

$$\begin{aligned} \xi_\alpha\xi_\beta + \eta_\alpha\eta_\beta + \zeta_\alpha\zeta_\beta &= 1, \text{ for } \alpha = \beta; \\ &= 0, \text{ for } \alpha \neq \beta. \end{aligned} \tag{A2.6}$$

By introducing these substitutions in eq. (A2.2), we find that the integration w.r.t. ϕ_1 can be carried out and yields

$$\overline{\Phi K_1} = K_{11}(c)c_\alpha/t_\alpha + K_{12}(c)(c_\alpha c_\beta - \tfrac{1}{3}\delta_{\alpha\beta}c^2)/t_{\alpha\beta}, \tag{A2.7}$$

in which ζ_α was eliminated by noting from (1.54) that $\zeta_\alpha = c_\alpha/c$, and K_{11} and K_{12} are given by:

$$K_{11}(c) = -\frac{(2\pi)^{-\frac{1}{2}}}{c} \int_0^\infty\int_0^\pi (c_1^2 - \tfrac{5}{2})c_1^3 g \exp(-c_1^2)\sin 2\theta_1 \, d\theta_1 \, dc_1, \tag{A2.8}$$

$$K_{12}(c) = \frac{(2\pi)^{-\frac{1}{2}}}{c^2} \int_0^\infty\int_0^\pi (3\sin^2\theta_1 - 2)c_1^4 g \exp(-c_1^2)\sin\theta_1 \, d\theta_1 \, dc_1. \tag{A2.9}$$

The variables of integration are next changed in (A2.8) to c_1 and $\cos\theta_1$, and in (A2.9) to c_1 and g, paying attention to the range of variation of the new limits of integration. Upon performing the integrations we obtain

$$K_{11}(c) = \frac{(2\pi)^{-\frac{1}{2}}}{2c^2}\left[e^{-c^2} - \frac{1}{c}\int_0^c e^{-x^2}dx\right], \tag{A2.10}$$

$$K_{12}(c) = (2\pi)^{-\frac{1}{2}}\frac{3}{4c^4}\left[e^{-c^2} + (\tfrac{2}{3}c - \tfrac{1}{c})\int_0^c e^{-x^2}dx\right]. \tag{A2.11}$$

B. Determination of $\overline{\Phi K_2}$

From eq. (3.22) this is given as follows:

$$\begin{aligned} \overline{\Phi K_2} &= \int_{-\infty}^{\infty} \Phi_1 K_2(\vec{c},\vec{c}_1)\exp(-c_1^2)d\vec{c}_1 \\ &= -2^{-\frac{1}{2}}\pi^{-3/2}\int_{-\infty}^{\infty}\{(c_1^2-\tfrac{5}{2})c_{1\alpha}/t_\alpha + (c_{1\alpha}c_{1\beta}-\tfrac{1}{3}\delta_{\alpha\beta}c_1^2)/t_{\alpha\beta}\}\frac{2}{g}. \\ &\quad .\exp\left[(|\vec{c}\Lambda\vec{c}_1|/g)^2 - c_1^2\right]d\vec{c}_1, \end{aligned} \tag{A2.12}$$

by substituting for Φ from (A2.1) and for K_2 from (3.29). The transformation made use of in the determination of $\overline{\Phi K_1}$ is introduced again here, whereby coordinates $\tilde{c}_{1\alpha}$ (with $\tilde{c}_{1_z}$ taken in the direction of $\vec{c}$) replace $c_{1\alpha}$, and introduced subsequently are the polar coordinates c_1, θ_1, ϕ_1, followed by the integration w.r.t. ϕ_1. The result may be obtained from eq. (A2.7) by replacing in (A2.8) and (A2.9) the expression of K_1 of (3.28) by the expression of K_2 of (3.29), since both K_1 and K_2 are independent of ϕ_1. Hence we can write

$$\overline{\Phi K_2} = K_{21}(c)\ c_\alpha/t_\alpha + K_{22}(c)\ (c_\alpha c_\beta - \tfrac{1}{3}\delta_{\alpha\beta}c^2)/t_{\alpha\beta}, \qquad \text{(A2.13)}$$

where

$$K_{21}(c) = -\frac{(2\pi)^{-\frac{1}{2}}}{c}\int_0^\infty\int_0^\pi \frac{2}{g}(c_1^2-\tfrac{5}{2})c_1^3 \exp\left[(|\vec{c}\wedge\vec{c}_1|/g)^2-c_1^2\right]\sin 2\theta_1 d\theta_1 dc_1, \qquad \text{(A2.14)}$$

$$K_{22}(c) = \frac{(2\pi)^{-\frac{1}{2}}}{c^2}\int_0^\infty\int_0^\pi \frac{2}{g}(3\sin^2\theta_1-2)c_1^4 \exp\left[(|\vec{c}\wedge\vec{c}_1|/g)^2-c_1^2\right]\sin\theta_1 d\theta_1 dc_1. \qquad \text{(A2.15)}$$

In these two expressions, the variables of integration c_1, θ_1 are replaced by g, $(\pi-\nu_1)$ where $(\pi-\nu_1)$ is the angle between $\vec{g}$ and $\vec{c}$, the limits of integration remaining unaltered. The quantity in the exponential takes the form

$$(|\vec{c}\wedge\vec{c}_1|/g)^2-c_1^2 = -(g-c\cos\nu_1)^2, \qquad \text{(A2.16)}$$

which further suggests that $(g-c\cos\nu_1)$ should be introduced as the variable of integration instead of g. The integrations in K_{21} and K_{22} can then be performed yielding the results

$$K_{21}(c) = (2\pi)^{-\frac{1}{2}}\left[e^{-c^2}\{-\tfrac{2}{3}c^2 + \tfrac{11}{6} - \tfrac{1}{4c^2}\}+\{-\tfrac{4}{3}c^3+3c+\tfrac{1}{4c^3}\}\int_0^c e^{-x^2}dx\right], \qquad \text{(A2.17)}$$

$$K_{22}(c) = \frac{(2\pi)^{-\frac{1}{2}}}{2c^2}\left[e^{-c^2}\{-c^2+1+\tfrac{3}{4c^2}\}+\{-2c^3+c-\tfrac{1}{2c}-\tfrac{3}{4c^3}\}\int_0^c e^{-x^2}dx\right]. \qquad \text{(A2.18)}$$

C. Determination of $\overline{\Phi K_4}$

By eq. (3.22) we have

$$\overline{\Phi K_4} = \int_{-\infty}^{\infty}\Phi_1 K_4(\Phi,\vec{c},\vec{c}_1)\exp(-c_1^2)d\vec{c}_1 \qquad \text{(A2.19)}$$

in which K_4 depends on Φ itself and, from (3.26), is given by

$$K_4 = 2^{\frac{1}{2}}\pi^{-3/2} g \int_0^{\pi/2} \exp(-g^2 tg^2\psi)\frac{\sin\psi}{\cos^3\psi}d\psi\{\frac{1}{2\pi}\int_0^{2\pi}\Phi(\vec{c}+gtg\psi\vec{n}_1)\exp(-2|\vec{c}\Lambda\vec{c}_1|\, tg\psi\cos\epsilon)d\epsilon\}. \qquad (A2.20)$$

Thus, the determination of $\overline{\Phi K_4}$ involves five integrations.

Consider initially the function K_4. The integrand of K_4 contains the quantity $\Phi(\vec{c}+gtg\psi\vec{n}_1)$, which is the function (A2.1) but with argument $\vec{c}+gtg\psi\vec{n}_1$, where $\vec{n}_1$ is a unit vector perpendicular to $\vec{g}$ in the $(\vec{R},\vec{g},\vec{R}_1)$ plane (see Fig. 4). The components of $\vec{c}$ in the direction of arbitrary coordinates x, y, z, are assumed to be known. Hence, the components of $\vec{n}_1$ along the same coordinate axes must be found and expressed in terms of the variables of integration ψ and ϵ of eq. (A2.20). The angle ψ lies in the $(\vec{R},\vec{g},\vec{R}_1)$ plane and is measured from the direction of $\vec{g}$. It is recalled that in passing from eq. (3.19) to (3.20) the notation $\epsilon_1, \vec{c}', \vec{R}$ of Fig. 4 was replaced by $\epsilon, \vec{c}_1, \vec{g}$, respectively. So that, in analogy with ϵ_1, the angle ϵ is the angle between the $(\vec{c}_1,\vec{g})$ plane and the $(\vec{g}.\vec{R})$ plane and is measured from the former plane.

Let the unit vector $\vec{n}_1$ have the components $n_{1\alpha}$ on an arbitrary set of rectangular coordinates. Also, let $\tilde{n}_{1\alpha}$ be another set of axes such that $\tilde{n}_{1_z}$ lies in the direction of $\vec{g}$. Then, by section (1.5), and recalling that $\vec{n}_1$ is perpendicular to $\vec{g}$, we have

$$n_{1\alpha} = \xi_\alpha\, \tilde{n}_{1_x} + \eta_\alpha\, \tilde{n}_{1_y}, \qquad (A2.21)$$

where the direction cosines are given by

$$\xi_1 = (g^2-g_x^2)^{\frac{1}{2}}/g\ ; \quad \xi_2 = -\, g_x g_y/g(g^2-g_x^2)^{\frac{1}{2}}\ ; \quad \xi_3 = -g_x g_z/g(g^2-g_x^2)^{\frac{1}{2}}\ ;$$

$$\eta_1 = 0 \quad ; \quad \eta_2 = g_z/(g^2-g_x^2)^{\frac{1}{2}} \quad ; \quad \eta_3 = -g_y/(g^2-g_x^2)^{\frac{1}{2}} \quad . \qquad (A2.22)$$

Using the same polar angles ψ and ϵ as in (A2.20), the components $\tilde{n}_{1\alpha}$ may be expressed as

$$\vec{n}_1 = (\tilde{n}_{1_x}, \tilde{n}_{1_y}, 0) = (-\cos\epsilon, \mp\sin\epsilon, 0). \qquad (A2.23)$$

Thus the required components $n_{1\alpha}$ are known in terms of ϵ. However, before we can actually establish the function $\Phi(\vec{c}+gtg\psi\vec{n}_1)$, the product $g\vec{c}.\vec{n}_1$ is required in terms of ϵ. The vector $\vec{c}$ lies in the $(\vec{c}_1,\vec{g})$ plane from which ϵ is measured, hence, by resolving $\vec{c}$ into components perpendicular and parallel to $\vec{g}$, we determine

$$g\vec{c}.\vec{n}_1 = |\vec{g}\Lambda\vec{c}|\cos\epsilon. \qquad (A2.24)$$

The function $\Phi(\vec{c}+gtg\psi\vec{n}_1)$ may now be written down in terms of ψ and ϵ; using eq. (A2.1) we get

$$\Phi(\vec{c}+g\,\mathrm{tg}\psi\vec{n}_1) = \Phi(\vec{c}) - \Big[(c_\alpha/t_\alpha-\delta_{\alpha\beta}/3t_{\alpha\beta})g^2\mathrm{tg}^2\psi+\{((c^2-5/2+g^2\mathrm{tg}^2\psi)/t_\alpha +$$

$$+ c_\beta(1/t_{\alpha\beta}+1/t_{\beta\alpha})\}g\,\mathrm{tg}\psi n_{1\alpha}+g^2\mathrm{tg}^2\psi n_{1\alpha}n_{1\beta}/t_{\alpha\beta} + (c_\alpha/t_\alpha-\delta_{\alpha\beta}/3t_{\alpha\beta})2a\; g\,\mathrm{tg}\psi\cos\epsilon +$$

$$+ 2ag^2\mathrm{tg}^2\psi\cos\epsilon\, n_{1\alpha}/t_\alpha\Big]; \qquad a = |\vec{c}\wedge\vec{c}_1|/g. \tag{A2.25}$$

Next, transform the expression for K_4 by substituting $\nu=g\,\mathrm{tg}\psi$ in (A2.20), obtaining

$$K_4 = (2\pi)^{-5/2}\,\frac{4}{g}\int_0^\infty\int_0^{2\pi}\exp(-\nu^2-2a\nu\cos\epsilon)\;\Phi(\vec{c}+\nu\vec{n}_1)\;\nu\;d\epsilon\, d\nu. \tag{A2.26}$$

Consider the integration w.r.t. ϵ; using eqs. (A2.21) to (A2.23), the contributing parts of $\Phi(\vec{c}+\nu\vec{n}_1)$ to (A2.26) are

$$\Phi(\vec{c}+\nu\vec{n}_1) = \Phi(\vec{c})-\Big[\{((c_\alpha-2a\;\xi_\alpha)/t_\alpha+(\xi_\alpha\xi_\beta-\delta_{\alpha\beta}/3)/t_{\alpha\beta}\}\;\nu^2-\nu^3\;\cos\epsilon\;\xi_\alpha/t_\alpha +$$

$$+\nu\;\cos\epsilon\{-(c^2-3/2)\xi_\alpha/t_\alpha + (c_\alpha/t_\alpha - \delta_{\alpha\beta}/3t_{\alpha\beta})2a-c_\beta\xi_\alpha(1/t_{\alpha\beta}+1/t_{\beta\alpha}) +$$

$$+ (\xi_\alpha\xi_\beta - \eta_\alpha\eta_\beta)/2at_{\alpha\beta}\}\Big]. \tag{A2.27}$$

Further, substitute in eq. (A2.26)

$$r\cos\mu = \nu\cos\epsilon + a\;; \qquad r\sin\mu = \nu\sin\epsilon, \tag{A2.28}$$

thereby yielding for K_4 the expression

$$K_4 = (2\pi)^{-5/2}\,\frac{4}{g}\exp(a^2)\int_0^\infty\int_0^{2\pi}\exp(-r^2)\Phi(\vec{c}+\nu\vec{n}_1)r\;d\mu\;dr. \tag{A2.29}$$

Expressing the function $\Phi(\vec{c}+\nu\vec{n}_1)$ of (A2.27) in terms of r and μ, the integrations in (A2.29) can be carried out giving the result

$$K_4 = (2\pi)^{-3/2}\,\frac{2}{g}\exp(a^2)\Big[\Phi(\vec{c})-\{((c_\alpha/t_\alpha-\delta_{\alpha\beta}/3t_{\alpha\beta})(1-a^2)+(\xi_\alpha\xi_\beta+\eta_\alpha\eta_\beta)/2t_{\alpha\beta} +$$

$$+ a^2\xi_\alpha\xi_\beta/t_{\alpha\beta} - a^3\xi_\alpha/t_\alpha + (c^2-3/2)a\xi_\alpha/t_\alpha + ac_\beta\xi_\alpha(1/t_{\alpha\beta}+1/t_{\beta\alpha})\}\Big]. \tag{A2.30}$$

Substituting in this for $\Phi(\vec{c})$, and noting from (A2.22) that

$$(\xi_\alpha\xi_\beta + \eta_\alpha\eta_\beta)/t_{\alpha\beta} = -(g_\alpha g_\beta/g^2 - \delta_{\alpha\beta})/t_{\alpha\beta}, \tag{A2.31}$$

and that from (A2.25)

$$a = |\vec{c}\wedge\vec{c}_1|/g = |\vec{c}\wedge\vec{g}|/g = c\;\sin\nu_1, \tag{A2.32}$$

where $(\pi-\nu_1)$ is the angle between $\vec{g}$ and $\vec{c}$. The function K_4 may then be expressed as

$$K_4 = -(2\pi)^{-3/2}\frac{2}{g}\exp(a^2)\Big[(c^2\cos^2\nu_1-5/2)(c_\alpha+a\xi_\alpha)/t_\alpha+\{(c_\alpha+a\xi_\alpha)(c_\beta+a\xi_\beta) -$$

$$-\delta_{\alpha\beta}c^2\cos^2\nu_1/3\}/t_{\alpha\beta}+(c_\alpha+a\xi_\alpha)/t_\alpha-(g_\alpha g_\beta/g^2-\delta_{\alpha\beta}/3)/2t_{\alpha\beta}\Big]. \quad (A2.33)$$

Next, since $\vec{\xi}$ is a unit vector perpendicular to $\vec{g}$ in the $(\vec{g},\vec{c}_1,\vec{c})$ plane from which the angle ϵ is measured, a simple vector diagram will show that

$$\vec{c}+a\vec{\xi} = -c\cos\nu_1\vec{n} \qquad (A2.34)$$

where $\vec{n}$ is a unit vector in the direction of $\vec{g}$. Using this in (A2.33) we may write

$$K_4 = -\frac{1}{2}K_2K_4^* \qquad (A2.35)$$

where

$$K_4^*(\vec{c},\vec{c}_1) = c\cos\nu_1(3/2-c^2\cos^2\nu_1)n_\alpha/t_\alpha+(c^2\cos^2\nu_1-\frac{1}{2})(n_\alpha n_\beta-\frac{1}{3}\delta_{\alpha\beta})/t_{\alpha\beta}, \quad (A2.36)$$

and K_2 is given by eq. (3.29). It may also be written in the form

$$K_2 = 2^{-\frac{1}{2}}\pi^{-3/2}\frac{2}{g}\exp(c^2\sin^2\nu_1). \qquad (A2.37)$$

It is seen that K_4 arises as the product of two weighting functions; namely K_2, which is involved in $\overline{\Phi K_2}$, and K_4^* which depends upon the orientation of the relative velocity but not upon its magnitude. Careful inspection of the result (3.20), which was derived in Chapter 3 for the purpose of transforming the Boltzmann equation, reveals that K_4 must satisfy the relationship

$$\int_{-\infty}^{\infty} K_4\exp(-c_1^2)d\vec{c}_1 = \overline{\Phi K_2}/2. \qquad (A2.38)$$

This requirement has been verified using the expression for K_4 just found.

There still remains three further integrations to be effected for the complete determination of $\overline{\Phi K_4}$. From eqs. (A2.19), (A2.35) and (A2.37), and upon the introduction of polar coordinates g, $\pi-\nu_1$, ϕ_1, where $(\pi-\nu_1)$ is the angle between $\vec{g}$ and $\vec{c}$, we may write

$$\overline{\Phi K_4} = 2(2\pi)^{-3/2}\int_0^{\pi}\int_0^{2\pi}\Delta_o(\nu_1,\phi_1)K_4^*\sin\nu_1\,d\phi_1\,d\nu_1. \qquad (A2.39)$$

The function K_4^* of (A2.36) depends on ν_1, ϕ_1 only, and Δ_o is defined by

$$\Delta_o(\nu_1,\phi_1) = -\int_0^{\infty}\Phi_1\exp(-\{g-c\cos\nu_1\}^2)g\,dg = -\int_{-y}^{\infty}\Phi_1\exp(-x^2)(x+y)dx, \quad (A2.40)$$

$$K_4 = -(2\pi)^{-3/2}\,\frac{2}{g}\exp(a^2)\Big[(c^2\cos^2\nu_1-5/2)(c_\alpha+a\xi_\alpha)/t_\alpha+\{(c_\alpha+a\xi_\alpha)(c_\beta+a\xi_\beta) -$$

$$-\,\delta_{\alpha\beta}c^2\cos^2\nu_1/3\}/t_{\alpha\beta} +(c_\alpha+a\xi_\alpha)/t_\alpha - (g_\alpha g_\beta/g^2 - \delta_{\alpha\beta}/3)/2t_{\alpha\beta}\Big]. \quad (A2.33)$$

Next, since $\vec{\xi}$ is a unit vector perpendicular to $\vec{g}$ in the $(\vec{g},\vec{c}_1,\vec{c})$ plane from which the angle ϵ is measured, a simple vector diagram will show that

$$\vec{c} + a\vec{\xi} = -c\cos\nu_1\vec{n} \qquad (A2.34)$$

where $\vec{n}$ is a unit vector in the direction of $\vec{g}$. Using this in (A2.33) we may write

$$K_4 = -\frac{1}{2}K_2K_4^* \qquad (A2.35)$$

where

$$K_4^*(\vec{c},\vec{c}_1) = c\,\cos\nu_1(3/2-c^2\cos^2\nu_1)n_\alpha/t_\alpha+(c^2\cos^2\nu_1-\tfrac{1}{2})(n_\alpha n_\beta-\tfrac{1}{3}\delta_{\alpha\beta})/t_{\alpha\beta}, \quad (A2.36)$$

and K_2 is given by eq. (3.29). It may also be written in the form

$$K_2 = 2^{-\frac{1}{2}}\pi^{-3/2}\,\frac{2}{g}\exp(c^2\sin^2\nu_1). \qquad (A2.37)$$

It is seen that K_4 arises as the product of two weighting functions; namely K_2, which is involved in $\overline{\Phi K_2}$, and K_4^* which depends upon the orientation of the relative velocity but not upon its magnitude. Careful inspection of the result (3.20), which was derived in Chapter 3 for the purpose of transforming the Boltzmann equation, reveals that K_4 must satisfy the relationship

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This requirement has been verified using the expression for K_4 just found.

There still remains three further integrations to be effected for the complete determination of $\overline{\Phi K_4}$. From eqs. (A2.19), (A2.35) and (A2.37), and upon the introduction of polar coordinates g, $\pi-\nu_1$, ϕ_1, where $(\pi-\nu_1)$ is the angle between $\vec{g}$ and $\vec{c}$, we may write

$$\overline{\Phi K_4} = 2(2\pi)^{-3/2}\int_0^{\pi}\int_0^{2\pi} \Delta_o(\nu_1,\phi_1)K_4^*\sin\nu_1\,d\phi_1\,d\nu_1. \qquad (A2.39)$$

The function K_4^* of (A2.36) depends on ν_1, ϕ_1 only, and Δ_o is defined by

$$\Delta_o(\nu_1,\phi_1) = -\int_0^{\infty}\Phi_1\exp(-\{g-c\,\cos\nu_1\}^2)g\,dg = -\int_{-y}^{\infty}\Phi_1\,\exp(-x^2)(x+y)dx, \quad (A2.40)$$

where we have introduced $x=g-c\cos\nu_1$, and $y=c\cos\nu_1$. By eq. (A2.1),

$$-\Phi(\vec{c}_1)=(c^2-5/2+g^2-2cg\cos\nu_1)(g_\alpha+c_\alpha)/t_\alpha+\{(g_\alpha+c_\alpha)(g_\beta+c_\beta)-\frac{1}{3}\delta_{\alpha\beta}(c^2+g^2-$$

$$-2cg\cos\nu_1)\}/t_{\alpha\beta}. \tag{A2.41}$$

Expressing Φ_1 in terms of x and y, noting that $g_\alpha=gn_\alpha$, and then introducing the result in eq. (A2.40), the integration w.r.t. x can be carried out without difficulty, yielding for $\Delta_o(\nu_1,\phi_1)$ the expression

$$\Delta_o=\left(\frac{c_\alpha}{t_\alpha}b_{o1}+\frac{c_\alpha c_\beta}{t_{\alpha\beta}}b_{o2}+\frac{1}{t_{\alpha\alpha}}b_{o3}\right)+n_\alpha\left(\frac{b_{11}}{t_\alpha}+b_{12}c_\beta\{\frac{1}{t_{\alpha\beta}}+\frac{1}{t_{\beta\alpha}}\}\right)+n_\alpha n_\beta\frac{b_2}{t_{\alpha\beta}}, \tag{A2.42}$$

where

$$b_{o1}=(c^2-\frac{3}{2}-y^2)\frac{1}{2}e^{-y^2}+(c^2-2-y^2)y\int_{-y}^{\infty}e^{-x^2}dx,$$

$$b_{o2}=\frac{1}{2}e^{-y^2}+y\int_{-y}^{\infty}e^{-x^2}dx,$$

$$b_{o3}=-\frac{1}{3}(c^2+1-y^2)\frac{1}{2}e^{-y^2}-\frac{1}{3}(c^2+\frac{1}{2}-y^2)y\int_{-y}^{\infty}e^{-x^2}dx, \tag{A2.43}$$

$$b_{11}=(c^2-2-y^2)y\,\frac{1}{2}e^{-y^2}+\{y^2(c^2-5/2-y^2)+(c^2-1)\frac{1}{2}\}\int_{-y}^{\infty}e^{-x^2}dx,$$

$$b_{12}=y\,\frac{1}{2}e^{-y^2}+(y^2+\frac{1}{2})\int_{-y}^{\infty}e^{-x^2}dx,$$

$$b_2=(1+y^2)\frac{1}{2}e^{-y^2}+(y^2+\frac{3}{2})y\int_{-y}^{\infty}e^{-x^2}dx.$$

With $\Delta_o(\nu_1,\phi_1)$ known, eq. (A2.39) may be rewritten in the form

$$\overline{\Phi K_4}=(2\pi)^{-\frac{1}{2}}\,2\int_0^{\pi}\Delta_1(\nu_1)\sin\nu_1 d\nu_1, \tag{A2.44}$$

where

$$\Delta_1(\nu_1)=\frac{1}{2\pi}\int_0^{2\pi}\Delta_o(\nu_1,\phi_1)K_4^*(\nu_1,\phi_1)d\phi_1. \tag{A2.45}$$

By eq. (A2.36), K_4^* may be expressed as

$$K_4^*=d_o\frac{\delta_{\gamma\delta}}{t_{\gamma\delta}}+d_1\frac{n_\gamma}{t_\gamma}+d_2\frac{n_\gamma n_\delta}{t_{\gamma\delta}} \tag{A2.46}$$

where

$$d_o = -\frac{1}{3}(y^2 - \frac{1}{2}); \quad d_1 = y(\frac{3}{2} - y^2); \quad d_2 = (y^2 - \frac{1}{2}). \qquad (A2.47)$$

Substituting for Δ_o and K_4^* in (A2.45), we have

$$\Delta_1(y) = \frac{1}{2\pi}\int_o^{2\pi} \Big\{ \frac{d_o}{t_{\gamma\gamma}}(\frac{c_\alpha}{t_\alpha}b_{o1} + \frac{c_\alpha c_\beta}{t_{\alpha\beta}}b_{o2} + \frac{b_{o3}}{t_{\alpha\alpha}}) + n_\alpha\Big[\frac{d_o}{t_{\gamma\gamma}}(\frac{b_{11}}{t_\alpha} + b_{12}c_\beta\{\frac{1}{t_{\alpha\beta}} + \frac{1}{t_{\beta\alpha}}\} +$$

$$+ \frac{d_1}{t_\alpha}(\frac{c_\beta}{t_\beta}b_{o1} + \frac{c_\beta c_\gamma}{t_{\beta\gamma}}b_{o2} + \frac{b_{o3}}{t_{\beta\beta}})\Big] + n_\alpha n_\beta\Big[\frac{b_2 d_o}{t_{\alpha\beta}t_{\gamma\gamma}} + \frac{d_2}{t_{\alpha\beta}}(\frac{c_\gamma}{t_\gamma}b_{o1} + \frac{c_\gamma c_\delta}{t_{\gamma\delta}}b_{o2} + \frac{b_{o3}}{t_{\gamma\gamma}}) +$$

$$+ \frac{d_1}{t_\alpha}(\frac{b_{11}}{t_\beta} + b_{12}c_\gamma\{\frac{1}{t_{\beta\gamma}} + \frac{1}{t_{\gamma\beta}}\})\Big] + n_\alpha n_\beta n_\gamma\Big[\frac{b_2 d_1}{t_{\alpha\beta}t_\gamma} + \frac{d_2}{t_{\alpha\beta}}(\frac{b_{11}}{t_\gamma} + b_{12}c_\delta\{\frac{1}{t_{\gamma\delta}} + \frac{1}{t_{\delta\gamma}}\})\Big] +$$

$$+ n_\alpha n_\beta n_\gamma n_\delta \frac{d_2 b_2}{t_{\alpha\beta}t_{\gamma\delta}}\Big\} d\phi_1. \qquad (A2.48)$$

In this expression the components of the unit vector $\vec{n}$ depend upon ϕ_1. Making use of the transformation given in section (1.5), whereby the components n_α are expressed in terms of $(\pi - \nu_1)$ and ϕ_1 and of course the appropriate direction cosines, we obtain

$$n_\alpha = \sin\nu_1 \cos\phi_1 \, \xi_\alpha + \sin\nu_1 \sin\phi_1 \, \eta_\alpha - \cos\nu_1 \, \zeta_\alpha. \qquad (A2.49)$$

The direction cosines are given by eq. (1.54), but with $\vec{c}$ replacing $\vec{\Omega}$, and satisfy eq. (A2.6). Finally, recalling that $y = c\cos\nu_1$, eq. (A2.44) may be written as

$$\overline{\Phi K_4} = (2\pi)^{-\frac{1}{2}} \frac{2}{c}\int_{-c}^{c} \Delta_1(y)dy. \qquad (A2.50)$$

We have now all the necessary information to determine $\Delta_1(y)$ and subsequently $\overline{\Phi K_4}$, the integrations are straightforward but the algebra involved is lengthy. Ultimately we obtain for $\overline{\Phi K_4}$ the following expression:

$$\overline{\Phi K_4} = \frac{c_\alpha c_\beta}{t_\alpha t_\beta}K_{40}(c) + \frac{1}{t_\alpha t_\alpha}K_{41}(c) + \frac{c_\alpha c_\beta c_\gamma c_\delta}{t_{\alpha\beta}t_{\gamma\delta}}K_{42}(c) + \frac{1}{t_{\alpha\alpha}t_{\beta\beta}}K_{43}(c) +$$

$$+ (\frac{1}{t_{\alpha\beta}} + \frac{1}{t_{\beta\alpha}})(\frac{1}{t_{\alpha\beta}} + \frac{1}{t_{\beta\alpha}})K_{44}(c) + \frac{c_\alpha c_\beta}{t_{\alpha\beta}t_{\gamma\gamma}}K_{45}(c) + c_\alpha c_\beta(\frac{1}{t_{\alpha\gamma}} + \frac{1}{t_{\gamma\alpha}})(\frac{1}{t_{\beta\gamma}} + \frac{1}{t_{\gamma\beta}})K_{46}(c) +$$

$$+ \frac{c_\alpha}{t_\alpha t_{\beta\beta}}K_{47}(c) + \frac{c_\alpha}{t_\beta}(\frac{1}{t_{\alpha\beta}} + \frac{1}{t_{\beta\alpha}})K_{48}(c) + \frac{c_\alpha c_\beta c_\gamma}{t_{\alpha\beta}t_\gamma}K_{49}(c), \qquad (A2.51)$$

where the K's are various average weighting functions and are given by

$$K_{40} = \frac{(2\pi)^{-\frac{1}{2}}}{4}\left[e^{-c^2}\left(\frac{c^4}{5}-\frac{29}{15}c^2+\frac{77}{30}-\frac{1}{4c^2}-\frac{3}{16c^4}\right)+\left(\frac{2}{5}c^5-\frac{11}{3}c^3+7c-\frac{3}{2c}+\frac{1}{8c^3}+\frac{3}{16c^5}\right)\int_0^c e^{-x^2}dx\right] \tag{A2.52}$$

$$K_{41} = \frac{(2\pi)^{-\frac{1}{2}}}{4}\left[e^{-c^2}\left(-\frac{c^6}{15}+\frac{8}{15}c^4-\frac{19}{30}c^2-\frac{1}{3}+\frac{1}{16c^2}\right)+\left(-\frac{2}{15}c^7+c^5-\frac{2}{3}c^3-2c+\frac{3}{8c}-\frac{1}{16c^3}\right)\int_0^c e^{-x^2}dx\right] \tag{A2.53}$$

$$K_{42} = \frac{(2\pi)^{-\frac{1}{2}}}{4}\left[e^{-c^2}\left(\frac{1}{4}-\frac{1}{2c^2}-\frac{7}{4c^4}-\frac{5}{2c^6}-\frac{105}{64c^8}\right)+\left(\frac{c}{2}-\frac{3}{4c}-\frac{1}{4c^3}+\frac{3}{8c^5}+\frac{45}{32c^7}+\frac{105}{64c^9}\right)\int_0^c e^{-x^2}dx\right] \tag{A2.54}$$

$$K_{43} = \frac{(2\pi)^{-\frac{1}{2}}}{4}\left[e^{-c^2}\left(-\frac{11}{540}c^4-\frac{c^2}{270}-\frac{19}{180}-\frac{1}{6c^2}-\frac{3}{64c^4}\right)+\left(-\frac{11}{270}c^5-\frac{c^3}{36}+\frac{c}{4}+\frac{13}{72c}+\frac{13}{96c^3}+\frac{3}{64c^5}\right)\int_0^c e^{-x^2}dx\right] \tag{A2.55}$$

$$K_{44} = \frac{(2\pi)^{-\frac{1}{2}}}{4}\left[e^{-c^2}\left(\frac{c^4}{120}+\frac{c^2}{60}-\frac{1}{15}-\frac{3}{128}\,\frac{1}{c^4}\right)+\left(\frac{c^5}{60}+\frac{c^3}{24}-\frac{c}{8}-\frac{1}{16c}-\frac{1}{64c^3}+\frac{3}{128c^5}\right)\int_0^c e^{-x^2}dx\right] \tag{A2.56}$$

$$K_{45} = \frac{(2\pi)^{-\frac{1}{2}}}{4}\left[e^{-c^2}\left(\frac{c^2}{18}-\frac{1}{9}+\frac{7}{6c^2}+\frac{1}{c^4}+\frac{15}{32c^6}\right)+\left(\frac{c^3}{9}-\frac{c}{6}-\frac{1}{2c}-\frac{7}{12c^3}-\frac{11}{16c^5}-\frac{15}{32c^7}\right)\int_0^c e^{-x^2}dx\right], \tag{A2.57}$$

$$K_{46} = \frac{(2\pi)^{-\frac{1}{2}}}{4}\left[e^{-c^2}\left(-\frac{c^2}{12}+\frac{1}{6}+\frac{1}{4c^4}+\frac{15}{64c^6}\right)+\left(-\frac{c^3}{6}+\frac{1}{4c}+\frac{c}{4}+\frac{1}{8c^3}-\frac{3}{32c^5}-\frac{15}{64c^7}\right)\int_0^c e^{-x^2}dx\right] \tag{A2.58}$$

$$K_{47} = \frac{(2\pi)^{-\frac{1}{2}}}{4}\left[e^{-c^2}\left(-\frac{c^4}{45}+\frac{7}{30}c^2+\frac{127}{180}-\frac{1}{24c^2}\right)+\left(-\frac{2}{45}c^5+\frac{4}{9}c^3-c+\frac{1}{3c}+\frac{1}{24c^3}\right)\int_0^c e^{-x^2}dx\right] \tag{A2.59}$$

$$K_{48} = \frac{(2\pi)^{-\frac{1}{2}}}{4}\left[e^{-c^2}\left(-\frac{2}{15}c^4+\frac{11}{15}c^2-\frac{13}{30}+\frac{1}{4c^2}\right)+\left(-\frac{4}{15}c^5+\frac{4}{3}c^3-\frac{1}{c}-\frac{1}{4c^3}\right)\int_0^c e^{-x^2}dx\right], \tag{A2.60}$$

$$K_{49} = \frac{(2\pi)^{-\frac{1}{2}}}{4}\left[e^{-c^2}\left(\frac{c^2}{3}-\frac{13}{6}-\frac{5}{4c^2}-\frac{3}{8c^4}\right)+\left(\frac{2}{3}c^3-4c+\frac{3}{c}+\frac{1}{c^3}+\frac{3}{8c^5}\right)\int_0^c e^{-x^2}dx\right]. \tag{A2.61}$$

APPENDIX 3. INTEGRATIONS RELATING TO THE SHOCK WAVE EQUATIONS

In section (5.4) there arises integrations involving the one-dimensional gain term, $G(\vec{V},x)$, w.r.t. the molecular velocity components V_y and V_z. These are:

$$J_i(V_x,x) = \iint_{-\infty}^{\infty} (V_y^2 + V_z^2)^i \, G(\vec{V},x) \, dV_y \, dV_z, \quad i = 0,1; \tag{A3.1}$$

the function G and the quantities it contains are given in section (5.1). When G is substituted for from eq. (5.2) we get

$$J_i(V_x,x) = \pi^{-\frac{1}{2}} j_i(V_x,x) n(x)/\lambda(x)\beta^i(x) \tag{A3.2}$$

where

$$j_i(V_x,x) = \frac{1}{\pi}\iint_{-\infty}^{\infty} (v_y^2 + v_z^2)^i e^{-c^2}(K_o + \overline{\Phi K_2} + \overline{\Phi K_4}) dv_y \, dv_z, \tag{A3.3}$$

and, by using (3.3), non-dimensional velocity components are introduced. For the present case we have

$$v_x = c_x + u(x), \quad v_y = c_y, \quad v_z = c_z, \tag{A3.4}$$

and the functions K_o, $\overline{\Phi K_2}$ and $\overline{\Phi K_4}$ depend on c_y and c_z only through their dependence on the random speed c. Hence, by introducing in (A3.3) the substitutions

$$v_y = \rho\cos\mu, \quad v_z = \rho\sin\mu, \tag{A3.5}$$

we may write

$$\frac{1}{\pi}\iint_{-\infty}^{\infty}\{ \, \}dv_y \, dv_z = \frac{1}{\pi}\int_0^{\infty}\int_0^{2\pi}\{ \, \}\rho d\rho d\mu = 2\int_0^{\infty}\{ \, \}\rho d\rho, \tag{A3.6}$$

where the brackets symbolize the integrand. Equation (A3.6) suggests the further substitution

$$c^2 = c_x^2 + \rho^2. \quad cdc = \rho d\rho, \tag{A3.7}$$

in which event, (A3.3) takes the form

$$j_i(c_x,x) = 2\int_{c_x}^{\infty}(c^2 - c_x^2)^i e^{-c^2}(K_o + \overline{\Phi K_2} + \overline{\Phi K_4}) \, cdc. \tag{A3.8}$$

This relation involves a single integration w.r.t. the dummy variable c; by (3.27), K_o is a function of c alone, and by section (5.1), $\overline{\Phi K_2}$ and $\overline{\Phi K_4}$ depend on c through the weighting functions K's which have been obtained in Appendix 2. Thus, the integration in (A3.8) is straightforward, but the algebra is very elaborate and will not be given here. However, the types of integrals encountered in the determination of (A3.8) are presented in Appendix 1.

A. The result $j_o(c_x,x)$

For i = o, eq. (A3.8) reduces to

$$j_o(c_x,x) = 2\int_{c_x}^{\infty} e^{-c^2}(K_o + \overline{\Phi K_2} + \overline{\Phi K_4})\, c\,dc. \tag{A3.9}$$

Using section (5.1) and Appendix 2 to substitute for the unknown quantities in the integrand, and then integrating, we obtain (the subscript x in c_x is dropped),

$$j_o(c,x) = k_o + k_1/t_{xx} + k_2/t_x + k_3/t_{xx}^2 + k_4/t_x^2 + k_5/t_x t_{xx}. \tag{A3.10}$$

The k's are weighting functions which depend only on the component of the random speed in the x-direction. They have the following expressions:

$$k_o(c) = (2\pi)^{-\frac{1}{2}}e^{-c^2}\left[e^{-c^2}+2c\int_0^c e^{-x^2}dx + 2e^{c^2}\{\tfrac{\pi}{4}-(\int_0^c e^{-x^2}dx)^2\}\right], \tag{A3.11}$$

$$k_1(c) = \frac{(2\pi)^{-\frac{1}{2}}}{3}e^{-c^2}\left[e^{-c^2}(1-c^2)+(c-2c^3)\int_0^c e^{-x^2}dx\right], \tag{A3.12}$$

$$k_2(c) = \frac{(2\pi)^{-\frac{1}{2}}}{3}e^{-c^2}\left[e^{-c^2}(\tfrac{5}{2}c-2c^3)+(\tfrac{3}{2}+3c^2-4c^4)\int_0^c e^{-x^2}dx\right], \tag{A3.13}$$

$$k_3(c) = \frac{(2\pi)^{-\frac{1}{2}}}{270}e^{-c^2}\left[e^{-c^2}(-7-\tfrac{19}{2}c^2-c^4)+(\tfrac{75}{2}c-20c^3-2c^5)\int_0^c e^{-x^2}dx\right], \tag{A3.14}$$

$$k_4(c) = \frac{(2\pi)^{-\frac{1}{2}}}{60}e^{-c^2}\left[e^{-c^2}(-7+22c^2-17c^4+2c^6)+(-15c+55c^3-32c^5+4c^7)\int_0^c e^{-x^2}dx\right], \tag{A3.15}$$

$$k_5(c) = \frac{(2\pi)^{-\frac{1}{2}}}{180} e^{-c^2}\left[e^{-c^2}(24c-31c^3+2c^5)+(-30+135c^2-60c^4+4c^6)\int_0^c e^{-x^2}dx\right]. \tag{A3.16}$$

The result (A3.10) can be inspected by noting from (5.15) that the conservation of mass requires that

$$\pi^{-\frac{1}{2}}\int_{-\infty}^{\infty} j_o(c_x,x)dv_x = l_o(x), \tag{A3.17}$$

where l_o is given by (5.18a). In addition, the conservation of momentum requires that

$$\pi^{-\frac{1}{2}}\int_{-\infty}^{\infty} v_x j_o(c_x,x)dv_x = u(x)l_1(x), \tag{A3.18}$$

where l_1 is given by (5.18b). Both of these requirements have been verified.

B. <u>The result $j_1(c_x,x)$</u>

For i = 1, eq. (A3.8) may be written in the form

$$j_1(c_x,x) = \tilde{j}_1(c_x,x)-c_x^2 j_o(c_x,x), \tag{A3.19}$$

where

$$\tilde{j}_1(c_x,x) = 2\int_{c_x}^{\infty} e^{-c^2}(K_o+\overline{\Phi K_2}+\overline{\overline{\Phi}K_4})c^3dc, \tag{A3.20}$$

which is similar to (A3.9) except for the presence of c^3. Integrating, we obtain

$$\tilde{j}_1(c,x) = \tilde{\kappa}_o+\tilde{\kappa}_1/t_{xx}+\tilde{\kappa}_2/t_x+\tilde{\kappa}_3/t_{xx}^2+\tilde{\kappa}_4/t_x^2+\tilde{\kappa}_5/t_x t_{xx}, \tag{A3.21}$$

where the $\tilde{\kappa}$'s are given by

$$\tilde{\kappa}_o(c)=(2\pi)^{-\frac{1}{2}}e^{-c^2}\left[e^{-c^2}(\tfrac{3}{2}+c)+(4c+2c^3)\int_0^c e^{-x^2}dx+2e^{c^2}\{\tfrac{\pi}{4}-(\int_0^c e^{-x^2}dx)^2\}\right], \tag{A3.22}$$

$$\tilde{\kappa}_1(c)=\frac{(2\pi)^{-\frac{1}{2}}}{3}e^{-c^2}\left[e^{-c^2}(1-c^4)+(c-c^3-2c^5)\int_0^c e^{-x^2}dx+2e^{c^2}\{\tfrac{\pi}{4}-(\int_0^c e^{-x^2}dx)^2\}\right], \tag{A3.23}$$

$$\tilde{\kappa}_2(c)=\frac{(2\pi)^{-\frac{1}{2}}}{3}e^{-c^2}\left[e^{-c^2}(-\tfrac{1}{2}c+\tfrac{1}{2}c^3-2c^5)+(-\tfrac{3}{2}c^2-c^4-4c^6)\int_0^c e^{-x^2}dx\right], \qquad (A3.24)$$

$$\tilde{\kappa}_3(c)=\frac{(2\pi)^{-\frac{1}{2}}}{270}e^{-c^2}\left[e^{-c^2}(\tfrac{41}{2}-34c^2-\tfrac{21}{2}c^4-c^6)+(45c-\tfrac{35}{2}c^3-22c^5-2c^7)\int_0^c e^{-x^2}dx\right], \qquad (A3.25)$$

$$\tilde{\kappa}_4(c)=\frac{(2\pi)^{-\frac{1}{2}}}{60}e^{-c^2}\left[e^{-c^2}(1+3c^2+9c^4-15c^6+2c^8)+(\tfrac{15}{2}c+5c^3+31c^5-28c^7+4c^9)\int_0^c e^{-x^2}dx\right], \qquad (A3.26)$$

$$\tilde{\kappa}_5(c)=\frac{(2\pi)^{-\frac{1}{2}}}{180}e^{-c^2}\left[e^{-c^2}(44c-17c^3-29c^5+2c^7)+(75c^2+55c^4-56c^6+4c^8)\int_0^c e^{-x^2}dx\right]. \qquad (A3.27)$$

It may be verified, by inspection of eq. (5.15), that the conservation of energy requires that

$$\frac{1}{\pi^{\frac{1}{2}}}\int_{-\infty}^{\infty}\tilde{j}_1(c_x,x)dv_x = \frac{2}{\pi^{\frac{1}{2}}}\left[\frac{7}{4}-\frac{11}{720}\,\frac{1}{t_{xx}^2}+\frac{1}{768}\,\frac{1}{t_x^2}\right]. \qquad (A3.28)$$

Substituting for $\tilde{j}_1$ from (A3.21) and integrating, we find that this requirement is satisfied.

Finally, the knowledge of j_o and $\tilde{j}_1$ enables us to determine j_1 using eq. (A3.19). We find that

$$j_1(c_x,x) = \kappa_o+\kappa_1/t_{xx}+\kappa_2/t_x+\kappa_3/t_{xx}^2+\kappa_4/t_x^2+\kappa_5/t_xt_{xx}, \qquad (A3.29)$$

where the κ's are given as follows:

$$\kappa_o(c)=(2\pi)^{-\frac{1}{2}}e^{-c^2}\left[e^{-c^2}\tfrac{3}{2}+4c\int_0^c e^{-x^2}dx+2(1-c^2)e^{c^2}\{\tfrac{\pi}{4}-(\int_0^c e^{-x^2}dx)^2\}\right], \qquad (A3.30)$$

$$\kappa_1(c) = \frac{(2\pi)^{-\frac{1}{2}}}{3}e^{-c^2}\left[e^{-c^2}(1-c^2)+(c-2c^3)\int_0^c e^{-x^2}dx+2e^{c^2}\{\tfrac{\pi}{4}-(\int_0^c e^{-x^2}dx)^2\}\right], \qquad (A3.31)$$

$$\kappa_2(c)=\frac{(2\pi)^{-\frac{1}{2}}}{3}e^{-c^2}\left[e^{-c^2}(-\tfrac{1}{2}c-2c^3)+(-3c^2-4c^4)\int_0^c e^{-x^2}dx\right], \qquad (A3.32)$$

$$\kappa_3(c)=\frac{(2\pi)^{-\frac{1}{2}}}{270}e^{-c^2}\left[e^{-c^2}(\tfrac{41}{2}-27c^2-c^4)+(45c-55c^3-2c^5)\int_0^c e^{-x^2}dx\right], \qquad (A3.33)$$

$$\kappa_4(c)=\frac{(2\pi)^{-\frac{1}{2}}}{60}e^{-c^2}\left[e^{-c^2}(1+10c^2-13c^4+2c^6)+\left(\frac{15}{2}c+20c^3-24c^5+4c^7\right)\int_0^c e^{-x^2}dx\right], \tag{A3.34}$$

$$\kappa_5(c)=\frac{(2\pi)^{-\frac{1}{2}}}{180}e^{-c^2}\left[e^{-c^2}(44c-41c^3+2c^5)+(105c^2-80c^4+4c^6)\int_0^c e^{-x^2}dx\right]. \tag{A3.35}$$

APPENDIX 4. COMPUTER PROGRAMMING OF THE SHOCK WAVE EQUATIONS

The present Appendix is concerned with the details of the numerical method discussed in Chapter 6 for the solution of the shock wave equations.

Representation of the Shock Equations.

It is not practicable to handle on a computer infinite limits of integration such as those in the velocity and physical spaces that arise from computing the moments n(x) and T(x), using eqs. (5.23a) and (5.23c). However, by following Chahine (1965), these equations can be represented in forms more suitable for rapid numerical computations by noting that the integrands become smaller as v becomes larger and ultimately vanish as $v \to \pm \infty$. Further, on the basis of the Navier-Stokes equations, the solutions for the flow parameters rapidly converge to their Rankine-Hugoniot limits. These features of the equations enable us to truncate the infinite limits of integration and still achieve a substantial degree of accuracy in the calculations.

It is convenient to introduce the following dimensionless quantities:

$$\theta(x) = T(x)/T_1; \quad W(x) = U(x)/U_1 ; \qquad N(x) = n(x)/n_1 = 1/W(x);$$

$$S(x) = u(x) = U(x)/\{2RT(x)\}^{\frac{1}{2}} = (5/6)^{\frac{1}{2}}M_1 \; W(x)/\{\theta(x)\}^{\frac{1}{2}};$$

$$\Gamma(x) = \lambda(x)/\lambda_1 = \{\mu(T)/\mu_1\}/N\{\theta(x)\}^{\frac{1}{2}};$$

$$\eta = v_x = V_x/\{2RT(x)\}^{\frac{1}{2}};$$

$$1/t_{xx} = \frac{4}{\sqrt{\pi}} \, S(x) \, \frac{\Gamma(x)}{W(x)} \, \frac{dW(x)}{dx};$$

$$1/t_x = \frac{3}{\sqrt{\pi}} \, \frac{\Gamma(x)}{\theta(x)} \, \frac{d\theta(x)}{dx}. \qquad (A4.1)$$

In these equations x is the physical coordinate made dimensionless by using the Maxwellian mean free path λ_1, eq. (5.25), ahead of the shock layer. With this notation, the problem is characterized by the following constants:

$$N_2 = n_2/n_1 = 1/W_2 = 4M_1^2/(M_1^2+3);$$

$$\theta_2 = T_2/T_1 = (5M_1^4+14M_1^2-3)/16M_1^2;$$

$$\Gamma_2 = \lambda_2/\lambda_1 = (\mu_2/\mu_1)/N_2\sqrt{\theta_2} \; ;$$

$$S_1 = (5/6)^{\frac{1}{2}}M_1; \quad S_2 = \{\tfrac{5}{6}(M_1^2+3)/(5M_1^2-1)\}^{\frac{1}{2}};$$

$$\lambda_1 = (5\pi/6)^{\frac{1}{2}}M_1\mu_1/\rho_1 U_1. \qquad (A4.2)$$

Define a point ξ_1 far upstream and a point ξ_2 far downstream such that for $x < \xi_1$ and $x > \xi_2$ the flow parameters may be taken to be equal to their respective constant upstream and downstream values. In order to introduce ξ_1 and ξ_2 into the integration limits of (5.23), we define, following Chahine (1963b, 1965), a symbolic function H by

$$H(\alpha) = 1, \quad \alpha \geqslant 0; \qquad\qquad H(\alpha) = 0, \quad \alpha < 0. \tag{A4.3}$$

By making use of this function and the dimensionless quantities introduced above, eq. (5.23a) can be expressed as follows:

$$\begin{aligned}
2N(x) = {} & H(\xi_2 - x)\frac{2}{\sqrt{\pi}} \int_0^{-\infty} \int_x^{\xi_2} \frac{N(x')}{\Gamma(x')}\{j_o(\eta, x')/\eta\} \exp\{-h_o(x, x')/\eta\}\, dx'\, d\eta \\
& - H(x - \xi_1)\frac{2}{\sqrt{\pi}} \int_0^{\infty} \int_x^{\xi_1} \frac{N(x')}{\Gamma(x')}\{j_o(\eta, x')/\eta\} \exp\{-h_o(x, x')/\eta\}\, dx'\, d\eta \\
& - H(\xi_2 - x) N_2 \int_0^{-\infty} k_o(\eta - S_2) \exp\{-h_o(x, \xi_2)/\eta\}\, d\eta \\
& + H(x - \xi_1) \int_0^{\infty} k_o(\eta - S_1) \exp\{-h_o(x, \xi_1)/\eta\}\, d\eta \\
& - H(x - \xi_2) N_2 \int_0^{-\infty} k_o(\eta - S_2)\, d\eta \\
& + H(\xi_1 - x) \int_0^{\infty} k_o(\eta - S_1)\, d\eta .
\end{aligned} \tag{A4.4}$$

Similarly eq. (5.23c) may take the following form:

$$\begin{aligned}
& 3N(x)\theta(x) + 2N(x)\{S_1 W(x)\}^2 = \\
& = H(\xi_2 - x)\frac{2}{\sqrt{\pi}} \int_0^{-\infty} \int_x^{\xi_2} \theta(x') \frac{N(x')}{\Gamma(x')}\{\eta j_o(\eta, x') + j_1(\eta, x')/\eta\} \exp\{-h_2(x, x')/\eta\}\, dx'\, d\eta \\
& - H(x - \xi_1)\frac{2}{\sqrt{\pi}} \int_0^{\infty} \int_x^{\xi_1} \theta(x') \frac{N(x')}{\Gamma(x')}\{\eta j_o(\eta, x') + j_1(\eta, x')/\eta\} \exp\{-h_2(x, x')/\eta\}\, dx'\, d\eta \\
& - H(\xi_2 - x) N_2 \frac{S_2^2 + 3/2}{S_2^2 + 7/4}\theta_2 \int_0^{-\infty} \{\eta^2 k_o(\eta - S_2) + \kappa_o(\eta - S_2)\} \exp\{-h_2(x, \xi_2)/\eta\}\, d\eta \\
& + H(x - \xi_1) \frac{S_1^2 + 3/2}{S_1^2 + 7/4} \int_0^{\infty} \{\eta^2 k_o(\eta - S_1) + \kappa_o(\eta - S_1)\} \exp\{-h_2(x, \xi_1)/\eta\}\, d\eta
\end{aligned}$$

$$- H(x-\xi_2)N_2\theta_2 \frac{S_2^2+3/2}{S_2^2+7/4} \int_0^{-\infty} \{\eta^2 k_o(\eta-S_2)+\kappa_o(\eta-S_2)\} d\eta$$

$$+ H(\xi_1-x)\frac{S_1^2+3/2}{S_1^2+7/4} \int_0^{\infty} \{\eta^2 k_o(\eta-S_1)+\kappa_o(\eta-S_1)\} d\eta . \qquad (A4.5)$$

In deriving eqs. (A4.4) and A4.5) use has been made of the relations (5.18) and (5.21) to obtain

$$j_o(\eta,\xi_1) = k_o(\eta-S_1) \; ; \quad l_o(\xi_1) = 2/\sqrt{\pi},$$

$$j_o(\eta,\xi_2) = k_o(\eta-S_2) \; ; \quad l_o(\xi_2) = 2/\sqrt{\pi},$$

$$j_1(\eta,\xi_1) = \kappa_o(\eta-S_1) \; ; \quad l_2(\xi_1) = (2/\sqrt{\pi})(S_1^2+7/4)/(S_1^2+3/2),$$

$$j_1(\eta,\xi_2) = \kappa_o(\eta-S_2) \; ; \quad l_2(\xi_2) = (2/\sqrt{\pi})(S_2^2+7/4)/(S_2^2+3/2), \qquad (A4.6)$$

and the function $h_i(x,x')$ is given by

$$h_i(x,x') = \{\theta(x')\}^{-\frac{1}{2}} \int_{x'}^{x} \frac{\{\theta(x'')\}^{\frac{1}{2}}}{\Gamma(x'')} l_i(x'')dx'' = \{\theta(x')\}^{-\frac{1}{2}} \int_{x'}^{x} L_i(x'')dx'' . \quad (A4.7)$$

The arguments x and x' of h_i represent, respectively, the upper and lower limits of the integral w.r.t. x''. For the four shock cases for which computations are made we have, by the analysis of Chapter 5, $h_i(x,x')/\eta \geqslant 0$ and the integrands, L_i, are bounded and do not change sign. However, from a numerical computation point of view the limit of $h_i(x,x')/\eta$ as $x' \rightarrow x$ and $\eta \rightarrow 0$ is undeterminate. This problem can be avoided by applying a Gaussian integration formula. Equations (A4.4) and (A4.5) represent the computational analogue to the shock equations (5.23) and form the basis for the computer programme given at the end of the present Appendix.

Saddle Point of the B.G.K. Shock Equations

Chahine and Narasimha (1963) and Chahine (1965) evaluated the saddle point, η_o, of the integrand w.r.t. η of the B.G.K. shock equations and determined the following approximations:

$$\eta_o \simeq S(x)\left[1 + \tfrac{1}{2}P - \tfrac{1}{2}P^2 + \tfrac{7}{8}P^3\right], \quad P < \tfrac{3}{4}, \; \eta > 0 \qquad (A4.8)$$

$$\eta_o \simeq S(x)\left[\tfrac{1}{3} + (\tfrac{P}{2})^{\frac{1}{3}}\right], \qquad P > \tfrac{3}{4}, \; \eta > 0 \qquad (A4.9)$$

$$\eta_o \simeq 0 \qquad , \quad P < \tfrac{1}{3}, \quad \eta < 0 \tag{A4.10}$$

$$\eta_o \simeq S(x)\left[\tfrac{1}{3} - (\tfrac{P}{2})^{\frac{1}{3}}\right], \quad P > \tfrac{1}{3}, \quad \eta < 0 \tag{A4.11}$$

where

$$P = h(x,x')/S^3(x). \tag{A4.12}$$

Function of Programme Components.

STRUCTURE OF SHOCK WAVE - Main programme organizes the job and the iteration scheme, as follows:

1) Number of iterations required and Navier-Stokes data for $N(x)$, $W(x)$, $\theta(x)$, $dW(x)/dx$ and $d\theta(x)/dx$ are specified. Programme evaluates the shock constants, eqs. (A4.2)

2) Tabulates values of the space-dependent quantities appearing in the shock equations and, subsequently, obtains their interpolated curves using SPLCON.

3) Values of x are specified where shock equations are to be evaluated.

4) Using PRMTS, the programme obtains newly computed data for the five basic quantities and extends them by computing rate of decay, then repeats from step (2) until number of iterations required is achieved.

SUBROUTINE PRMTS - Values of x and initial data are prescribed, the routine evaluates one iteration to the five basic quantities, as follows:

1) Using VAL and AUX1, the routine determines the values of $h_i(x,\xi_1)$ and $h_i(x,\xi_2)$ at all points x; then using VAL and AUX2, it evaluates the four onefold integrals of (A4.4) and (A4.5).

2) Using VAL and AUX3, the routine separately determines the contributions of the first two terms for a given value of x(the integration w.r.t. η is carried out by AUX3). Calculations are then repeated for all points x.

3) New data for $N(x)$, $W(x)$ and $\theta(x)$ are formed and the corresponding values of $dW(x)/dx$ and $d\theta(x)/dx$ are determined by a numerical differentiation. The results are communicated to the main programme.

SUBROUTINE SPLCON (X,Y,M,C) - An interpolation formula which connects each pair of adjacent points, of a given set of points, with a section of a third order polynomial (Pennington 1965, p. 404) and matches up the sections so that the first and second derivatives are continuous at each point. Values of a function Y are specified at points X whose number is M. The routine evaluates in each segment the four constants, C, of the polynomial.

SUBROUTINE SPLINE (X,Y,M,C,XI,YI) - Searching and interpolating routine. Values X,Y,M,C (where the constants C have been previously computed and stored) are specified together with a point XI. The routine determines which two points the given value XI lies between, then uses the interpolation formula appropriate to the segment to find YI.

SUBROUTINE VAL or GAL (A,B,ANS,AUXL,X,F,NOS,STEM) - A threepoint Gaussian formula (Mineur 1952, pp. 261-264) applied in a subdivided range of integration on the limits of which no restrictions are imposed (see Fig. 15 for block diagram). Specified are the lower limit A and the upper limit B, the initial length of a subinterval STEM and an auxiliary routine AUXL where information is to be found about the integrands F whose number is NOS. The routine calculates three values X (the Gaussian abscissae) and obtains the corresponding values of F from AUXL; simultaneously, it receives instructions regarding the length of the next subinterval, STEM. The routine forms the integral over the subinterval according to the Gaussian formula and repeats the procedure until all subintervals are covered. The accumulated sum represents the value ANS of the integral and is communicated to the calling routine.

SUBROUTINE AUX1 (X,F,NOS,STEM) - An auxiliary routine for evaluating the integrands $L_i(x'')$, eq. (A4.7). Given a point X, the routine evaluates, using SPLINE, the integrands F whose number is NOS and the next subinterval length, STEM.

SUBROUTINE AUX2 (U,YY,NOST,STER) - An auxiliary routine for evaluating the integrands of the four onefold integrals of eqs. (A4.4) and (A4.5) where $h_i(x,\xi_1)$ and $h_i(x,\xi_2)$ have been previously computed for all points x. Given a value U of the speed variable, the routine determines simultaneously the values of all the integrands at all points x. The results YY numbering NOST and next subinterval length, STER, are communicated to VAL.

SUBROUTINE AUX3 (R,QQ,NOST,STER) - Given specific values of x and x′, this auxiliary routine evaluates the integration w.r.t. η of the first two terms of eqs. (A4.4) and (A4.5). A point R, representing x′, is specified. Depending on the location of R in the physical space, the routine initially chooses the length of the next subinterval of integration, STER (Chahine 1965, p. 96). Then, by using GAL and AUX1, it evaluates $h_i(x,x')$ and the saddle point η_o. Finally, by using GAL and AUX4, it evaluates the required integrands QQ the number of which is NOST and, together with STER, communicates them to VAL.

SUBROUTINE AUX4 (ETA,Q,NIST,STEM) - An auxiliary routine for evaluating the integrands of the first two terms of eqs. (A4.4) and (A4.5), where all functions of x′, $h_i(x,x')$ and the corresponding saddle point η_o have been previously computed for specific values of x and x′. Depending on the given value ETA of the speed variable, the routine makes use of the value of η_o to decide on the subinterval length, STEM. The computed values of the integrands are returned to GAL.

FUNCTIONS - The weighting functions k_o, ..., k_5, κ_o, ..., κ_5, which are available in an analytical form, are defined as functions of the computer systems. In order to use these functions it is only necessary to write their names with suitable expressions for arguments.

Principal Symbols of Computer Programme

C1,C3,C4,C6,C7,C8,C9,CC,CP - Constants of interpolation formula
COBAR(1,N) = $h_o(x_j,\xi_2)$; COBAR(2,N) = $h_o(x_j,\xi_1)$
C2BAR(1,N) = $h_2(x_j,\xi_2)$; C2BAR(2,N) = $h_2(x_j,\xi_1)$
D = 0.816
DAN(N,1) = $N(x_j)$; DAN(N,3) = $\theta(x_j)$; DAN(N,5) = $W(x_j)$
DOB(N) = $(\pi^{\frac{1}{2}}/2)l_o(x_i)$; D2B(N) = $(\pi^{\frac{1}{2}}/2)l_2(x_i)$
DOBAR(N) = $(\pi^{\frac{1}{2}}/2)L_o(x_i)$; D2BAR(N) = $(\pi^{\frac{1}{2}}/2)L_2(x_i)$
DNN1DX(N) = $(dN/dx)_{x_i}$; DTT1DX(N) = $(d\theta/dx)_{x_i}$; DUU1DX(N) = $(dW/dx)_{x_i}$
EE = η_o, saddle point ; EM = M_1
EN2N1 = N_2 ; ENN1(N) = $N(x_i)$
EX - A specific value x_j of x
FAN(N,3) = $(d\theta/dx)_{x_j}$; FAN(N,5) = $(dW/dx)_{x_j}$

FC08B(Z,ERF) - Library routine for evaluating error function

F1F2 = $1/\Gamma_2$

HXY1 = $h_o(x,x')$; HXY2 = $h_2(x,x')$

III - Number of iterations required

JZ - Number of points at which data are given or required

KKK - Number of iterations performed

NXT - Number of points at which data are available for computations

N - An integer representing a point on the physical axis

PEL - A factor varying between 0.1 and 1.0 depending on accuracy required

PI = π ; PPI = $\pi^{\frac{1}{2}}$

QM1 = $j_o(\eta,x)$; QM2 = $j_1(\eta,x)$

QUPDUU(N) = $1/t_{xx}(x_i)$; QUPDTT(N) = $1/t_x(x_i)$

S1 = S_1 ; S2 = S_2 ; S(N) = $S(x_i)$

SAMINT(N) = $N(x_i)/\Gamma(x_i)$; SAMH(N) = $\{\theta(x_i)\}^{\frac{1}{2}}/\Gamma(x_i)$

SCR - A factor varying between 10^{-3} and 10^{-2} depending on accuracy required

STEP - Subinterval length of integration

TS1 = $(S_1^2+7/4)/(S_1^2+3/2)$; TS2 = $(S_2^2+7/4)/(S_2^2+3/2)$

T2T1 = θ_2 ; TT1(N) = $\theta(x_i)$

U2U1 = W_2 ; UU1(N) = $W(x_i)$

X(N) = x_j, coordinates of points of input or output data

Y(N) = x_i, coordinates of points of data which include asymptotic decay and are actually used in computations

Y(1) = ξ_2 ; Y(NXT) = ξ_1

ZAA(Z) = $k_o(c)$; ZAB(Z) = $k_1(c)$; ZAC(Z) = $k_2(c)$

ZAD(Z) = $k_3(c)$; ZAE(Z) = $k_4(c)$; ZAF(Z) = $k_5(c)$

ZBA(Z) = $\kappa_o(c)$; ZBB(Z) = $\kappa_1(c)$; ZBC(Z) = $\kappa_2(c)$

ZBD(Z) = $\kappa_3(c)$; ZBE(Z) = $\kappa_4(c)$; ZBF(Z) = $\kappa_5(c)$

V0042 BATTAT LIST PROGRAM

```
*FORTRAN
C     STRUCTURE OF SHOCK WAVE
      PUBLIC EN2N1,U2U1,T2T1,TS1,TS2,F1F2,S1,S2,PI,PPI,PEL,SCR,NXT,JZ,Y,
     XX,D0BAR,D2BAR,QUPDUU,QUPDTT,TT1,S,SAMINT,C8,C9,C1,C4,C3,C7,C6,DAN,
     XFAN
      DIMENSION Y(300),ENN1(300),UU1(300),TT1(300),S(300),SAMINT(300),SA
     XMH(300),QUMU1(300),DNN1DX(300),DUU1DX(300),DTT1DX(300),QUPDUU(300)
     X,QUPDTT(300),D0B(300),D0BAR(300),D2B(300),D2BAR(300),DAN(300,5),FA
     XN(300,5),X(300),C1(4,300),C8(4,300),C9(4,300),C4(4,300),C3(4,300),
     XC6(4,300),C7(4,300)
  105 FORMAT(1H0)
  110 FORMAT(1H1,51H                                          I N P U T)
  115 FORMAT(1H1,51H                                        O U T P U T)
  140 FORMAT(1H0,6H   X,13H            NN1,20H                 TT1,21H
     X                UU1)
  800 FORMAT(6F13.7)
      READ INPUT TAPE 5,2050,III
  400 READ INPUT TAPE 5,500,EM,SCR,D,PEL
      KKK=0
      EN2N1=4.*EM**2/(EM**2+3.)
      U2U1=1./EN2N1
      T2T1=(5.*EM**4+14.*EM**2-3.)/(16.*EM**2)
      F1F2=EN2N1*SQRTF(T2T1)/(T2T1**D)
      S1=EM*SQRTF(5./6.)
      CONST=S1
      S2=SQRTF(5./6.)*SQRTF(EM**2+3.)/SQRTF(5.*EM**2-1.)
      TS=1./SQRTF(T2T1)
      TS1=(S1**2+1.75)/(S1**2+1.5)
      TS2=(S2**2+1.75)/(S2**2+1.5)
      PI=3.1415926536
      PPI=SQRTF(PI)
      WRITE OUTPUT TAPE 6,110
      WRITE OUTPUT TAPE 6,105
      WRITE OUTPUT TAPE 6,450
  450 FORMAT(1H0,8H      M1,11H       STEW,10H     OMEGA,11H      DELTA)
  500 FORMAT(4F10.6)
      WRITE OUTPUT TAPE 6,2000,EM,SCR,D,PEL
 2000 FORMAT(1H0,4F10.3)
      WRITE OUTPUT TAPE 6,105
      WRITE OUTPUT TAPE 6,140
      READ INPUT TAPE 5,2050,JZ
      READ INPUT TAPE 5,800,(X(N),DAN(N,3),DAN(N,5),DAN(N,1),FAN(N,3),FA
     XN(N,5),N=1,JZ)
 2577 FORMAT(1H0,F10.5,F15.8,2F20.8)
      KY=0
      GO TO 221
  551 READ INPUT TAPE 5,2050,KY
      READ INPUT TAPE 5,2100,(Y(N),N=1,KY)
      DO 270 N=1,3
      ZN=1./DAN(N,1)
      ZT=DAN(N,3)
      DAN(N,5)=ZN
```

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 270 DAN(N,3)=ZT
 550 EN=LOGF((EN2N1-DAN(3,1))/(EN2N1-DAN(1,1)))
     EN=EN/(X(1)-X(3))
     BN=X(3)+(LOGF(EN2N1-DAN(3,1))/EN)
     AT=LOGF((T2T1-DAN(3,3))/(T2T1-DAN(1,3)))
     AT=AT/(X(1)-X(3))
     BT=X(3)+(LOGF(T2T1-DAN(3,3))/AT)
     WRITE OUTPUT TAPE 6,140
     DO 220 JT=1,KY
     ENN1(JT)=EN2N1-EXPF(-EN*(Y(JT)-BN))
     UU1(JT)=1./ENN1(JT)
     TT1(JT)=T2T1-EXPF(-AT*(Y(JT)-BT))
     QUMU1(JT)=TT1(JT)**D
     DNN1DX(JT)=EN*(EN2N1-ENN1(JT))
     DUU1DX(JT)=-DNN1DX(JT)/(ENN1(JT)**2)
     DTT1DX(JT)=AT*(T2T1-TT1(JT))
 220 PUNCH 800,Y(JT),TT1(JT),UU1(JT),ENN1(JT),DTT1DX(JT),DUU1DX(JT)
 221 DO 1802 N=1,JZ
     JT=N+KY
     Y(JT)=X(N)
     ENN1(JT)=DAN(N,1)
     UU1(JT)=DAN(N,5)
     TT1(JT)=DAN(N,3)
     DUU1DX(JT)=FAN(N,5)
     DTT1DX(JT)=FAN(N,3)
1802 QUMU1(JT)=TT1(JT)**D
     JZ=JZ+KY
     NXT=JZ
     WRITE OUTPUT TAPE 6,2577,(Y(N),ENN1(N),TT1(N),UU1(N),N=1,JZ)
     CALL OUTBRK(6)
3425 FORMAT(1HO,6H    EX,21H         EN-EN1/EN2-EN1,17H        U-U1/U2-U1,
    X18H        T-T1/T2-T1)
3430 FORMAT(1HO,F10.4,F15.8,2F20.8)
1814 WRITE OUTPUT TAPE 6,105
     WRITE OUTPUT TAPE 6,3425
     DO 1804 N=1,JZ
     EXXX=Y(N)
     DNN=(ENN1(N)-1.)/(EN2N1-1.)
     DUU=EN2N1*(UU1(N)-1.)/(1.-EN2N1)
     DTT=(TT1(N)-1.)/(T2T1-1.)
     WRITE OUTPUT TAPE 6,3430,EXXX,DNN,DUU,DTT
1804 CONTINUE
     CALL OUTBRK(6)
     IF (KKK-III) 1810,3310,3310
1810 DO 1820 N=1,NXT
     S(N)=CONST*UU1(N)/SQRTF(TT1(N))
     SAMH(N)=TT1(N)*ENN1(N)/QUMU1(N)
     SAMINT(N)=(SQRTF(TT1(N))*ENN1(N)**2)/QUMU1(N)
     QUPDUU(N)=4./PPI*CONST*DUU1DX(N)/SAMH(N)
     QUPDTT(N)=3./PPI*DTT1DX(N)/(SAMH(N)*SQRTF(TT1(N)))
     DOB(N)=1.-1./180.*QUPDUU(N)**2-1./64.*QUPDTT(N)**2
     D2B(N)=(S(N)**2*DOB(N)+S(N)*(-5./12.*QUPDTT(N)+1./60.*QUPDUU(N)*QU
    XPDTT(N))+1.75-11./720.*QUPDUU(N)**2+1./768*QUPDTT(N)**2)/(S(N)**2+
    X1.5)
     DOBAR(N)=SAMH(N)*DOB(N)
```

```
      D2BAR(N)=SAMH(N)*D2B(N)
 1820 CONTINUE
      WRITE OUTPUT TAPE 6,105
      WRITE OUTPUT TAPE 6,1821
 1821 FORMAT(1HO,6H    EX,16H          MUPDUU,16H          MUPDTT,13H
     X       DOB,16H          D2B)
      WRITE OUTPUT TAPE 6,1822,(Y(N),QUPDUU(N),QUPDTT(N),DOB(N),D2B(N),N
     X=1,NXT)
 1822 FORMAT(1HO,F10.4,4F16.8)
      CALL OUTBRK(6)
      CALL SPLCON(Y,SAMINT,NXT,C1)
      CALL SPLCON(Y,DOBAR,NXT,C8)
      CALL SPLCON(Y,D2BAR,NXT,C9)
      CALL SPLCON(Y,S,NXT,C4)
      CALL SPLCON(Y,TT1,NXT,C3)
      CALL SPLCON(Y,QUPDUU,NXT,C6)
      CALL SPLCON(Y,QUPDTT,NXT,C7)
      WRITE OUTPUT TAPE 6,115
      KKK=KKK+1
      WRITE OUTPUT TAPE 6,2039,KKK
 2039 FORMAT(1HO,47H                    START ITERATION NUMBER KKK=,I3)
 2040 READ INPUT TAPE 5,2050,JZ
 2050 FORMAT(I5)
      READ INPUT TAPE 5,2100,(X(N),N=1,JZ)
 2100 FORMAT(7F11.7)
      CALL PRMTS
      GO TO 551
 3310 GO TO EXIT
      END



*FORTRAN
      SUBROUTINE PRMTS
      EXTERNAL AUX1
      PUBLIC EN2N1,T2T1,TS1,TS2,F1F2,S1,S2,PI,PPI,PEL,SCR,E1Z,NXT,JZ,EX,
     XRO,STEP,NOSIM,NOSM,I2,I1,A,B1,A2,X(300),STEW,NOSS,Y(300),COBAR,C2B
     XAR,DOBAR(300),D2BAR(300),QUPDTT(300),QUPDUU(300),TT1(300),S(300),S
     XAMINT(300),C8(4,300);C9(4,300),C1(4,300),C4(4,300),C3(4,300),C7(4,
     X300),C6(4,300),A22,DAN(300,5),U2U1,FAN(300,5)
      DIMENSION COBAR(2,59),C2BAR(2,59),QQ(2),ANS(2),AN(5),ANSWER(240),Y
     XY(240),P4(2),A1(2),CC(4,60),CP(4,60),DAN1(60),DAN3(60)
  105 FORMAT(1HO)
  125 FORMAT(1HO,70H                    B A T T A T  I T E R A T I V
     XE  S O L U T I O N)
      STEP=0.2
 2106 CONTINUE
 2181 FORMAT(1HO,I6,F15.4,4F22.8)
      WRITE OUTPUT TAPE 6,105
      WRITE OUTPUT TAPE 6,125
      WRITE OUTPUT TAPE 6,105
      WRITE OUTPUT TAPE 6,2107
 2107 FORMAT(1HO,6H     N,10H        EX,24H          COBAR(EX,Y2),21H
```

```
     X        COBAR(EX,Y1),24H            C2BAR(EX,Y2),21H         C2BAR
     X(EX,Y1))
      NOSIM=2
      B=Y(1)
      PQ=T2T1
      IN=1
      N=0
2110  N=N+1
      EX=X(N)
      GO TO (2111,2113),IN
2111  IF (EX-Y(1)) 2114,2112,2112
2112  COBAR(IN,N)=0.
      C2BAR(IN,N)=0.
      GO TO 2136
2113  IF (Y(NXT)-EX) 2114,2112,2112
2114  CALL VAL(EX,B,A1,AUX1,R,P4,NOSIM,STEP)
      COBAR(IN,N)=2.*A1(1)/SQRTF(PQ*PI)
      C2BAR(IN,N)=2.*A1(2)/SQRTF(PQ*PI)
2136  IF (N-JZ) 2110,2140,2140
2140  B=Y(NXT)
      PQ=1.
      IN=IN+1
      N=0
      GO TO (2110,2110,2150),IN
2150  WRITE OUTPUT TAPE 6,2181,(N,X(N),COBAR(1,N),COBAR(2,N),C2BAR(1,N),
     XC2BAR(2,N),N=1,JZ)
      CALL OUTBRK(6)
      WRITE OUTPUT TAPE 6,105
      WRITE OUTPUT TAPE 6,2177
2177  FORMAT(1H0,5H    N,15H INTGR(ENN1,V-),15H INTGR(ENN1,V+),15H  INTG
     XR(TT1,V-),15H  INTGR(TT1,V+))
      NOSM=4*JZ
      JZJ=JZ
      READ=6.+S1
      EXTERNAL AUX2
      CALL VAL(0.,READ,ANSWER,AUX2,U,YY,NOSM,STEP)
      DO 2178 N=1,JZ
      N11=N
      N12=2*JZJ+N
      N13=JZJ+N
      N14=3*JZJ+N
      WRITE OUTPUT TAPE 6,2180,N,ANSWER(N11),ANSWER(N12),ANSWER(N13),ANS
     XWER(N14)
2180  FORMAT(1H0,I5,4F15.8)
2178  CONTINUE
      CALL OUTBRK(6)
      WRITE OUTPUT TAPE 6,2190
2190  FORMAT(1H1,6H    EX,18H        ENN1(ITER),18H         TT1(ITER),20
     XH           UU1(ITER))
2192  FORMAT(1H0,75H                             FORCED CONVERGENCE
     X            UU1=1./ENN1)
      WRITE OUTPUT TAPE 6,105
      WRITE OUTPUT TAPE 6,2192
      WRITE OUTPUT TAPE 6,105
2197  CONTINUE
```

```
     N=0
2200 N=N+1
     NOSS=2
     EX=X(N)
     IF (EX+3.) 2202,2204,2204
2204 E1Z=1.9
     GO TO 2220
2202 E1Z=0.9
2220 B1=0.
     AA=Y(1)
     AN(1)=0.
     AN(2)=0.
     I2=0
     IF (EX-Y(1)) 2250,2230,2230
2230 ANS(1)=0.
     ANS(2)=0.
     GO TO 2550
2250 I1=1
     STEW=SCR
     RO=EX
     A2=0.
     A22=0.
     EXTERNAL AUX3
     CALL VAL(EX,AA,ANS,AUX3,R,QQ,NOSS,STEW)
2550 AN(1)=AN(1)+ANS(1)
     AN(2)=AN(2)+ANS(2)
     WRITE OUTPUT TAPE 6,2571,EX,AN(1),AN(2)
2571 FORMAT(1H0,F10.4,F15.8,F20.8)
     I2=I2+1
     I3=I2+1
     GO TO (2560,2570),I2
2560 A=0.
     B1=6.+S1
     AA=Y(NXT)
     IF (Y(NXT)-EX) 2250,2230,2230
2570 JZ3=N+2*JZ
     JZ4=N+3*JZ
     JZ6=N+JZ
     AN(1)=AN(1)+ANSWER(N)+ANSWER(JZ3)
     AN(2)=AN(2)+ANSWER(JZ6)+ANSWER(JZ4)
     AN(1)=AN(1)/2.
     AN(2)=AN(2)/3.
     AN(5)=1./AN(1)
     AN(3)=AN(2)/AN(1)-(2./3.)*((S1*AN(5))**2)
     WRITE OUTPUT TAPE 6,2575,EX,AN(1),AN(3),AN(5)
2575 FORMAT(1H0,F10.4,F15.8,2F20.8)
     CALL OUTBRK(6)
     IF (AN(1)-EN2N1) 305,305,310
 310 GO TO EXIT
 305 IF (AN(5)-U2U1) 320,315,315
 320 GO TO EXIT
 315 IF (AN(3)-T2T1) 330,330,325
 325 GO TO EXIT
 330 CONTINUE
     DO 2580 I=1,5,2
```

```
 2580 DAN(N,I)=AN(I)
      IF (N-JZ) 2200,3300,3300
 3300 DO 3304 N=1,JZ
      DAN1(N)=DAN(N,1)
 3304 DAN3(N)=DAN(N,3)
      CALL SPLCON(X,DAN1,JZ,CC)
      CALL SPLCON(X,DAN3,JZ,CP)
      DO 3301 N=1,JZ-1
      FAN(N,1)=-3.*CC(1,N)*(X(N+1)-X(N))**2-CC(3,N)+CC(4,N)
      FAN(N,3)=-3.*CP(1,N)*(X(N+1)-X(N))**2-CP(3,N)+CP(4,N)
 3301 FAN(N,5)=-FAN(N,1)/(DAN(N,1)**2)
      FAN(JZ,1)=3.*CC(2,JZ-1)*(X(JZ)-X(JZ-1))-CC(3,JZ-1)+CC(4,JZ-1)
      FAN(JZ,3)=3.*CP(2,JZ-1)*(X(JZ)-X(JZ-1))-CP(3,JZ-1)+CP(4,JZ-1)
      FAN(JZ,5)=-FAN(JZ,1)/(DAN(JZ,1)**2)
      WRITE OUTPUT TAPE 6,105
      WRITE OUTPUT TAPE 6,3302
 3302 FORMAT(1H0,6H    EX,13H       DNN1DX)
      WRITE OUTPUT TAPE 6,3303,(X(N),FAN(N,1),N=1,JZ)
 3303 FORMAT(F10.5,F16.8)
      CALL OUTBRK(6)
      RETURN
      END
```

```
*FORTRAN
      SUBROUTINE SPLCON (X,Y,M,C)
      DIMENSION X(300),Y(300),D(300),P(300),E(300),C(4,300),A(300,3),B(3
     X00),Z(300)
      MM=M-1
      DO 2 K=1,MM
      D(K)=X(K+1)-X(K)
      P(K)=D(K)/6.
    2 E(K)=(Y(K+1)-Y(K))/D(K)
      DO 3 K=2,MM
    3 B(K)=E(K)-E(K-1)
      A(1,2)=-1.-D(1)/D(2)
      A(1,3)=D(1)/D(2)
      A(2,3)=P(2)-P(1)*A(1,3)
      A(2,2)=2.*(P(1)+P(2))-P(1)*A(1,2)
      A(2,3)=A(2,3)/A(2,2)
      B(2)=B(2)/A(2,2)
      DO 4 K=3,MM
      A(K,2)=2.*(P(K-1)+P(K))-P(K-1)*A(K-1,3)
      B(K)=B(K)-P(K-1)*B(K-1)
      A(K,3)=P(K)/A(K,2)
    4 B(K)=B(K)/A(K,2)
      Q=D(M-2)/D(M-1)
      A(M,1)=1.+Q+A(M-2,3)
      A(M,2)=-Q-A(M,1)*A(M-1,3)
      B(M)=B(M-2)-A(M,1)*B(M-1)
      Z(M)=B(M)/A(M,2)
      MN=M-2
```

```
      DO 6 I=1,MN
      K=M-I
    6 Z(K)=B(K)-A(K,3)*Z(K+1)
      Z(1)=-A(1,2)*Z(2)-A(1,3)*Z(3)
      DO 7 K=1,MM
      Q=1./(6.*D(K))
      C(1,K)=Z(K)*Q
      C(2,K)=Z(K+1)*Q
      C(3,K)=Y(K)/D(K)-Z(K)*P(K)
    7 C(4,K)=Y(K+1)/D(K)-Z(K+1)*P(K)
      RETURN
  101 FORMAT(2E16.8)
      END
```

```
*FORTRAN
      SUBROUTINE SPLINE(X,Y,M,C,XI,YI)
      DIMENSION X(300),Y(300),C(4,300)
      IF (XI-X(1)) 2,1,7
    1 YI=Y(1)
      RETURN
    2 K=1
    3 IF (XI-X(K+1)) 5,4,6
    4 YI=Y(K+1)
      RETURN
    5 K=K+1
      IF (M-K) 7,7,3
    6 YI=(X(K+1)-XI)*(C(1,K)*(X(K+1)-XI)**2+C(3,K))
      YI=YI+(XI-X(K))*(C(2,K)*(XI-X(K))**2+C(4,K))
      RETURN
    7 PRINT 101
      GO TO EXIT
  101 FORMAT(31H OUT OF RANGE FOR INTERPOLATION)
      END
```

```
*FORTRAN
      SUBROUTINE VAL(A,B,ANS,AUXL,X,F,NOS,STEM)
      EXTERNAL AUXL
      DIMENSION ANS(240),F(240),FA(240),GCOW(3),GAU(5)
C     THREEPOINT INTEGRATION GAUSSIAN FOR INTEGRANDS F LENGTH NOS WITH V
C    XARIABLE SUBDIVISIONS STEM,AUXL DETERMINES F,NO RESTRICTION ON A,B.
      GCOW(3)=0.8888888889
      GCOW(1)=0.7745966692
      GCOW(2)=0.5555555556
      Y=A
      DO 100 K=1,NOS
  100 ANS(K)=0.
  101 IF (A-B) 102,102,103
```

```
102 SSSP=ABSF(STEM)
    IF (Y+SSSP-B)104,105,105
103 SSSP=-1.*ABSF(STEM)
    IF (Y+SSSP-B)105,105,104
105 SSSP=B-Y
104 M=0
    ICOUNT=0
    N1=3
    M1=2
    GAU(1)=Y
    GAU(2)=Y+SSSP
106 M=M+1
    IF (M-2) 107,108,107
107 GAU(4)=0.5*(GAU(2)+GAU(1))
    GAU(5)=0.5*(GAU(2)-GAU(1))
    IF (ABSF(GAU(5))-0.00001) 109,109,110
109 DO 111 K=1,NOS
111 F(K)=0.
    GO TO 118
110 DO 112 K=1,NOS
112 FA(K)=0.
    IG=1
    JG=N1
113 IF (JG-IG) 114,115,116
114 DO 117 K=1,NOS
117 F(K)=FA(K)*GAU(5)
118 DO 119 K=1,NOS
119 ANS(K)=ANS(K)+F(K)
108 M=M-1
    IF (M) 120,120,121
121 ICOUNT=ICOUNT+1
    I=IG+1
    DO 122 K=1,NOS
122 FA(K)=FA(K)+F(K)*GCOW(I)
    IF (ICOUNT-M1) 123,124,125
123 IG=IG+2
    GO TO 113
115 IG=IG-1
    GAU(3)=0.
    GO TO 126
116 I=IG
    GAU(3)=-GAU(5)*GCOW(I)
    GO TO 126
125 IG=IG+1
    GO TO 123
124 IG=IG-1
    I=IG
    GAU(3)=GAU(5)*GCOW(I)
126 X=GAU(4)+GAU(3)
    CALL AUXL(X,F,NOS,STEM)
    STEM=STEM
    GO TO 106
120 Y=GAU(2)
    IF (A-B) 127,127,128
127 IF (Y-B) 101,129,129
```

```
  128 IF (Y-B) 129,129,101
  129 RETURN
      END




*FORTRAN
      SUBROUTINE GAL(A,B,ANS,AUXL,X,F,NOS,STEM)
      EXTERNAL AUXL
      DIMENSION ANS(240),F(240),FA(240),GCOW(3),GAU(5)
C     THREEPOINT INTEGRATION GAUSSIAN FOR INTEGRANDS F LENGTH NOS WITH V
C    XARIABLE SUBDIVISIONS STEM,AUXL DETERMINES F,NO RESTRICTION ON A,B.
      GCOW(3)=0.8888888889
      GCOW(1)=0.7745966692
      GCOW(2)=0.5555555556
      Y=A
      DO 100 K=1,NOS
  100 ANS(K)=0.
  101 IF (A-B) 102,102,103
  102 SSSP=ABSF(STEM)
      IF (Y+SSSP-B)104,105,105
  103 SSSP=-1.*ABSF(STEM)
      IF (Y+SSSP-B)105,105,104
  105 SSSP=B-Y
  104 M=0
      ICOUNT=0
      N1=3
      M1=2
      GAU(1)=Y
      GAU(2)=Y+SSSP
  106 M=M+1
      IF (M-2) 107,108,107
  107 GAU(4)=0.5*(GAU(2)+GAU(1))
      GAU(5)=0.5*(GAU(2)-GAU(1))
      IF (ABSF(GAU(5))-0.00001) 109,109,110
  109 DO 111 K=1,NOS
  111 F(K)=0.
      GO TO 118
  110 DO 112 K=1,NOS
  112 FA(K)=0.
      IG=1
      JG=N1
  113 IF (JG-IG) 114,115,116
  114 DO 117 K=1,NOS
  117 F(K)=FA(K)*GAU(5)
  118 DO 119 K=1,NOS
  119 ANS(K)=ANS(K)+F(K)
  108 M=M-1
      IF (M) 120,120,121
  121 ICOUNT=ICOUNT+1
      I=IG+1
      DO 122 K=1,NOS
  122 FA(K)=FA(K)+F(K)*GCOW(I)
```

```
      IF (ICOUNT-M1) 123,124,125
  123 IG=IG+2
      GO TO 113
  115 IG=IG-1
      GAU(3)=0.
      GO TO 126
  116 I=IG
      GAU(3)=-GAU(5)*GCOW(I)
      GO TO 126
  125 IG=IG+1
      GO TO 123
  124 IG=IG-1
      I=IG
      GAU(3)=GAU(5)*GCOW(I)
  126 X=GAU(4)+GAU(3)
      CALL AUXL(X,F,NOS,STEM)
      STEM=STEM
      GO TO 106
  120 Y=GAU(2)
      IF (A-B) 127,127,128
  127 IF (Y-B) 101,129,129
  128 IF (Y-B) 129,129,101
  129 RETURN
      END
```

```
*FORTRAN
      SUBROUTINE AUX1(X,F,NOS,STEM)
      PUBLIC  F1F2,T2T1,TS1,TS2,NXT,Y(300),DOBAR(300),D2BAR(300),C8(4,30
     X0),NOSIM,C9(4,300),STEP,STPP
      DIMENSION F(2)
      STEM=STEM
      IF (X-Y(1)) 2120,2115,2115
 2115 F(1)=F1F2*SQRTF(T2T1)
      F(2)=F(1)*TS2
      GO TO 2135
 2120 IF (X-Y(NXT)) 2125,2125,2130
 2125 F(1)=1.
      F(2)=TS1
      GO TO 2135
 2130 CALL SPLINE(Y,DOBAR,NXT,C8,X,F1)
      CALL SPLINE(Y,D2BAR,NXT,C9,X,F2)
      F(1)=F1
      F(2)=F2
 2135 RETURN
      END
```

```
*FORTRAN
      SUBROUTINE AUX2(U,YY,NOST,STER)
      PUBLIC S1,S2,EN2N1,T2T1,TS1,TS2,JZ,X(59),C0BAR(2,59),C2BAR(2,59),N
     XOSM,STEP
      DIMENSION YY(240)
      STER=STEP
      IN=1
      Z=ABSF(U+S2)
      KN=0
      DO 2160 J=1,JZ
      KN=KN+1
      BB1=ZAA(Z)*EXPF(-ABSF(C0BAR(IN,J)/U))
      IF (ABSF(BB1)-0.000001) 2151,2152,2152
 2151 YY(KN)=0.
      GO TO 2160
 2152 YY(KN)=BB1*EN2N1
 2160 CONTINUE
      DO 2165 J=1,JZ
      KN=KN+1
      BB2=((U**2)*ZAA(Z)+ZBA(Z))*EXPF(-ABSF(C2BAR(IN,J)/U))
      IF (ABSF(BB2)-0.000001) 2161,2162,2162
 2161 YY(KN)=0.
      GO TO 2165
 2162 YY(KN)=BB2*EN2N1*T2T1/TS2
 2165 CONTINUE
      IN=2
      ZE=ABSF(U-S1)
      DO 2170 J=1,JZ
      KN=KN+1
      BBB1=ZAA(ZE)*EXPF(-ABSF(-C0BAR(IN,J)/U))
      IF (ABSF(BBB1)-0.000001) 2163,2164,2164
 2163 YY(KN)=0.
      GO TO 2170
 2164 YY(KN)=BBB1
 2170 CONTINUE
      DO 2175 J=1,JZ
      KN=KN+1
      BBB2=((U**2)*ZAA(ZE)+ZBA(ZE))*EXPF(-ABSF(-C2BAR(IN,J)/U))
      IF (ABSF(BBB2)-0.000001) 2171,2172,2172
 2171 YY(KN)=0.
      GO TO 2175
 2172 YY(KN)=BBB2/TS1
 2175 CONTINUE
      RETURN
      END
```

```
*FORTRAN
      SUBROUTINE AUX3(R,QQ,NOST,STER)
      PUBLIC E1C,E2C,E4C,E8C,EFC,EE,NISS,STEE,WTEE,ES,HXY1,HXY2,P9,P10,F
     X1F2,T2T1,TS1,TS2,NXT,Y(300),STPP,DOBAR(300),D2BAR(300),C8(4,300),C
     X9(4,300),S1,S2,PEL,SCR,E1Z,EX,STEW,SAMINT(300),S(300),TT1(300),QUP
     XDUU(300),QUPDTT(300),C1(4,300),C4(4,300),C3(4,300),C7(4,300),C6(4,
     X300),A2,A,B1,I1,I2,PI,PPI,RO,NOSS,EN2N1,A22,E6C
      DIMENSION QQ(2),A11(2),P44(2),Q(2),V(2)
      IF (ABSF(R-EX)-PEL) 2245,2256,2256
 2256 IF (ABSF(R-EX)-E1Z) 2255,2254,2254
 2254 IF (ABSF(R)-5.0) 2246,2246,2247
 2247 IF (R+20.0) 2248,2257,2257
 2245 STER=SCR
      GO TO 2259
 2255 STER=0.20
      GO TO 2259
 2246 STER=0.50
      GO TO 2259
 2257 STER=2.0
      GO TO 2259
 2248 STER=5.0
      GO TO 2259
 2259 IF (R-Y(1)) 2270,2260,2260
 2260 EL=EN2N1*F1F2
      P8=1.0/EN2N1
      ES=S2
      P7=T2T1
      P5=F1F2*SQRTF(T2T1)
      P9=0.0
      P10=0.0
      GO TO 2294
 2270 IF (R-Y(NXT)) 2280,2280,2290
 2280 EL=1.
      P8=1.
      ES=S1
      P7=1.
      P9=0.
      P10=0.
      GO TO 2294
 2290 CALL SPLINE(Y,SAMINT,NXT,C1,R,EL)
      CALL SPLINE(Y,S,NXT,C4,R,ES)
      CALL SPLINE(Y,TT1,NXT,C3,R,P7)
      CALL SPLINE(Y,QUPDUU,NXT,C6,R,P9)
      CALL SPLINE(Y,QUPDTT,NXT,C7,R,P10)
 2294 CONTINUE
      STPP=(ABSF(R-RO))
 2300 EXTERNAL AUX1
      CALL GAL(RO,R,A11,AUX1,SS,P44,2,STPP)
      A2=A2+A11(1)
      A22=A22+A11(2)
      RO=R
 2370 HXY1=2.*A2 /SQRTF(P7*PI)
      HXY2=2.*A22/SQRTF(P7*PI)
      H1=ABSF(HXY2)
      HH=H1/(ES**3)
```

```
      IF (ABSF(R-EX)-3.) 2380,2380,2372
2372  IF (ABSF(R-EX)-8.) 2374,2374,2376
2374  I4=2
      GO TO 2380
2376  I4=3
2380  I1=I1
      I3=I2+1
      GO TO (2506,2508),I3
2506  A=-ABSF(6.-ES)
6509  IF (HH-0.3) 2402,2402,2404
2402  EE=0.
      GO TO 2500
2404  EE=-((H1/2.0)**0.333333)+ES/3.0
      GO TO 2500
2508  B1=6.0+ES
      IF (HH-0.75) 2502,2502,2504
2502  EE=ES*(1.0+HH/2.0-(HH**2)/2.0+7.0*(HH**3)/8.0)
      GO TO 2500
2504  EE=((H1/2.0)**0.3333333)+ES/3.0
      GO TO 2500
2500  IF (ES-H1) 2590,2590,2592
2590  WTEE=ES/10.0
      GO TO 2503
2592  WTEE=H1/10.0
2503  STEE=WTEE
      IF (WTEE-0.12) 2505,2505,2507
2505  IF (WTEE-0.001) 2501,2501,2509
2501  WTEE=0.001
      GO TO 2509
2507  WTEE=0.12
2509  E1C=10.0*WTEE
      E2C=20.0*WTEE
      E4C=3.0*E2C
      E6C=7.0*E2C
      E8C=15.0*E2C
      EFC=81.0*E2C
      NISS=2
      EXTERNAL AUX4
      CALL GAL(A,B1,V,AUX4,ETA,Q,NISS,STEE)
2565  QQ(1)=V(1)*EL*2./PPI
      QQ(2)=V(2)*EL*P7*2./PPI
      RETURN
      END
```

```
*FORTRAN
      SUBROUTINE AUX4(ETA,Q,NIST,STEM)
      PUBLIC E1C,E2C,E4C,E6C,E8C,EFC,EE,NISS,STEE,WTEE,ES,P9,P10,HXY1,HX
     XY2
      DIMENSION Q(2)
      ZR=ABSF(ETA-ES)
      IF(ETA-ES)2537,2538,2538
 2537 QM1=ZAA(ZR)+ZAB(ZR)*P9-ZAC(ZR)*P10+ZAD(ZR)*P9**2+ZAE(ZR)*P10**2-ZA
     XF(ZR)*P9*P10
      QM2=ZBA(ZR)+ZBB(ZR)*P9-ZBC(ZR)*P10+ZBD(ZR)*P9**2+ZBE(ZR)*P10**2-ZB
     XF(ZR)*P9*P10
      GO TO 2539
 2538 QM1=ZAA(ZR)+ZAB(ZR)*P9+ZAC(ZR)*P10+ZAD(ZR)*P9**2+ZAE(ZR)*P10**2+ZA
     XF(ZR)*P9*P10
      QM2=ZBA(ZR)+ZBB(ZR)*P9+ZBC(ZR)*P10+ZBD(ZR)*P9**2+ZBE(ZR)*P10**2+ZB
     XF(ZR)*P9*P10
 2539 IF (ABSF(ETA)-E1C) 2511,2511,2540
 2540 IF (ABSF(ETA-EE)-E2C) 2511,2511,2541
 2541 IF (ABSF(ETA-EE)-E4C) 2513,2513,2542
 2542 IF (ABSF(ETA)-EE-E6C) 2517,2517,2519
 2519 IF (ABSF(ETA-EE)-E8C) 2531,2531,2533
 2533 IF (ABSF(ETA-EE)-EFC) 2534,2534,2535
 2511 STEM=(10.0/3.0)*WTEE
      GO TO 2548
 2513 STEM=10.*WTEE
      GO TO 2548
 2517 STEM=20.0*WTEE
      GO TO 2548
 2531 STEM=40.0*WTEE
      GO TO 2548
 2534 STEM=132.0*WTEE
      GO TO 2548
 2535 STEM=(EFC-E8C)/3.0
 2548 QF=ABSF(-(ETA-ES)**2+HXY2/ETA)
      IF (QF-36.) 2562,2562,2563
 2562 Q(1)=QM1*EXPF(-ABSF(-HXY1/ETA))
      Q(2)=(QM1*ETA**2+QM2)*EXPF(-ABSF(-HXY2/ETA))
      Q(1)=Q(1)/(-ETA)
      Q(2)=Q(2)/(-ETA)
      GO TO 5200
 2563 Q(1)=0.
      Q(2)=0.
 5200 RETURN
      END
```

```
*FORTRAN
      FUNCTION Z1Y(Z)
      PI=3.1415926536
      Z1Y=(1./SQRTF(2.*PI))*EXPF(-2.*Z**2)
      RETURN
      END
*FORTRAN
      FUNCTION Z2Y(Z)
      CALL FC08B(Z,ERF)
      Z2Y=(1./SQRTF(8.))*EXPF(-Z**2)*ERF
      RETURN
      END
*FORTRAN
      FUNCTION Z3Y(Z)
      CALL FC08B(Z,ERF)
      PI=3.1415926536
      Z3Y=(SQRTF(PI/32.))*(1.-ERF**2)
      RETURN
      END
*FORTRAN
      FUNCTION ZAA(Z)
      F111=1.
      F112=2.*Z
      ZAA=F111*Z1Y(Z)+F112*Z2Y(Z)+2.*Z3Y(Z)
      RETURN
      END
*FORTRAN
      FUNCTION ZAB(Z)
      F121=1./3.*(1.-Z**2)
      F122=1./3.*(Z-2.*Z**3)
      ZAB=F121*Z1Y(Z)+F122*Z2Y(Z)
      RETURN
      END
*FORTRAN
      FUNCTION ZAC(Z)
      F131=5./6.*Z-2./3.*Z**3
      F132=0.5+Z**2-4./3.*Z**4
      ZAC=F131*Z1Y(Z)+F132*Z2Y(Z)
      RETURN
      END
*FORTRAN
      FUNCTION ZAD(Z)
      F141=0.25*(-14./135.-19./135.*Z**2-2./135.*Z**4)
      F142=0.25*(5./9.*Z-8./27.*Z**3-4./135.*Z**5)
      ZAD=F141*Z1Y(Z)+F142*Z2Y(Z)
      RETURN
      END
*FORTRAN
      FUNCTION ZAE(Z)
      F151=1./60.*(-7.+22.*Z**2-17.*Z**4+2.*Z**6)
      F152=0.25*(-Z+11./3.*Z**3-32./15.*Z**5+4./15.*Z**7)
      ZAE=F151*Z1Y(Z)+F152*Z2Y(Z)
      RETURN
      END
```

```
*FORTRAN
       FUNCTION ZAF(Z)
       F161=0.25*(8./15.*Z-31./45.*Z**3+2./45.*Z**5)
       F162=0.25*(-2./3.+3.*Z**2-4./3.*Z**4+4./45.*Z**6)
       ZAF=F161*Z1Y(Z)+F162*Z2Y(Z)
       RETURN
       END
*FORTRAN
       FUNCTION ZBA(Z)
       F211=1.5
       F212=4.*Z
       ZBA=F211*Z1Y(Z)+F212*Z2Y(Z)+2.*(1.-Z**2)*Z3Y(Z)
       RETURN
       END
*FORTRAN
       FUNCTION ZBB(Z)
       F221=1./3.*(1.-Z**2)
       F222=1./3.*(Z-2.*Z**3)
       ZBB=F221*Z1Y(Z)+F222*Z2Y(Z)+2./3.*Z3Y(Z)
       RETURN
       END
*FORTRAN
       FUNCTION ZBC(Z)
       F231=-1./6.*Z-2./3.*Z**3
       F232=-Z**2-4./3.*Z**4
       ZBC=F231*Z1Y(Z)+F232*Z2Y(Z)
       RETURN
       END
*FORTRAN
       FUNCTION ZBD(Z)
       F241=0.25*(41./135.-2./5.*Z**2-2./135.*Z**4)
       F242=0.25*(2./3.*Z-22./27.*Z**3-4./135.*Z**5)
       ZBD=F241*Z1Y(Z)+F242*Z2Y(Z)
       RETURN
       END
*FORTRAN
       FUNCTION ZBE(Z)
       F251=0.25*(1./15.+2./3.*Z**2-13./15.*Z**4+2./15.*Z**6)
       F252=0.25*(0.5*Z+4./3.*Z**3-8./15.*Z**5+4./15.*Z**7)
       ZBE=F251*Z1Y(Z)+F252*Z2Y(Z)
       RETURN
       END
*FORTRAN
       FUNCTION ZBF(Z)
       F261=0.25*(44./45.*Z-41./45.*Z**3+2./45.*Z**5)
       F262=0.25*(7./3.*Z**2-16./9.*Z**4+4./45.*Z**6)
       ZBF=F261*Z1Y(Z)+F262*Z2Y(Z)
       RETURN
       END
```

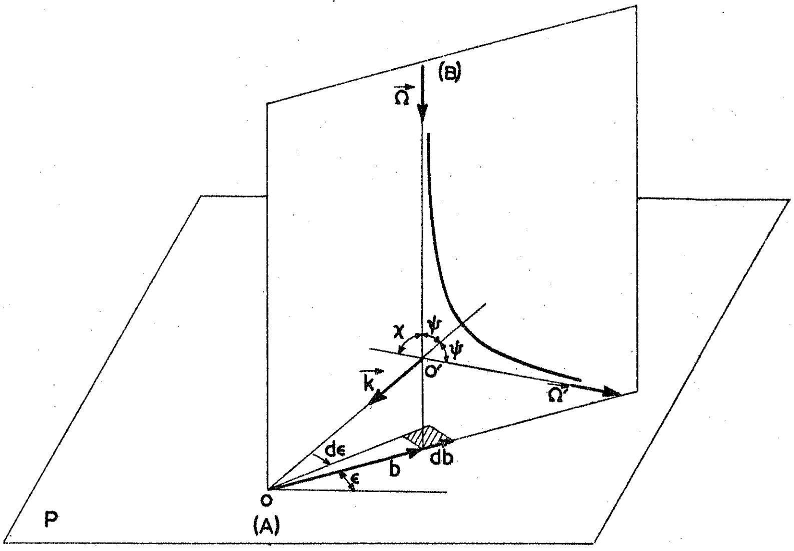

FIG. 1. ENCOUNTER PARAMETERS.

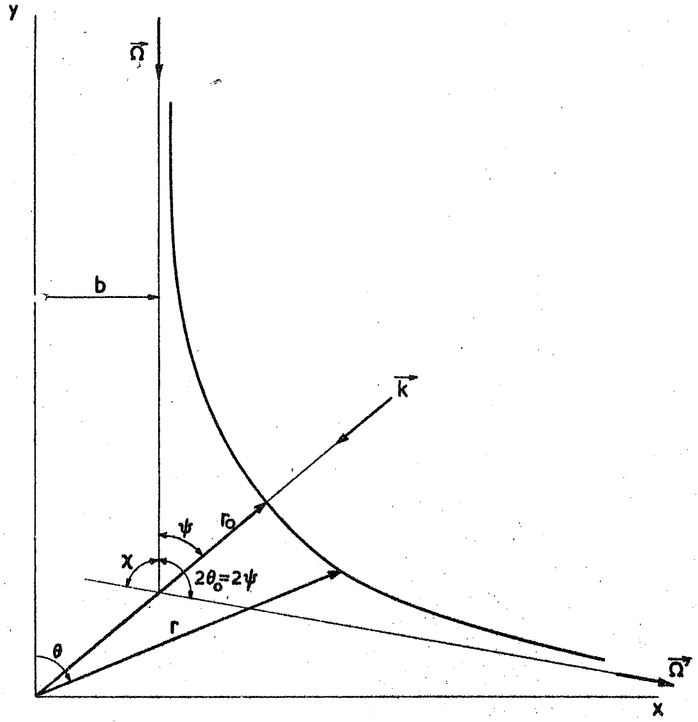

FIG. 2. RELATIVE TRAJECTORY OF CENTRE OF FORCE MOLECULES.

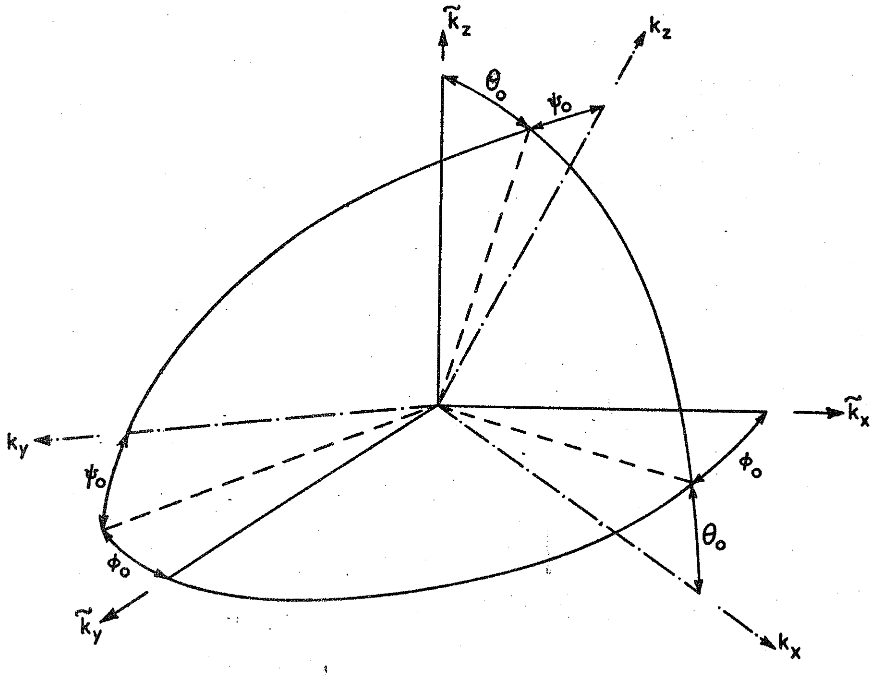

FIG. 3. TRANSFORMATION OF CO-ORDINATE AXIS.

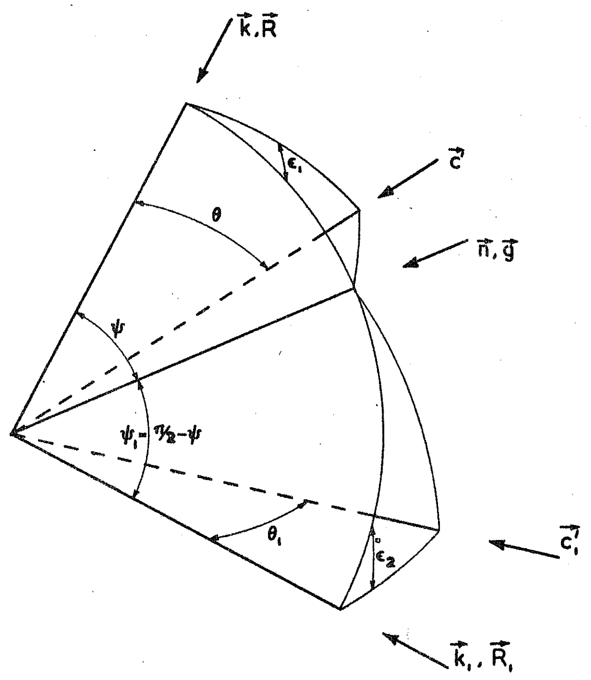

FIG. 4. GEOMETRY OF THE TRANSFORMATION OF VELOCITIES.

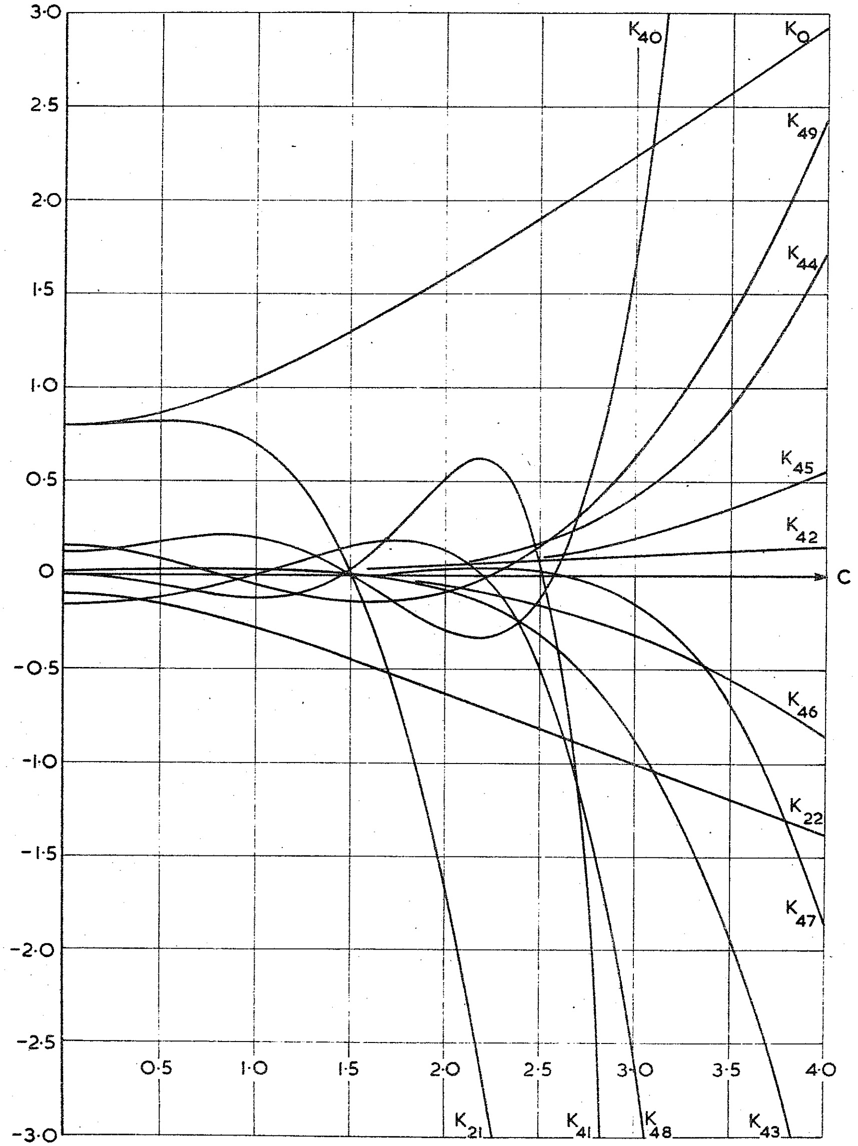

FIG. 5. WEIGHTING FUNCTIONS OF THE MODEL EQUATION

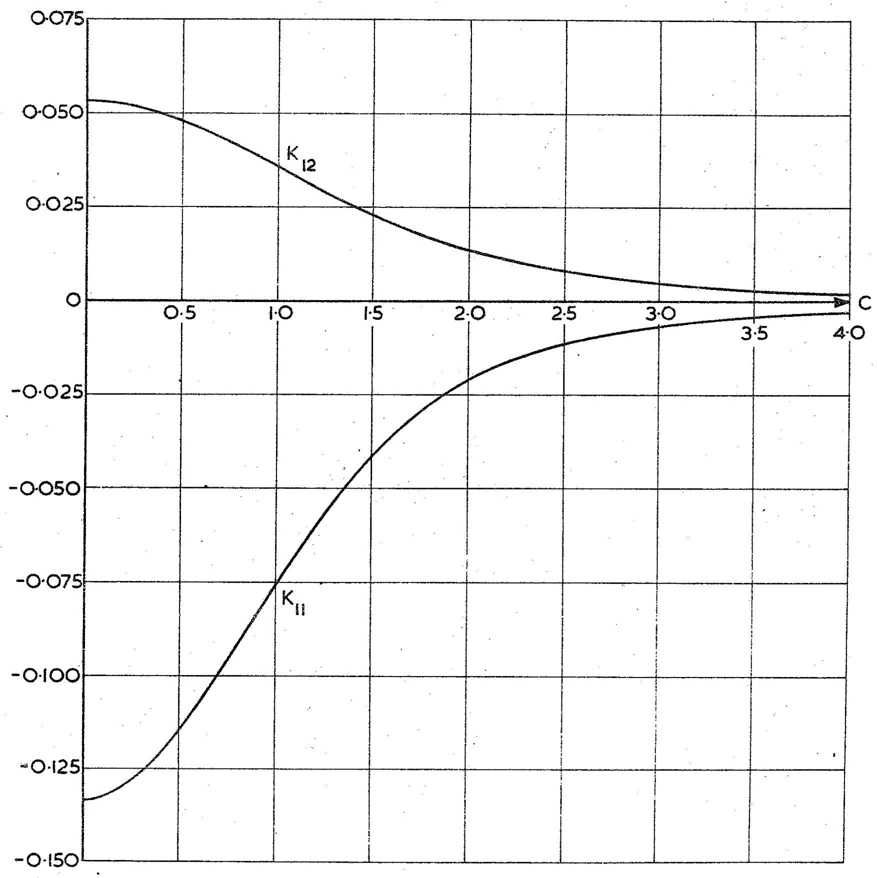

FIG. 6. WEIGHTING FUNCTIONS OF THE MODEL EQUATION.

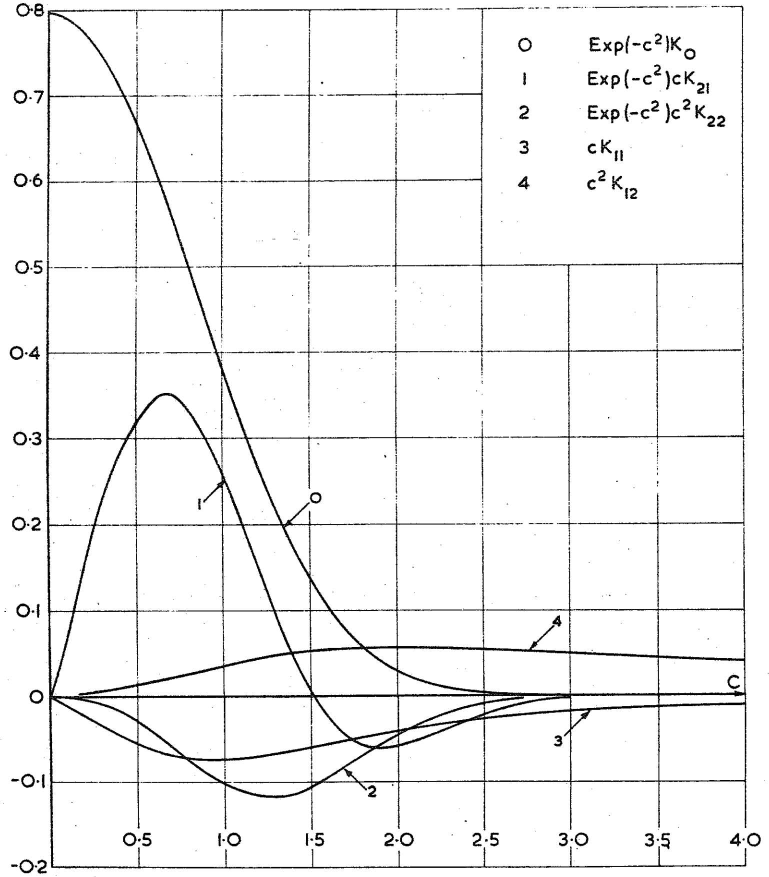

FIG. 7. EFFECTIVE CONTRIBUTION OF WEIGHTING FUNCTIONS.

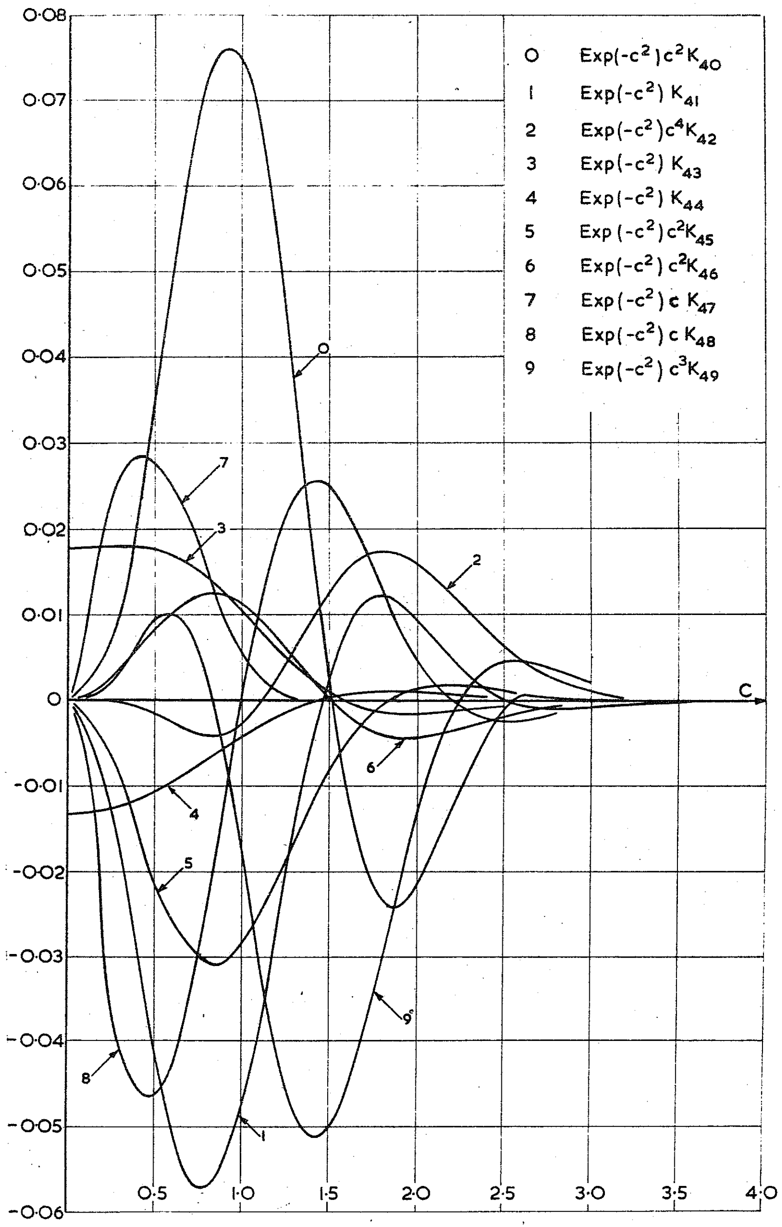

FIG. 8. EFFECTIVE CONTRIBUTION OF WEIGHTING FUNCTIONS.

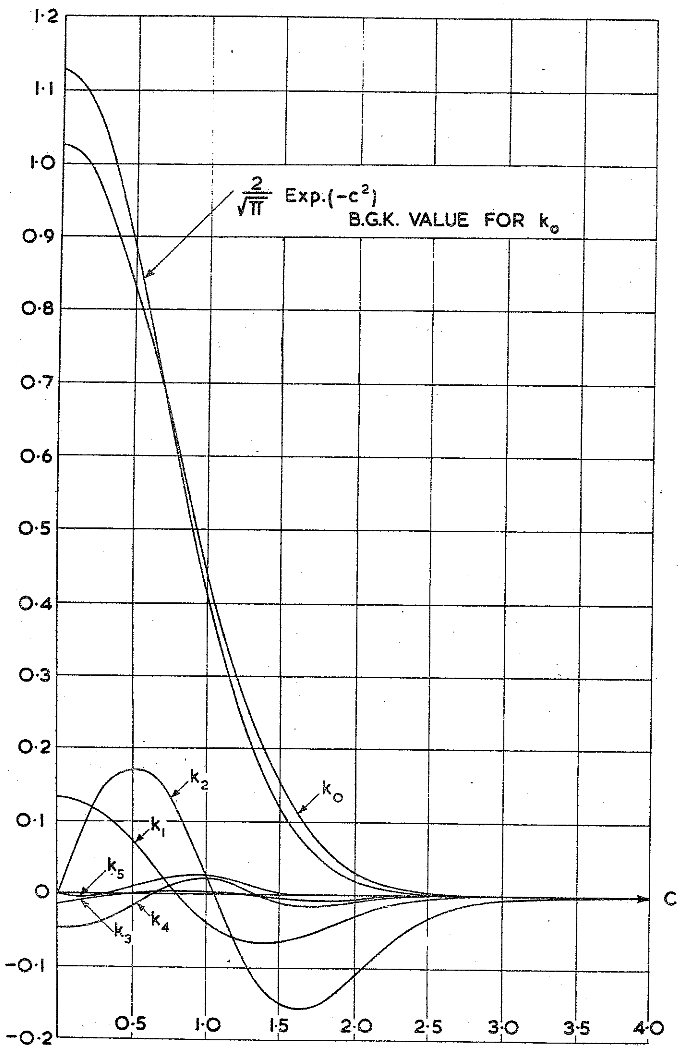

FIG. 9. WEIGHTING FUNCTIONS OF SHOCK EQUATIONS.

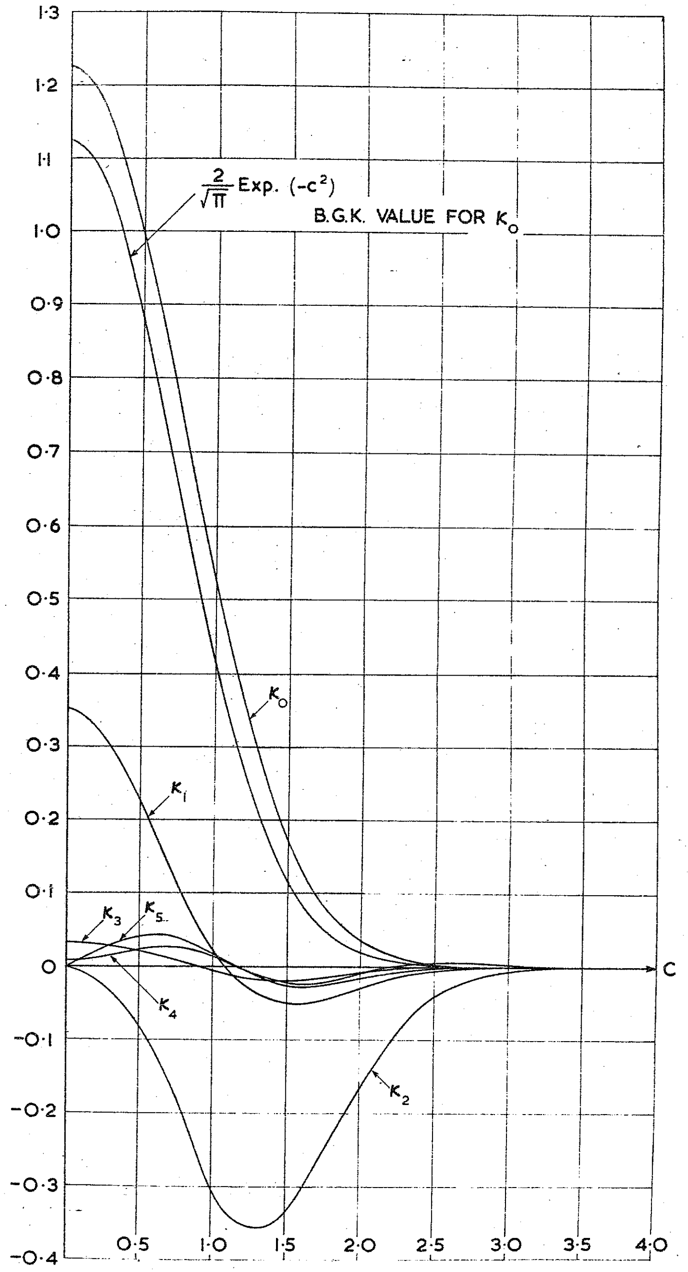

FIG. 10. WEIGHTING FUNCTIONS OF SHOCK EQUATIONS.

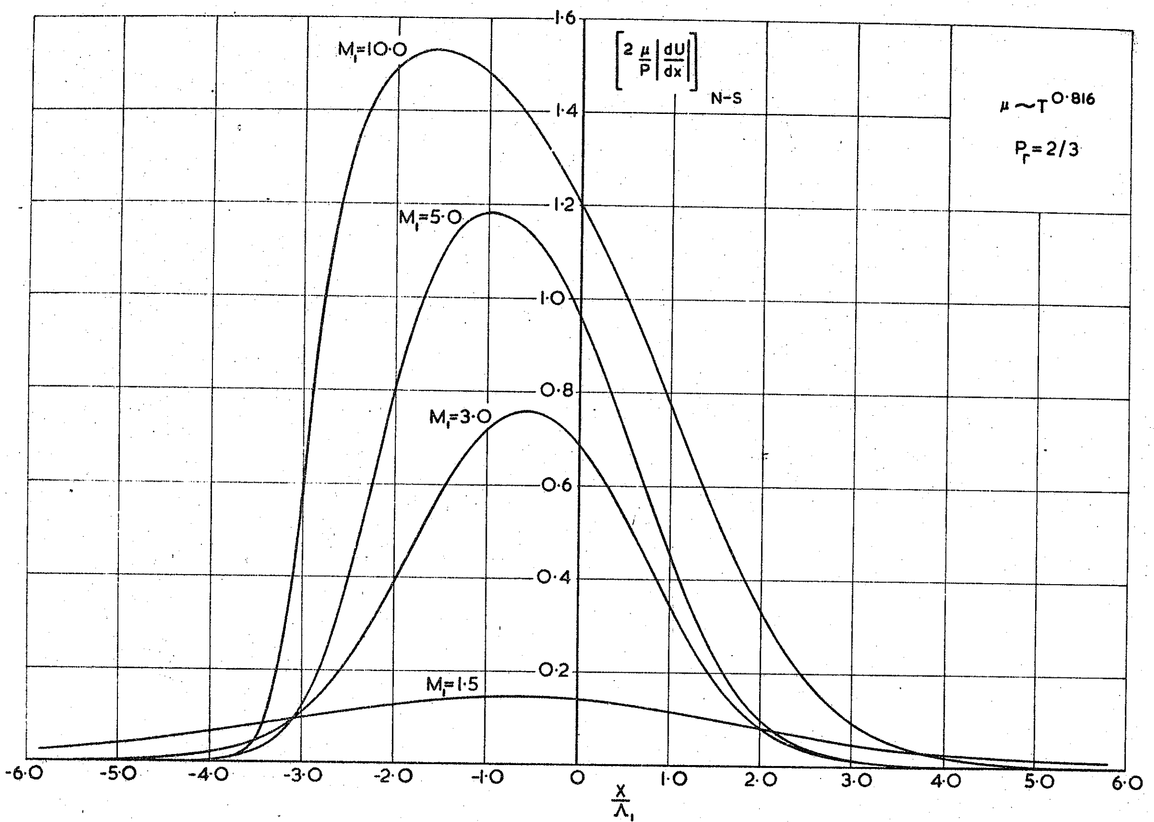

FIG.11. THE NAVIER-STOKES VALUE OF THE VELOCITY PARAMETER ACROSS A SHOCK-WAVE.

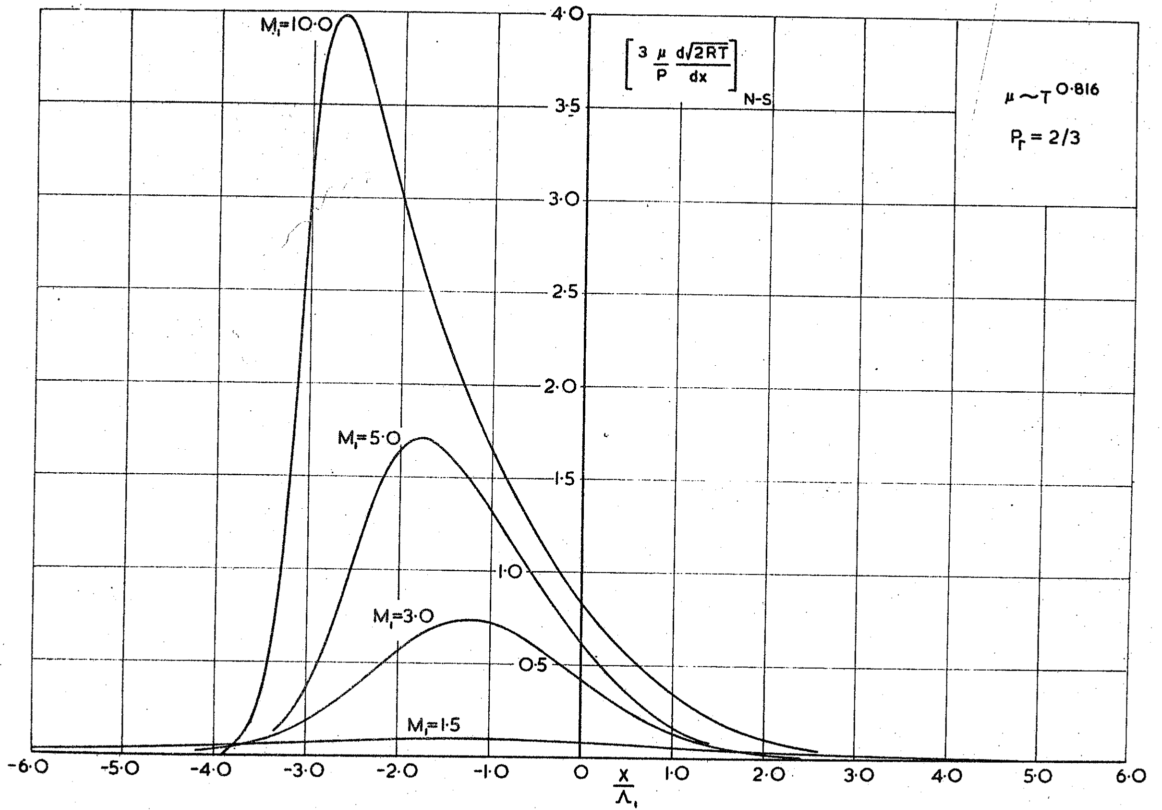

FIG.12. THE NAVIER-STOKES VALUE OF THE TEMPERATURE PARAMETER ACROSS A SHOCK-WAVE.

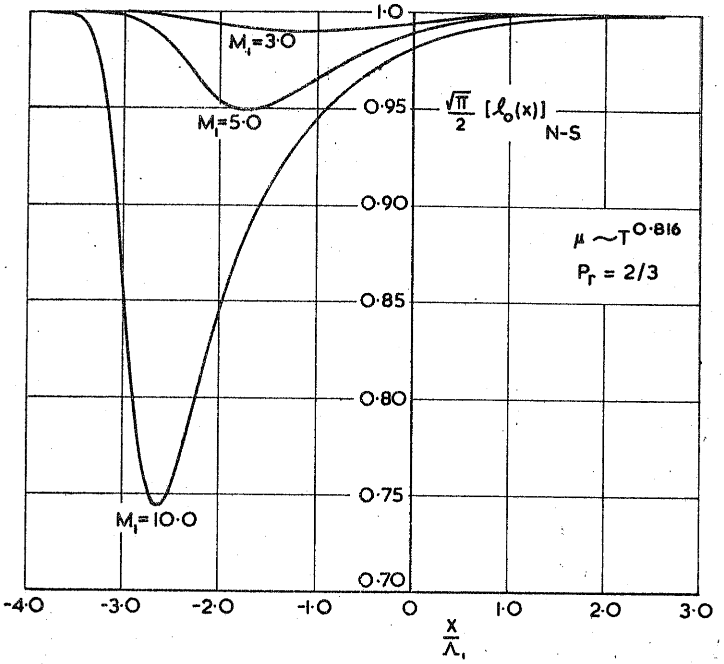

FIG. 13. THE NAVIER-STOKES VALUE OF ℓ_0, EQ. (5·18).

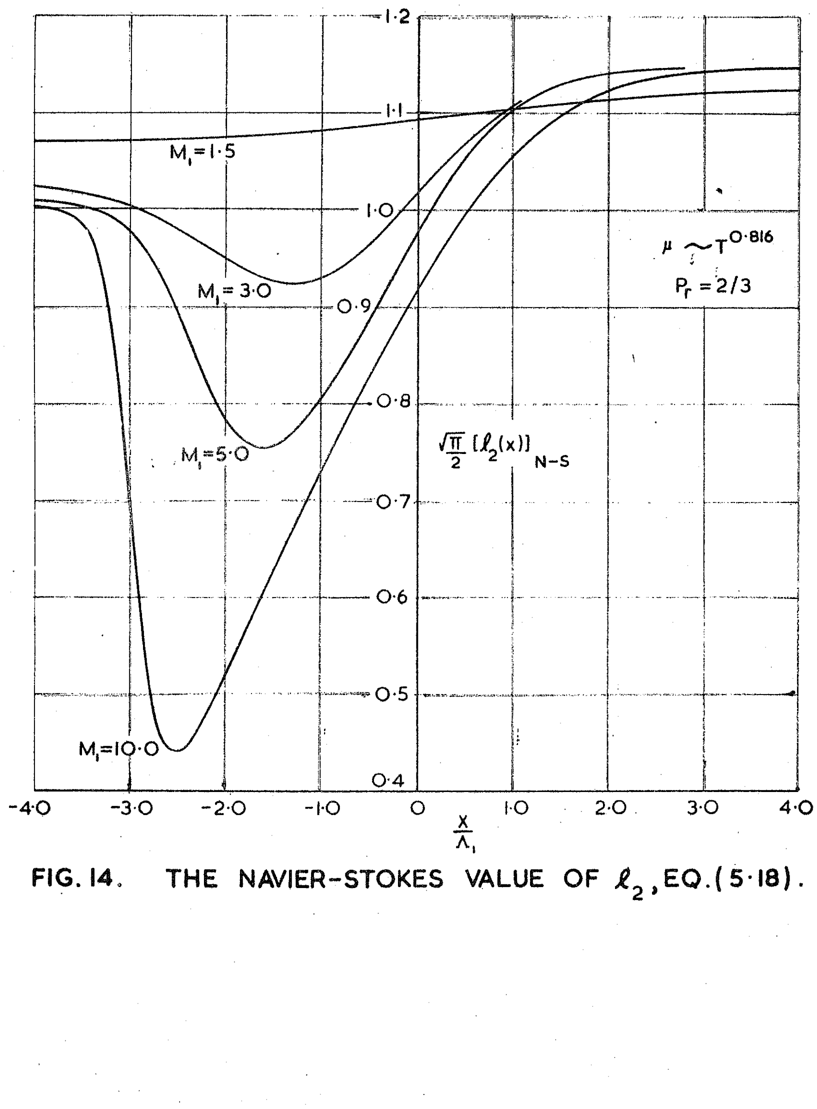

FIG. 14. THE NAVIER-STOKES VALUE OF ℓ_2, EQ. (5·18).

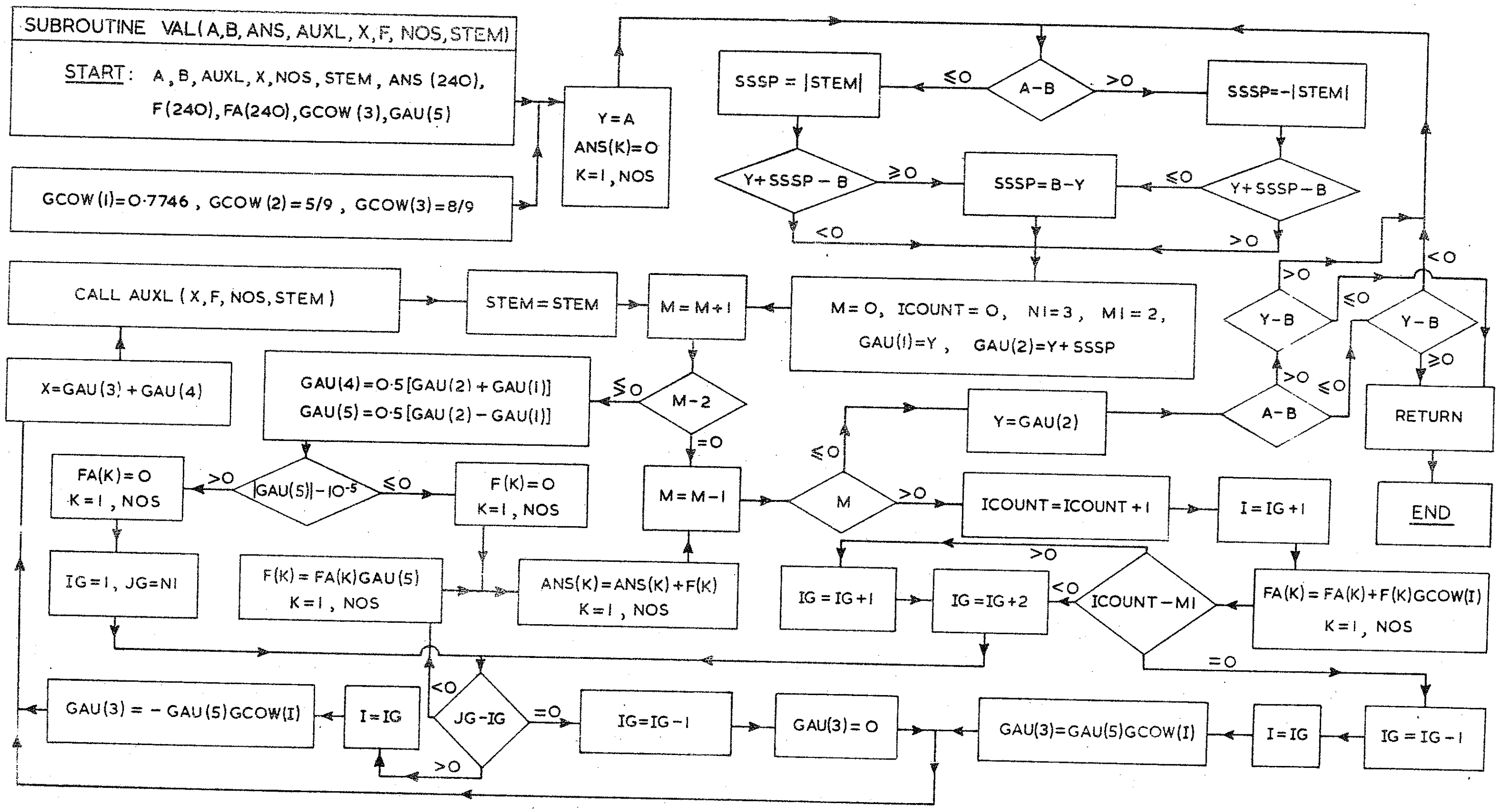

FIG. 15. BLOCK DIAGRAM OF A THREEPOINT GAUSSIAN INTEGRATION ROUTINE.

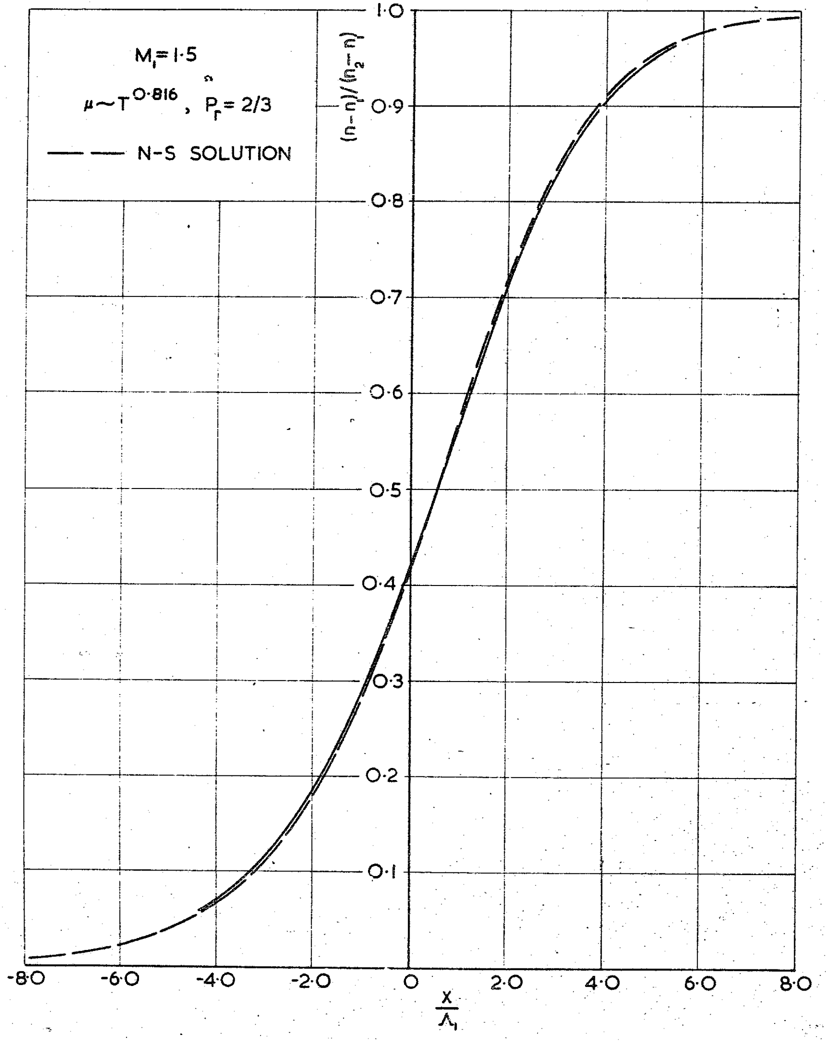

FIG. 16. SHOCK-WAVE DENSITY PROFILES.

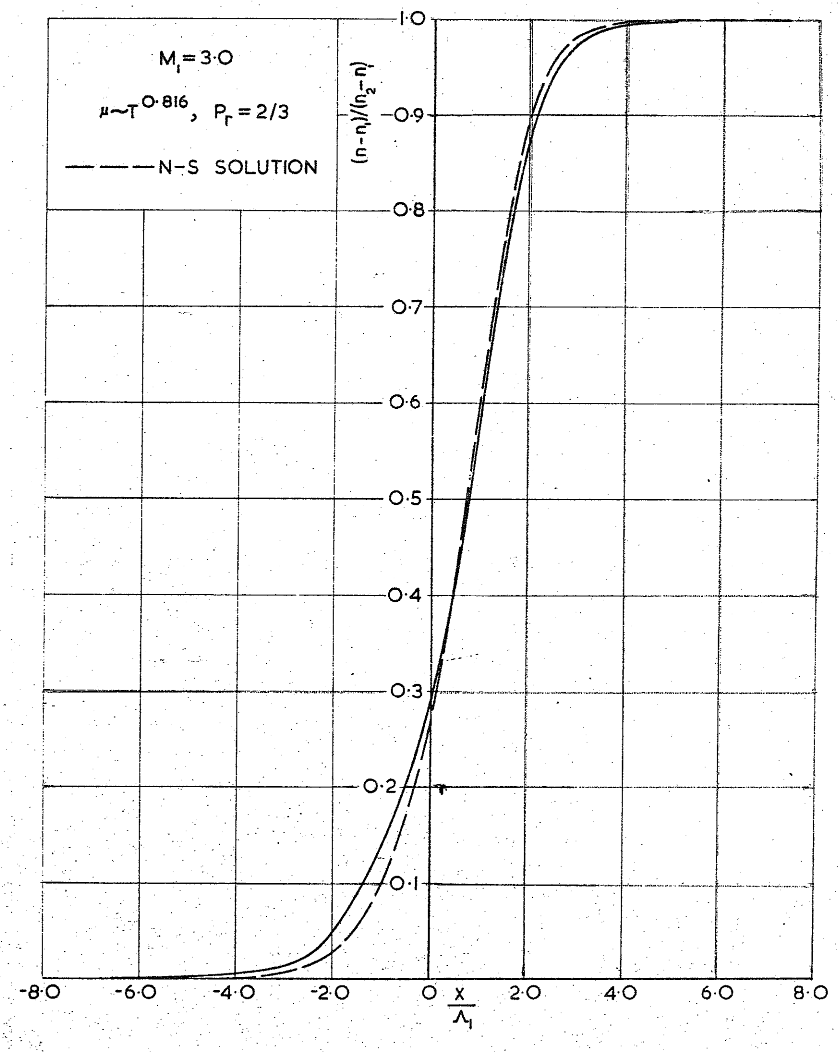

FIG. 17. SHOCK-WAVE DENSITY PROFILES.

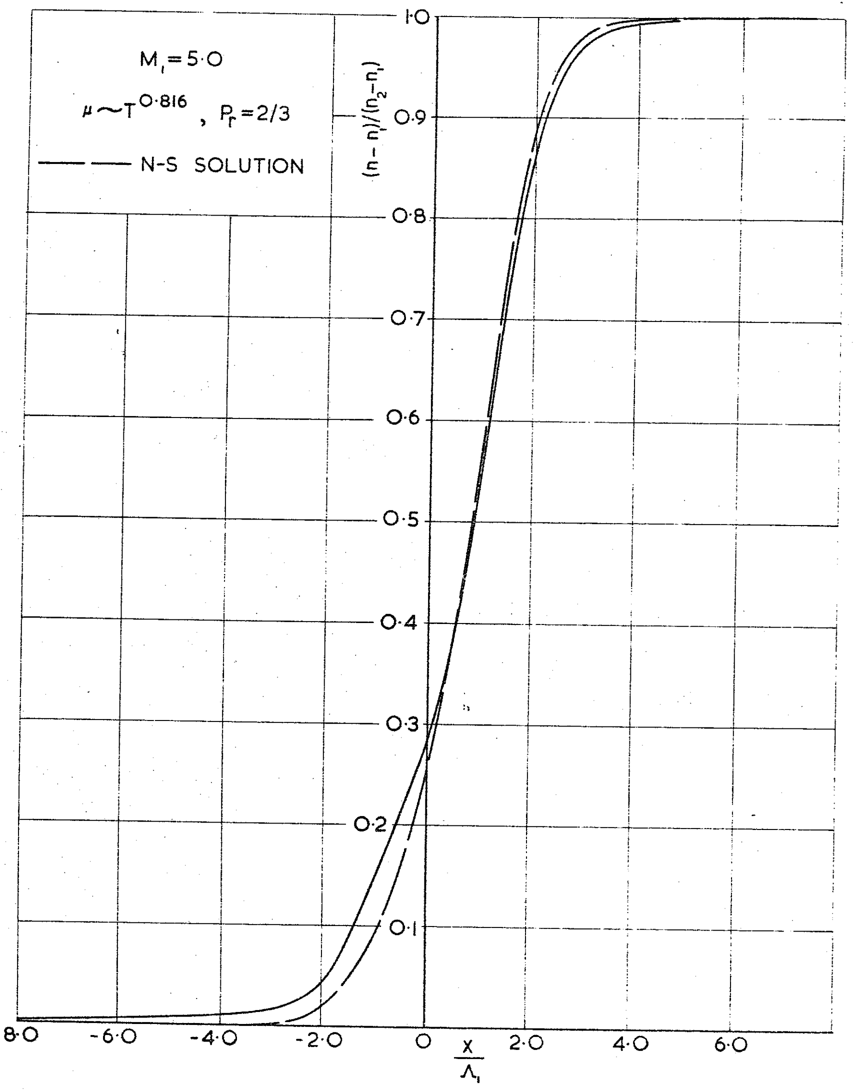

FIG. 18. SHOCK-WAVE DENSITY PROFILES.

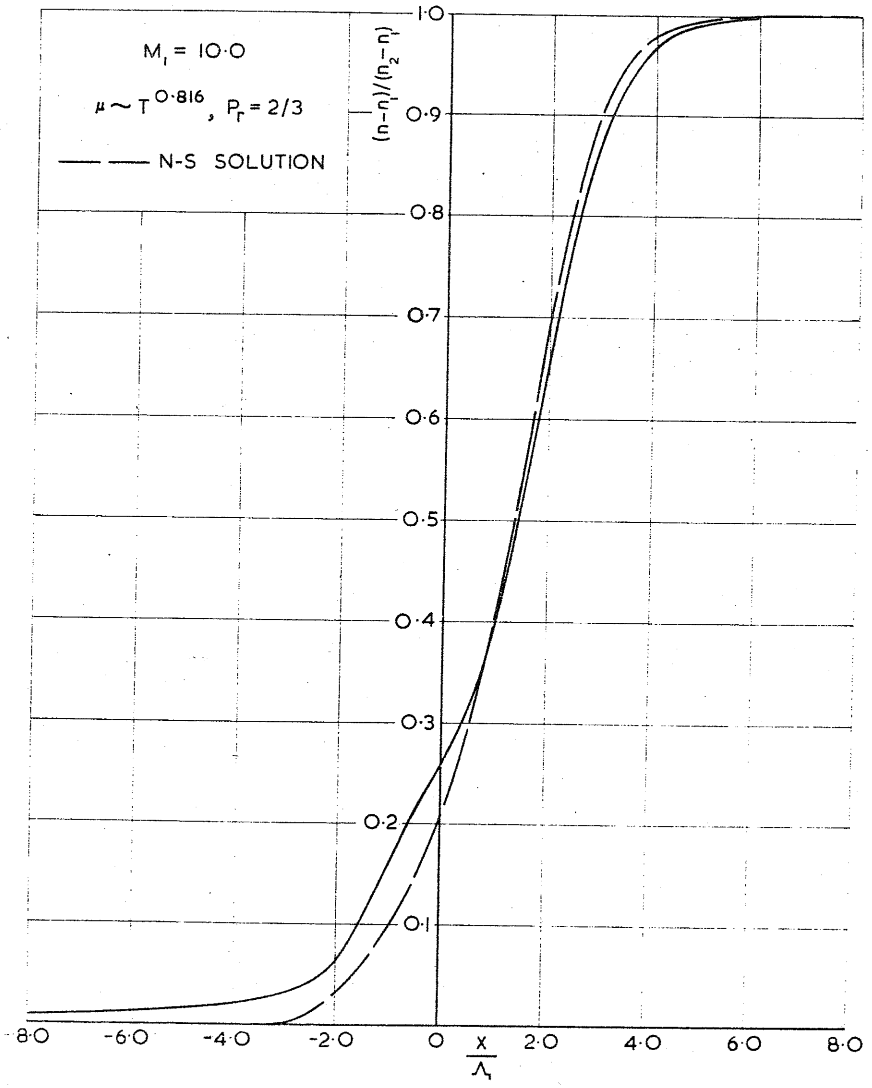

FIG. 19. SHOCK-WAVE DENSITY PROFILES.

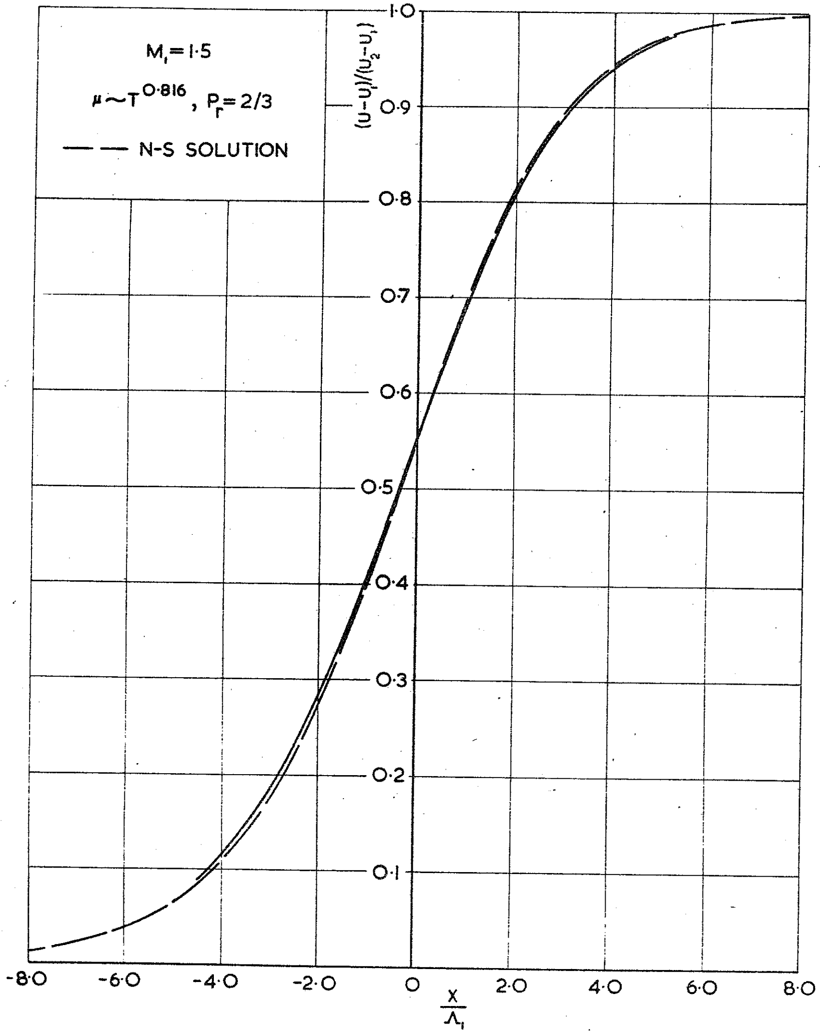

FIG. 20. SHOCK-WAVE VELOCITY PROFILES.

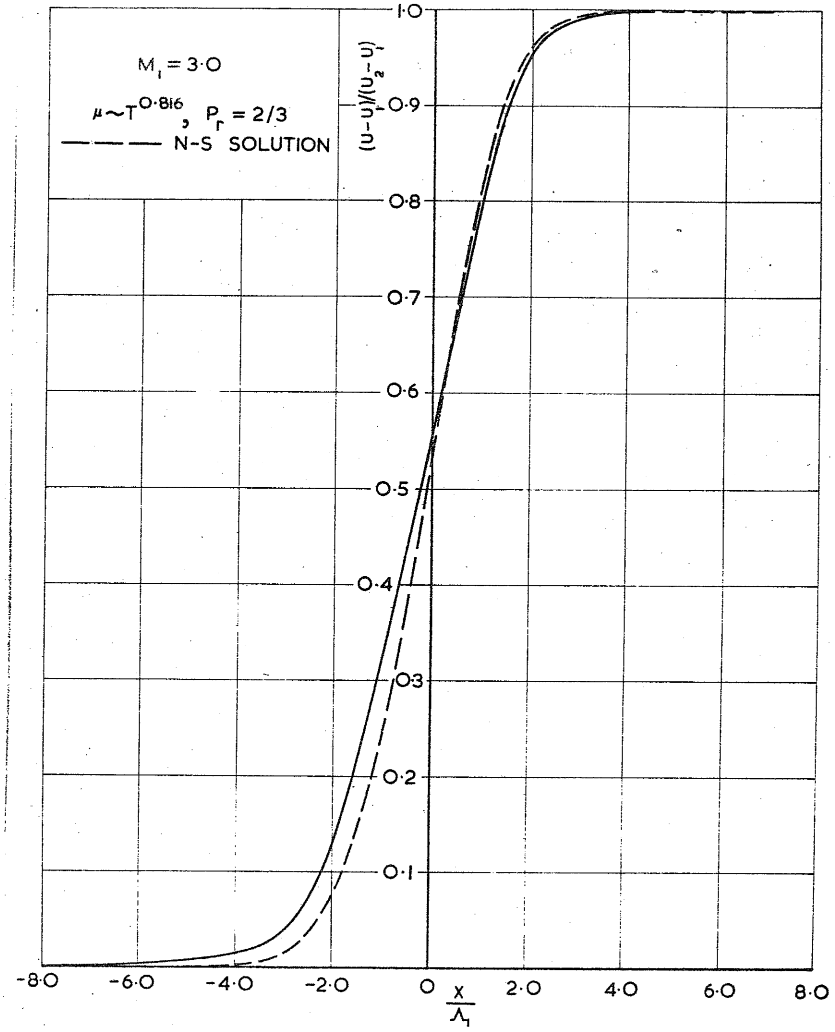

FIG. 21. SHOCK-WAVE VELOCITY PROFILES.

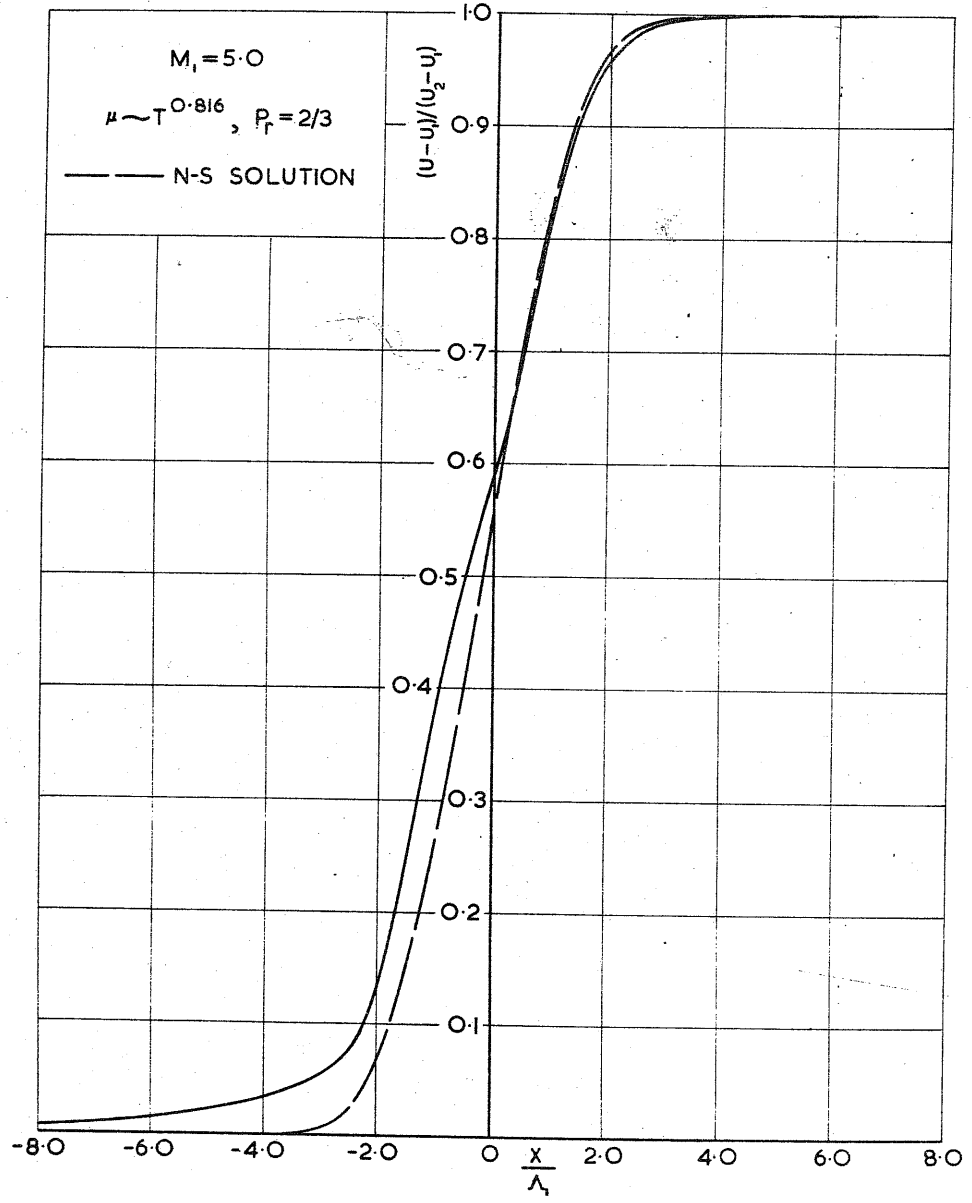

FIG. 22. SHOCK-WAVE VELOCITY PROFILES

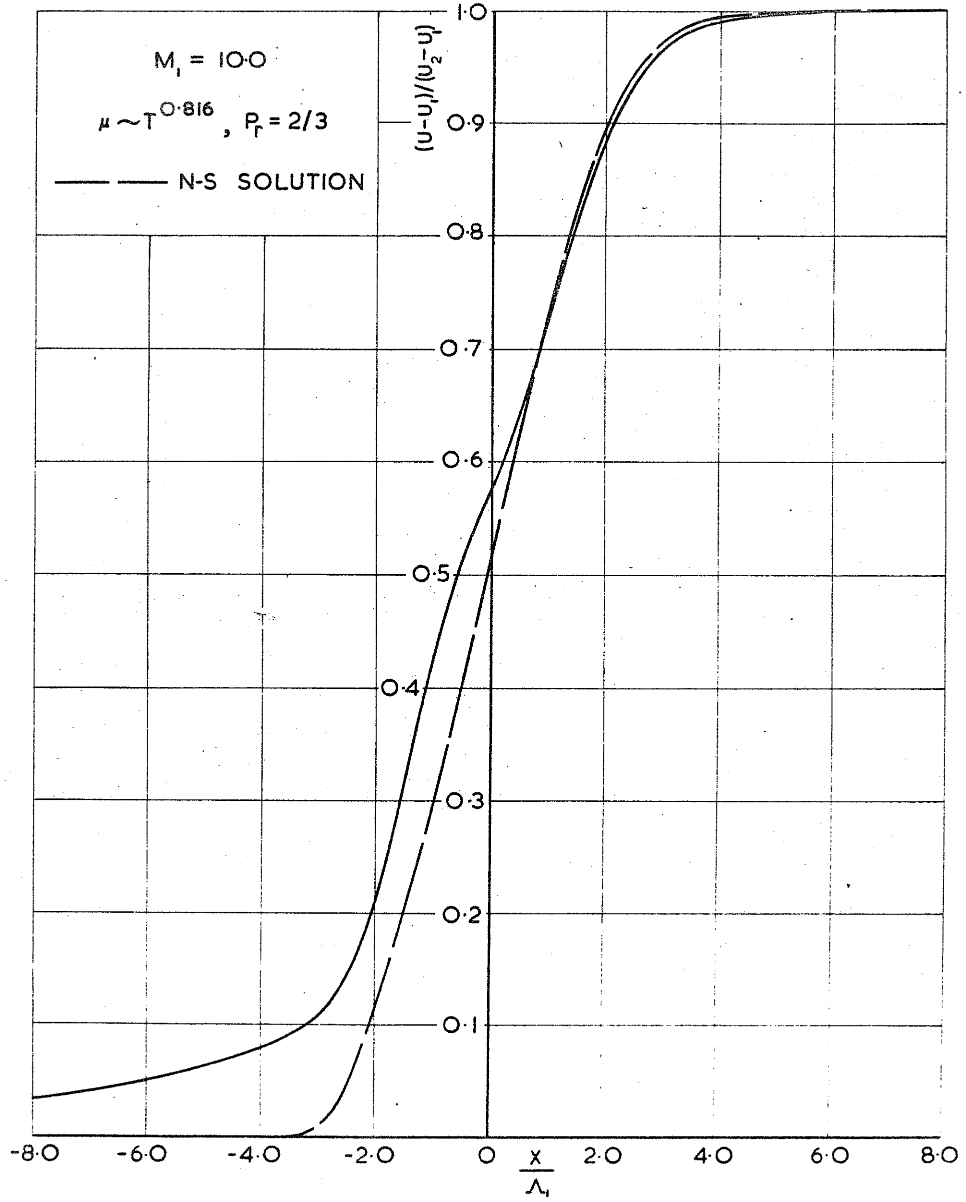

FIG. 23. SHOCK-WAVE VELOCITY PROFILES.

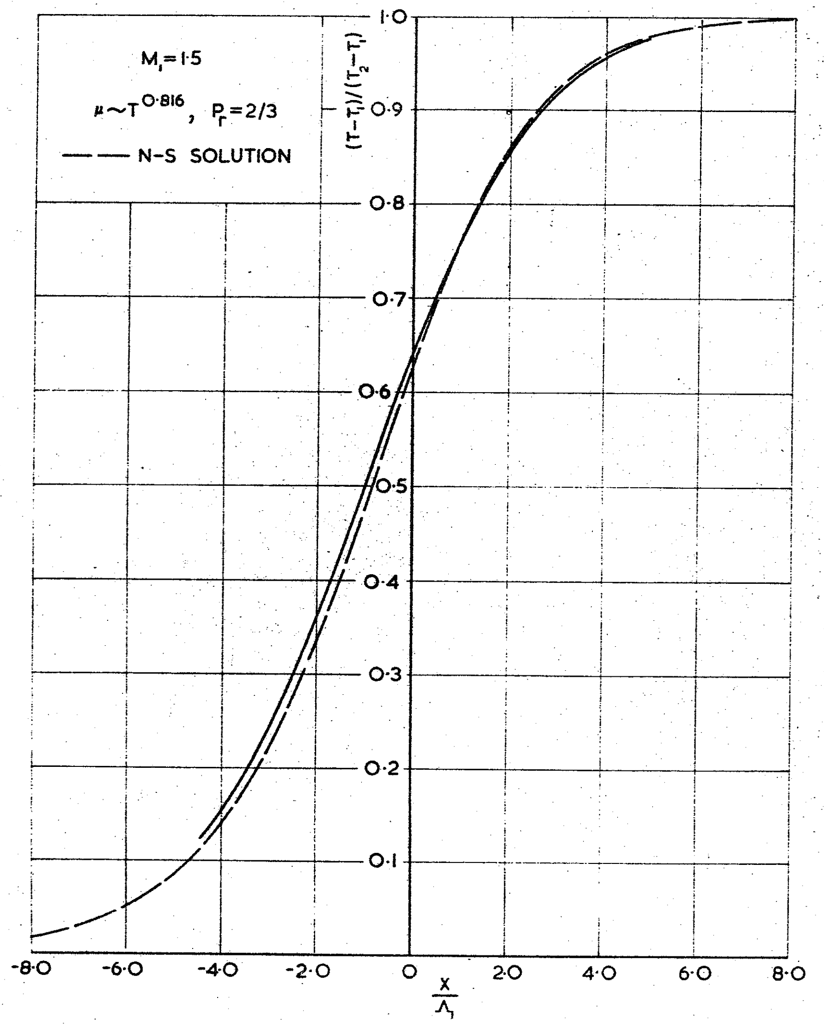

FIG. 24. SHOCK-WAVE TEMPERATURE PROFILES.

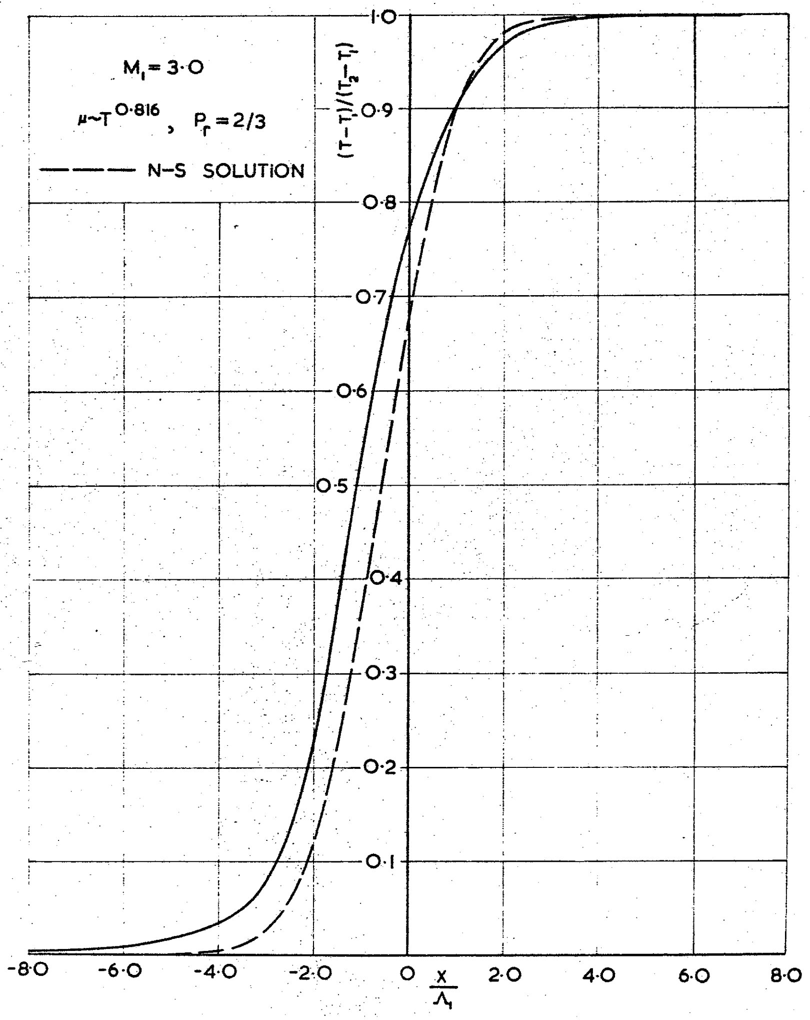

FIG. 25. SHOCK-WAVE TEMPERATURE PROFILES.

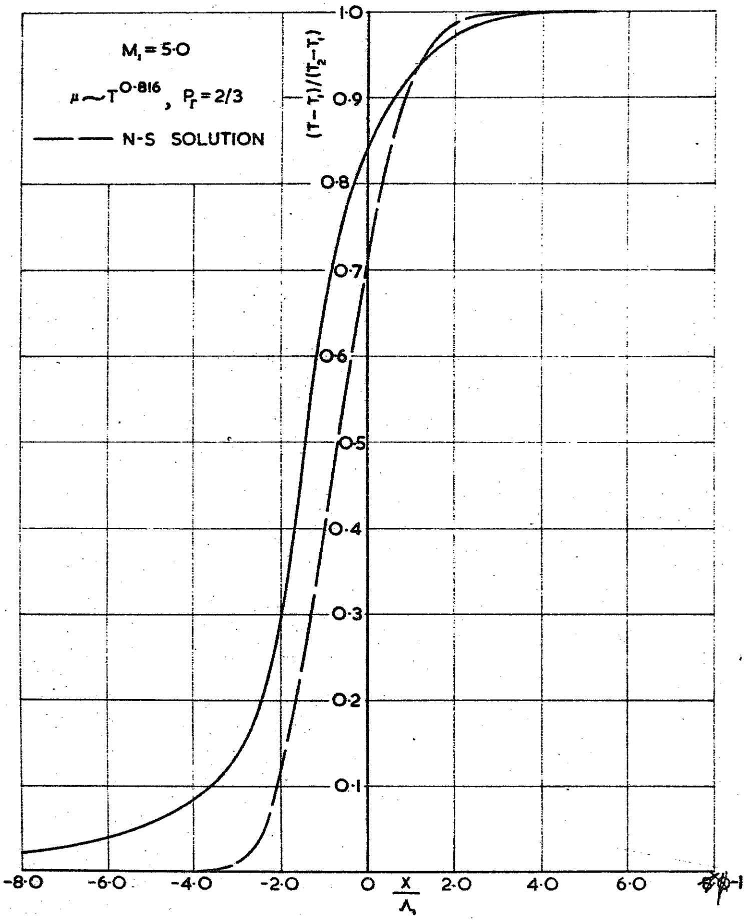

FIG. 26. SHOCK-WAVE TEMPERATURE PROFILES.

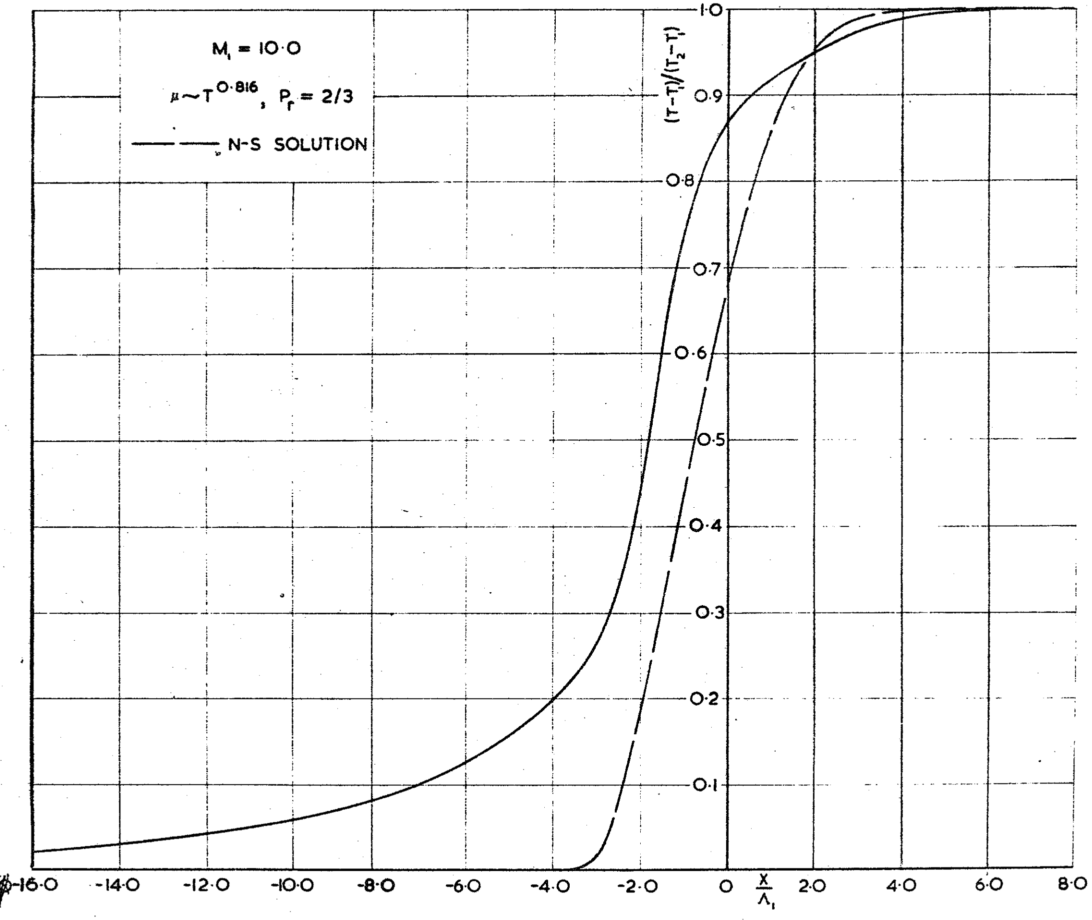

FIG. 27. SHOCK-WAVE TEMPERATURE PROFILES.

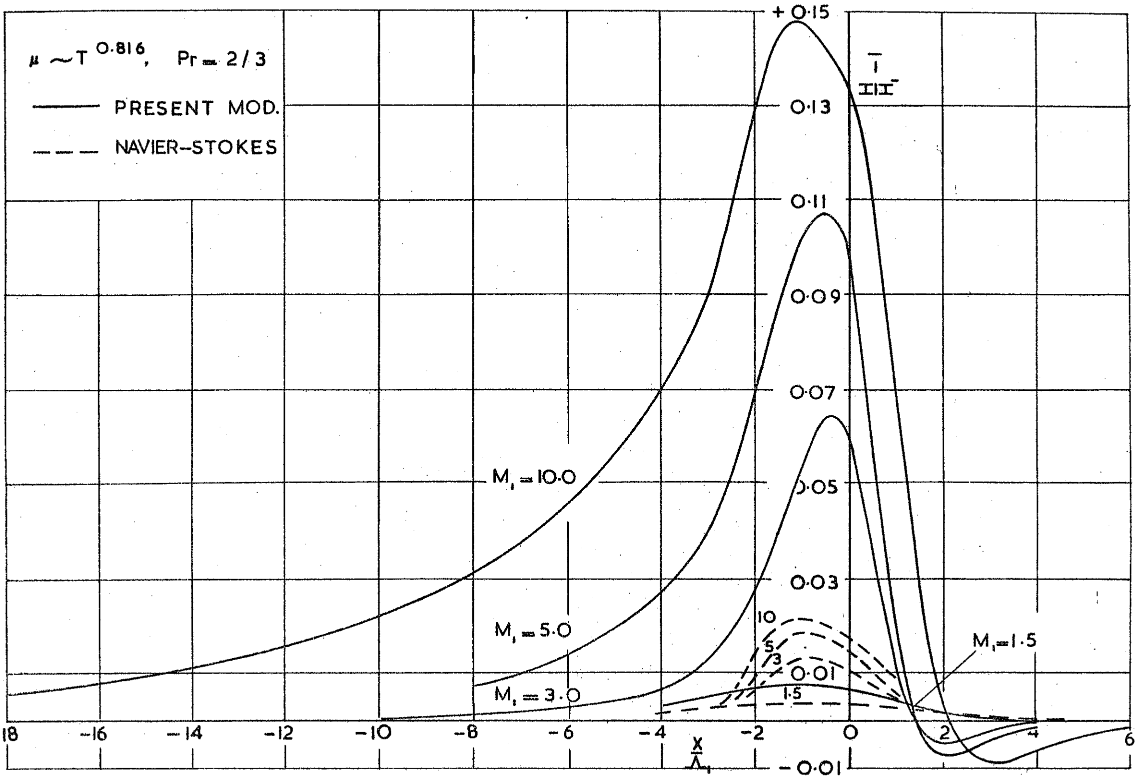

FIG.28. VARIATION OF THE TOTAL ENTHALPY ACROSS THE SHOCK-WAVE