Continuum equations in the dynamics of rarefied gases

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A procedure is given for translating boundary-value problems of gas dynamics from microscopic form into approximately equivalent continuum form. The continuum formulations involve state-variables that are either half-space moments, or complete moments of the molecular distribution functions. Moment equations derived from the kinetic equations are reduced to a determinate set by representing the distribution functions as sums of 'modified Maxwellian functions based on various characteristic temperatures and velocities'. The particular choice of such a representation depends on the Knudsen number and on the nature of the microscopic boundary conditions.

1. Introduction

Considerable progress has been made in the study of gaseous systems whose behaviour is governed by the Navier–Stokes equations. These equations are, however, valid only in cases where departures from local thermodynamic equilibrium are uniformly small at all positions and times. There are many systems of interest that involve considerable departures from states of local thermodynamic equilibrium. Such systems can be treated only within the framework of a more general formalism than the Navier–Stokes formalism.

Kinetic theory provides a microscopic, and therefore rather general, formulation of gas dynamics. However, very few problems of the theory can be handled completely and explicitly in microscopic form. Instead, we usually proceed by first translating a microscopically formulated problem into an 'approximately equivalent' macroscopic (i.e. continuum) form. We then attempt to solve the mathematically simpler continuum problem. From a practical standpoint, the microscopic theory is general for just the reason that it constitutes the basis for generating an unlimited number of distinct types of continuum theory. In this paper we shall discuss procedures for translating microscopically formulated boundary-value problems of gas dynamics into approximately equivalent continuum problems.

The microscopic state of a system is specified by molecular distribution functions, one for each species of molecule in the system. The microscopic equations of motion then have the form of non-linear integro-differential equations which can be solved only approximately, if at all. As indicated above, we usually begin by deriving from the kinetic equations a system of differential equations for a finite set of macroscopic variables. The macroscopic variables may be interpreted formally as state-variables that specify the state of some continuum; the differential equations are then interpreted as the equations of motion for that continuum. Different types of continua are distinguished one from another by the number of independent state-variables, by the physical significance of those state-variables, and by the particular form of the equations of motion.

For any gaseous system the quantities of direct physical interest are various macroscopic fields such as density, flow velocity, stress, etc. These variables can be expressed as simple functions of low-order moments of the molecular velocity distributions. An approximation method may then be counted as adequate if it leads to an accurate prediction for the behaviour of the lower-order moments, even when it determines high-order moments with poor accuracy.

When the physical interaction of gas molecules with boundaries of the system has been specified, we can formulate the (microscopic) boundary conditions to be satisfied by the distribution functions. In the translation of a specific microscopic problem into an approximately equivalent continuum problem, our choice of a suitable continuum formalism will depend intimately on the nature of the microscopic boundary data, and on the values of certain dimensionless parameters (Knudsen number K, Mach number M, etc.) that characterize the system of interest. In particular, it is important that we use a continuum formalism which permits an adequate (approximate) representation of the physical boundary data in terms of the state-variables of the theory.

The methods to be presented in this paper will be formulated with specific reference to one-dimensional problems for a simple gas in the absence of external fields (the extension to more complex cases is quite straightforward in principle). The microscopic state of a system is then specified by a single distribution function $f(\mathbf{v}, x, t)$, which is a function of the velocity variables $\mathbf{v} \equiv (v_1, v_2, v_3)$, of a position co-ordinate x, and of the time t.

The number density $n(x, t)$, the flow velocity $\mathbf{q}(x, t)$, and the kinetic temperature $T(x, t)$ are defined by the usual relations (see Chapman & Cowling 1939)

$$\left.\begin{aligned} n = \int f\,d\mathbf{v}, \quad n\mathbf{q} = \int \mathbf{v} f\,d\mathbf{v}, \\ \frac{3nkT}{m} = \int (\mathbf{v}-\mathbf{q})^2 f\,d\mathbf{v}, \end{aligned}\right\} \tag{1.1}$$

where m is the molecular mass, k is Boltzmann's constant, and the integrations extend over the whole velocity space. It is convenient to introduce also a stress tensor $p_{i,j}(x, t)$ and a heat flux vector $\mathbf{h}(x, t)$ defined by

$$p_{i,j} = \int m(v_i - q_i)(v_j - q_j) f\,d\mathbf{v} \quad (i,j = 1, 2, 3), \tag{1.2}$$

$$\mathbf{h} = \int \tfrac{1}{2} m(\mathbf{v}-\mathbf{q})^2 (\mathbf{v}-\mathbf{q}) f\,d\mathbf{v}. \tag{1.3}$$

The behaviour of the system is governed by the kinetic equation

$$\frac{\partial f}{\partial t} + v_1 \frac{\partial f}{\partial x} = \frac{\delta f}{\delta t}. \tag{1.4}$$

$\delta f/\delta t$ denotes a non-linear functional of f, whose explicit form depends on the model used to represent the molecular interactions, e.g. the Maxwell–Boltzmann model, the Fokker–Planck model (for ionized gases), and various types of ‘statistical model’. In the Maxwell–Boltzmann model, the interaction term has the form of a collision integral (see Chapman & Cowling 1939):

$$\frac{\delta f}{\delta t} = \iiint \{-f(\mathbf{v})\,f(\mathbf{w})+f(\mathbf{v}')\,f(\mathbf{w}')\}\,gb\,db\,d\epsilon\,d\mathbf{w}, \tag{1.5}$$

where $g = |g| = |\mathbf{w}-\mathbf{v}|$, and $\mathbf{v}', \mathbf{w}'$ are the final velocities of two molecules in a binary collision with initial velocities $\mathbf{v}$, $\mathbf{w}$, with impact parameter b, and with orientation of the plane of the relative orbit specified by the angle ϵ. For conciseness, the arguments x, t of the distribution functions have not been exhibited explicitly in the integrand of equation (2.3). Statistical models will be discussed in § 12.

2. Moments as state-variables

Let us ignore, for the moment, any limitations that might be imposed by the nature of the boundary data. Multiplying the kinetic equation (1.1) in turn by 1, $\mathbf{v}$ and $\frac{1}{2}m\mathbf{v}^2$, and integrating over velocity space, we can derive five continuum equations* in which $\rho = nm$, $\mathbf{q}$ and T appear as independent state-variables (see Chapman & Cowling 1939) thus:

$$\left.\begin{aligned}\frac{\partial \rho}{\partial t}+q_1\frac{\partial \rho}{\partial x}+\rho\frac{\partial q_1}{\partial x} &= 0,\\ \rho\frac{\partial q_i}{\partial t}+\rho q_1\frac{\partial q_i}{\partial x}+\frac{\partial p_{1,i}}{\partial x} &= 0,\\ \frac{\partial T}{\partial t}+q_1\frac{\partial T}{\partial x}+\frac{2}{3nk}\left[p_{1,j}\frac{\partial q_j}{\partial x}+\frac{\partial h_1}{\partial x}\right] &= 0.\end{aligned}\right\} \tag{2.1}$$

These equations are *formally* independent of the microscopic state of the gas, and of the special law of force between molecules. This is a consequence of the conservation of mass, momentum, and energy in molecular collisions. The conservation laws guarantee the elimination of all collision terms from the equations; in fact, the set of equations (2.1) makes maximum use of the simplifying consequences of the conservation theorems.

The equations (2.1) do not, however, constitute a determinate set. In addition to the basic state-variables ρ, $\mathbf{q}$ and T, they also involve the stress tensor $p_{i,j}$ and the heat flux vector $\mathbf{h}$. To make up a determinate set of continuum equations from the equations (2.1), we may proceed in either of two main ways.

On the one hand, we may elect to regard the quantities $p_{i,j}$ and $\mathbf{h}$ as *dependent* state-variables, and therefore expressible in terms of the basic state-variables ρ, $\mathbf{q}$, and T (and possibly also in terms of space gradients of ρ, $\mathbf{q}$, T). For cases in which departures from local thermodynamic equilibrium are uniformly small, the above equations can now be reduced to the Navier–Stokes equations by applying the Chapman–Enskog procedure to the kinetic equations. This derivation supplies not only the form of the Navier–Stokes equations, but also explicit formulae for the coefficients of viscosity, heat conduction, etc., as functionals of the laws of

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* The same set of equations is valid also for composite systems and for molecules with internal degrees of freedom, provided $\mathbf{q}$, T, $p_{i,j}$ and $\mathbf{h}$ are defined appropriately.

force between molecules. For cases in which appreciable departures from local thermodynamic equilibrium do occur, we might try to relate the variables $p_{i,j}$ and **h** to the basic state-variables in an entirely different manner. We would thereby obtain continua specified by exactly the same basic state-variables as the 'Navier–Stokes continuum', but obeying different equations of motion; such continua have, of course, to be counted as different from the Navier–Stokes continuum.

On the other hand, we may elect to assign to the stress components $p_{i,j}$, and possibly also to some velocity moments of still higher order, the status of basic state-variables on the same footing as ρ, **q**, and T. We can construct *formal* equations of motion for the new basic state-variables by multiplying through the kinetic equations with suitable functions of velocity, and then integrating over velocity space. The equations obtained in this way are again not a determinate set, and for two reasons.

In the first place, the new equations contain velocity moments which are not themselves basic state-variables, and which have therefore ultimately to be expressed as functions of the basic variables. In the second place, the equations contain non-vanishing moments of the collision integrals. These collision moments cannot be eliminated by invoking the conservation theorems, since those theorems have already been 'used up' in eliminating collision moments from equations (2.1). All the non-vanishing collision moments must ultimately also be expressed in terms of the basic state-variables.

Continuum theories of the above type are capable of representing the behaviour of gases which depart considerably from local thermodynamic equilibrium, provided only that the distribution functions at the system boundaries are not 'seriously' singular on surfaces in velocity space. This condition is usually satisfied in systems with very small Knudsen number.

In other cases, however, the distribution functions at the boundaries will generally be discontinuous on a plane in velocity space, e.g. when gas molecules that impinge on a wall are 'processed' by the wall before being returned to the gas. It is then necessary to use a continuum formalism that is adapted to the form of the microscopic boundary conditions (Krook 1955*a*, *b*). An appropriate formalism of this kind can be based on the use of half-space velocity moments as state-variables instead of complete moments.

For systems with small Knudsen number in which departures from local thermodynamic equilibrium are uniformly small, we would of course use the Navier–Stokes equations. In this paper, however, we shall be concerned primarily with problems in which the distribution functions exhibit steep gradients (or discontinuities), in the interior of the gas, or at boundaries, or both. (For cases in which linearization of the collision terms is permissible, the theory admits considerable simplification.)

3. Use of approximating forms

In any scheme for constructing a determinate set of macroscopic equations from the kinetic equation, an essential ingredient is the assignment of a specific form to the distribution function f in its dependence on certain of the independent variables **v**, x, and t. This form contains arbitrary parameters that are treated as unspecified functions of the remaining independent variables. In the Chapman–Enskog method, the arbitrary parameters appear as functions of the velocity $\mathbf{v}$. In Grad's method (Grad 1949), and also in the method of this paper, the unspecified parameters are interpreted as functions of position and time. An approximate solution of the problem is then known when the parameters have been determined as functions of x and t. In practice, however, it is generally more convenient to select particular moments of the velocity distributions to serve as state-variables, and to construct equations of motion for those moments.

We have noted that the formal properties of the distribution function depend markedly on the values of various dimensionless parameters that characterize the system. Of special importance for our consideration is the Knudsen number $K = l/|x_2 - x_1|$, where l is some typical value of the molecular mean free path, and $x = x_1$, $x = x_2$ are the boundaries of the system. For systems with boundaries at infinity (and sometimes also for systems with x_1 and x_2 finite), K has to be replaced (or supplemented) by a 'local Knudsen number' which is a measure of the steepness of local gradients in the gas. The most general type of approximating functions contemplated in this paper may reasonably be expected to provide representations that are, in a sense, uniformly valid over the whole range of Knudsen number, or of local Knudsen number.

In an approximation of order N, the distribution function is approximated by a function that involves N arbitrary parameters. The corresponding continuum equations are then a set of N differential equations for N state-variables (i.e. moments). The derivation of the continuum equations is of course only an intermediate step in the solution of any problem. These equations have still to be solved subject to appropriate initial and boundary conditions. The solution will be feasible only when the order of approximation N is not too large. It is therefore desirable that the approximating forms be chosen so as to yield optimum accuracy for given order N.

In this paper, the approximating functions will have the form of sums of 'modified Maxwellian functions based on various characteristic velocities and temperatures'. As we shall see, such representations can be motivated on physical grounds, and have the advantage that all (or most) of the mathematical manipulations involved in the construction of continuum equations can often be carried out analytically.

4. Auxiliary functions

The kinetic equation (1.4) has to be solved subject to conditions imposed at the boundaries of the system at $x = x_1$ and $x = x_2$ $(x_1 < x_2)$. In general, the physical interaction of gas molecules with a solid wall introduces a fundamental distinction between the velocity distributions of incoming and outgoing molecules at the wall. In fact, the distribution function is then singular on the plane $v_1 = 0$ in velocity space.

It is advantageous to recognize the singularity explicitly in the mathematical formalism by using different approximating forms for f in the two regions $v_1 > 0$ and $v_1 < 0$ of $\mathbf{v}$-space. To this end we introduce two auxiliary functions $f_+(\mathbf{v}, x, t)$ and $f_-(\mathbf{v}, x, t)$ defined only in the half-spaces $v_1 > 0$ and $v_1 < 0$ respectively (see

Krook 1955*a*, *b*; Gross, Jackson & Ziering 1957). Within their respective domains of definition, the values of f_+ and f_- are specified by the relation

$$f(\mathbf{v},x,t) = \begin{cases} f_+(\mathbf{v},x,t) & (v_1 > 0), \\ f_-(\mathbf{v},x,t) & (v_1 < 0). \end{cases} \tag{4.1}$$

Depending on the type of physical interaction at the walls, the mathematical boundary conditions may take the form of a specification of $f_+(\mathbf{v},x_1,t)$ and $f_-(\mathbf{v},x_2,t)$, or a specification of relations between f_+ and f_- at $x = x_1$ and $x = x_2$, or etc.

It is sometimes convenient, especially when the velocity distribution exhibits special symmetry, to refer velocity space to co-ordinates other than rectangular Cartesian. Thus, for the case of axial symmetry, we may use polar co-ordinates (v,θ,ϕ), and write $f = f(v,\mu,x,t)$ where $\mu \equiv \cos\theta$. The function $f_+(v,\mu,x,t)$ is defined only for $0 < \mu \leqslant 1$ and $f_-(v,\mu,x,t)$ is defined only for $-1 \leqslant \mu < 0$, so that

$$f(v,\mu,x,t) = \begin{cases} f_+(v,\mu,x,t) & (\mu > 0), \\ f_-(v,\mu,x,t) & (\mu < 0). \end{cases} \tag{4.2}$$

For systems with boundaries at finite values of x_1 and x_2, we shall generally have to use different representations for f_+ and f_-. In an approximation of order $N = N_+ + N_-$, f_+ and f_- are approximated by functional forms that involve N_+ and N_- arbitrary parameters, respectively.

In certain limiting situations (e.g. Knudsen number $K \ll 1$), it is sufficient to use a single approximating form for the complete distribution f. For systems with boundaries at infinity, f is generally not singular on the plane $v_1 = 0$, and a unified representation of f_+ and f_- is again admissible though not necessarily expedient.

5. Moments

With any function of velocity $\phi(\mathbf{v})$, we associate functionals $\mathscr{M}_+[\phi]$, $\mathscr{M}_-[\phi]$ and $\mathscr{M}[\phi]$, defined as functions of x and t by the relations

$$\mathscr{M}_\pm[\phi] \equiv \int_\pm \phi f \, d\mathbf{v} \equiv \int_\pm \phi f_\pm \, d\mathbf{v}, \tag{5.1a,b}$$

$$\mathscr{M}[\phi] \equiv \int \phi f \, d\mathbf{v} = \mathscr{M}_+[\phi] + \mathscr{M}_-[\phi], \tag{5.1c}$$

where $\int_+$ and $\int_-$ denote integration over the velocity half-spaces $v_1 > 0$ and $v_1 < 0$, respectively. The functions ϕ to be considered here generally have the form of a product of powers of the velocity components, (e.g. $v_1^{m_1} v_2^{m_2} v_3^{m_3}$ or $v^p \mu^q$), and sometimes the form of a sum of such terms (e.g. $v_1^p \mathbf{v}^2 \equiv v_1^p(v_1^2+v_2^2+v_3^2)$). The functionals (5.1) will be termed 'moments' of the distribution function; $\mathscr{M}_\pm[\phi]$ are half-space moments, and $\mathscr{M}[\phi]$ is a complete moment. Our continuum theories will involve either half-space moments or complete moments as basic state-variables.

With the function $\phi(\mathbf{v})$ we also associate half-space interaction moments $\mathscr{P}_+[\phi]$, $\mathscr{P}_-[\phi]$, and a complete interaction moment $\mathscr{P}[\phi]$, defined as functions of x and t by the relations

$$\mathscr{P}_\pm[\phi] \equiv \int_\pm \phi \frac{\delta f}{\delta t} d\mathbf{v}, \tag{5.2a,b}$$

$$\mathscr{P}[\phi] \equiv \int \phi \frac{\delta f}{\delta t} d\mathbf{v} = \mathscr{P}_+[\phi] + \mathscr{P}_-[\phi]. \tag{5.2c}$$

From the definitions (1.1) and (5.1), it then follows that

$$n = \mathscr{M}[1] = \mathscr{M}_+[1] + \mathscr{M}_-[1], \tag{5.3}$$

$$nq_i = \mathscr{M}[v_i] = \mathscr{M}_+[v_i] + \mathscr{M}_-[v_i] \quad (i = 1, 2, 3), \tag{5.4}$$

$$n\frac{3kT}{m} = \mathscr{M}[(\mathbf{v}-\mathbf{q})^2] = \mathscr{M}_+[(\mathbf{v}-\mathbf{q})^2] + \mathscr{M}_-[(\mathbf{v}-\mathbf{q})]. \tag{5.5}$$

The conservation laws for particle number, momentum and energy in molecular interactions imply the relations

$$\mathscr{P}[1] = 0, \quad \mathscr{P}[v_i] = 0, \quad \mathscr{P}[\mathbf{v}^2] = 0. \tag{5.6}$$

6. Moment equations

Let $\phi_1(\mathbf{v})$, $\phi_2(\mathbf{v}), \ldots, \phi_N(\mathbf{v})$ be any particular set of N simple functions, i.e. products of powers of velocity components or sums of such products. Multiplying the kinetic equation (1.4) by $\phi_j(\mathbf{v})$ and integrating (a) over the half-space $v_1 > 0$, (b) over the half-space $v_1 < 0$, we obtain two sets of half-space moment equations:

$$\frac{\partial}{\partial t}\mathscr{M}_+[\phi_j] + \frac{\partial}{\partial x}\mathscr{M}_+[v_1\phi_j] = \mathscr{P}_+[\phi_j] \quad (j = 1, 2 \ldots N), \tag{6.1a}$$

$$\frac{\partial}{\partial t}\mathscr{M}_-[\phi_j] + \frac{\partial}{\partial x}\mathscr{M}_-[v_1\phi_j] = \mathscr{P}_-[\phi_j] \quad (j = 1, 2 \ldots N). \tag{6.1b}$$

Integration over the whole velocity space, instead of the half-spaces, yields a single set of complete-moment equations

$$\frac{\partial}{\partial t}\mathscr{M}[\phi_j] + \frac{\partial}{\partial x}\mathscr{M}[v_1\phi_j] = \mathscr{P}[\phi_j] \quad (j = 1, 2 \ldots N) \tag{6.1c}$$

Considering for the present only the $2N$ half-moment equations (6.1a, b), we next define a set of $2N$ basic (independent) *state-variables* $M_j^{(+)}(x,t)$, $M_j^{(-)}(x,t)$, $(j = 1, 2 \ldots N)$, as the half-space moments that correspond to N particular simple functions $\psi_1(\mathbf{v}), \ldots, \psi_N(\mathbf{v})$, i.e.

$$M_j^{(+)} \equiv \mathscr{M}_+[\psi_j], \quad M_j^{(-)} \equiv \mathscr{M}_-[\psi_j] \quad (j = 1, 2 \ldots N). \tag{6.2a,b}$$

Moments $\mathscr{M}_\pm[\psi]$ that are not basic state-variables will be termed 'extraneous moments'. Our aim will be to construct, from the $2N$ formal equations (6.1a, b), a determinate set of equations of motion for the $2N$ independent state-variables $M_j^{(\pm)}$.

The choice of N functions ϕ_j in the equations (6.1), and of N functions ψ_j for the definitions (6.2), is largely arbitrary. In practice, the functions ϕ_j are usually selected to comprise simple functions of lowest degree. It is then convenient to select the N functions ψ_j in such a way that, in the formal equations (6.1 *a*, *b*), as many moments as possible are basic state-variables. For time-independent problems, the identification $\psi_j = v_1 \phi_j$ $(j = 1, 2 \ldots N)$, would result in the exclusive occurrence of basic state-variables on the left-hand sides of equations (6.1 *a*, *b*). However, certain moments will appear naturally in our approximating formulae, through definitions of characteristic local velocities and temperatures (see § 9). It is then convenient to include those moments among the basic state-variables.

In general the formal equations will involve some extraneous moments. Furthermore (except with the simpler types of statistical model), the interaction moments $\mathscr{P}_{\pm}[\phi_j]$ have purely formal significance, and are not directly expressible in terms of moments of f. In order to reduce the basic equations (6.1 *a*, *b*) to a determinate system, we have to express all extraneous moments and the $2N$ interaction moments in terms of the basic state-variables.

Similar considerations apply to the N complete-moment equations (6.1 *c*), with basic state-variables $\mathscr{M}_j(x,t)$ defined by the relations

$$M_j \equiv \mathscr{M}[\psi_j] = M_j^{(+)} + M_j^{(-)} \quad (j = 1, 2 \ldots N). \tag{6.2c}$$

7. Reduction procedure

The $2N$ formal equations (6.1 *a*, *b*) can be reduced to a determinate set by representing f_+ and f_- as specific functions of $\mathbf{v}$, involving $2N$ parameters $A_j^{(+)}$ and $A_j^{(-)}$ $(j = 1, 2 \ldots N)$; the parameters are interpreted as unknown functions of x and t. The more general types of approximating function to be considered here will depend on the state-variables $M_k^{(\pm)}$ as well as on the parameters $A_k^{(\pm)}$, thus

$$f_+(\mathbf{v}, x, t) = g_+(\mathbf{v}; A_k^{(+)}, M_k^{(+)}, M_k^{(-)}), \tag{7.1a}$$

$$f_-(\mathbf{v}, x, t) = g_-(\mathbf{v}; A_k^{(-)}, M_k^{(+)}, M_k^{(-)}), \tag{7.1b}$$

where g_+ and g_- are prescribed functions of the indicated arguments.

Using the approximations (7.1), we may evaluate the moments $M_j^{(\pm)} = \mathscr{M}_{\pm}[\psi_j]$ in the form

$$M_j^{(+)} = G_j^{(+)}(A_k^{(+)}; M_k^{(+)}, M_k^{(-)}) \quad (j = 1, 2 \ldots N), \tag{7.2a}$$

$$M_j^{(-)} = G_j^{(-)}(A_k^{(-)}; M_k^{(+)}, M_k^{(-)}) \quad (j = 1, 2 \ldots N), \tag{7.2b}$$

where the $G_j^{(+)}$ and $G_j^{(-)}$ are known functions of their arguments. For the approximating functions contemplated in this paper, $G_j^{(\pm)}$ will be linear functions of the parameters $A_k^{(\pm)}$, with coefficients that may depend on the state-variables.

Solving the two sets of (linear) equations (7.2), we obtain formulae for the parameters $A_j^{(\pm)}$ as functions of the state-variables:

$$A_j^{(+)} = H_j^{(+)}(M_k^{(+)}, M_k^{(-)}), \tag{7.3a}$$

$$A_j^{(-)} = H_j^{(-)}(M_k^{(+)}, M_k^{(-)}), \tag{7.3b}$$

where the $H_j^{(\pm)}$ are again known functions of their arguments. In the important special case that the functions (7.1 *a*, *b*) do not involve the state-variables explicitly, the functions $H_j^{(+)}$ and $H_j^{(-)}$ are simply linear functions of the state-variables $M_k^{(+)}$ and $M_k^{(-)}$, respectively.

Substitution of the formulae (7.3) for $A_j^{(\pm)}$ on the right-hand sides of equations (7.1) now provides representations for $f_\pm$ that contain only the state-variables, and not the parameters thus:

$$f_\pm = h_\pm(\mathbf{v};\, M_k^{(+)}, M_k^{(-)}), \tag{7.4a, b}$$

where h_+ and h_- are known functions of their arguments. Any functionals of f_+ and f_- can now be evaluated, at least in principle, as explicit functions of the $2N$ state-variables $M_k^{(\pm)}$. In particular, extraneous moments $\mathscr{M}_\pm[\psi]$, and interaction moments $\mathscr{P}_\pm[\phi_j]$, can thus be determined as functions of the state-variables. When these functions are substituted in the formal equations (6.1*a*, *b*), we obtain a determinate set of equations of motion for the state-variables.

An analogous process with complete moments M_j as state-variables, leads from the formal equations (6.1*c*) to a determinate set of N equations for the M_j.

The macroscopic boundary conditions satisfied by the state-variables $M_j^{(\pm)}$ are readily derived from the microscopic boundary conditions on f_+ and f_-. If, for example, the boundary values $f_+(\mathbf{v}, x_1)$ and $f_-(\mathbf{v}, x_2)$ are specified, direct integration provides the boundary values $M_j^{(+)}(x_1)$ and $M_j^{(-)}(x_2)$ for the state-variable.

The formulae for the interaction moments $\mathscr{P}_\pm[\phi_j]$ as functions of the state-variables involve coefficients that appear in the form of multiple integrals. Since the derivation of continuum equations is merely a preliminary step in the solution of a problem of gas dynamics, the usefulness of the procedure outlined above will depend crucially on the extent to which these multiple integrals can be evaluated in closed form. (The elimination of extraneous moments in closed form presents no difficulty.) This circumstance places severe restrictions on the types of approximating forms that can reasonably be used to represent the velocity distributions. Sums of modified Maxwellian functions provide satisfactory representations from this point of view, especially when used in conjunction with statistical models.

8. Modified Maxwellian functions

The normalized Maxwell distribution function corresponding to average velocity $\mathbf{Q}$ and temperature $\Theta \equiv m\alpha^2/k$ will be denoted by $\Psi(\mathbf{v}; \mathbf{Q}, \Theta)$ or $\Phi(\mathbf{v}; \mathbf{Q}, \alpha)$:

$$\begin{aligned}\Psi(\mathbf{v}; \mathbf{Q}, \Theta) &\equiv \left(\frac{m}{2\pi k\Theta}\right)^{\frac{3}{2}} \exp\left[-m(\mathbf{v}-\mathbf{Q})^2/2k\Theta\right] \\ &= \Phi(\mathbf{v}; \mathbf{Q}, \alpha) \equiv \left(\frac{1}{2\pi\alpha^2}\right)^{\frac{3}{2}} \exp\left[-(\mathbf{v}-\mathbf{Q})^2/2\alpha^2\right].\end{aligned} \tag{8.1}$$

A function $F(\mathbf{v}; \mathbf{Q}, \alpha)$ will be termed a 'modified Maxwellian function (*MM* function), based on $(\mathbf{Q}, \Theta)$ or on $(\mathbf{Q}, \alpha)$', when it has the form

$$F = \Psi(\mathbf{v}; \mathbf{Q}, \Theta)\, P\left(\frac{\mathbf{v}}{\alpha}\right) = \Phi(\mathbf{v}; \mathbf{Q}, \alpha)\, P\left(\frac{\mathbf{v}}{\alpha}\right), \tag{8.2}$$

where P represents a polynomial in the components of $\mathbf{v}/\alpha$, with coefficients that may be functions of x and t. The velocity $\mathbf{Q}$, and the temperature Θ or associated speed $\alpha = (k\Theta/m)^{\frac{1}{2}}$, may be prescribed constants or they may be functions of the basic state-variables. The modifying polynomial P in the formula (8.2) represents a distortion of the basic Maxwellian distribution $\Psi(\mathbf{v}; \mathbf{Q}, \Theta)$.

9. Characteristic velocities and temperatures

For any particular system, we can define a number of characteristic macroscopic velocities $\mathbf{V}_\lambda$ and associated temperatures Θ_λ ($\lambda = 1, 2 \ldots s$). Among such velocity-temperature pairs, we note in particular the following:

(*a*) Constant pairs $(\mathbf{Q}_1, T_1)$ and $(\mathbf{Q}_2, T_2)$ which generally appear in the specification of microscopic boundary conditions at $x = x_1$ and $x = x_2$, respectively.

(*b*) The pair $(\mathbf{q}, T)$ consisting of the local macroscopic velocity $\mathbf{q}(x,t)$ and kinetic temperature $T(x,t)$.

(*c*) Two pairs $(\mathbf{q}, T_+)$ and $(\mathbf{q}, T_-)$ where $T_+(x,t)$ and $T_-(x,t)$ are local kinetic temperatures associated with the half-space velocity distributions $v_1 > 0$ and $v_1 < 0$, respectively, thus

$$\frac{kT_\pm}{m} \equiv \beta_\pm^2 = \frac{\mathcal{M}_\pm[(\mathbf{v}-q)^2]}{3\mathcal{M}_\pm[1]}. \tag{9.1a,b}$$

(*d*) Two pairs $(\mathbf{q}_+, T'_+)$ and $(\mathbf{q}_-, T'_-)$ which provide a 'purer' characterization than (*c*) for the half-space velocity distributions. The velocities $\mathbf{q}_\pm(x,t)$ and temperatures $T'_\pm(x,t)$ are defined by the relations

$$(\mathbf{q}_\pm)_1 = q_1; \quad (\mathbf{q}_\pm)_j = \frac{\mathcal{M}_\pm[v_j]}{\mathcal{M}_\pm[1]} \quad (j = 2, 3), \tag{9.2a,b}$$

$$\frac{kT'_\pm}{m} \equiv (\beta'_\pm)^2 = \frac{\mathcal{M}_+[(\mathbf{v}-\mathbf{q}_\pm)^2]}{3\mathcal{M}_\pm[1]}. \tag{9.3a,b}$$

We note that the velocities and temperatures of (*b*), (*c*) and (*d*) are all expressible directly in terms of complete moments or half-space moments of the velocity distributions. A different type of characteristic local velocity and temperature will be introduced in § 11.

Instead of the velocity-temperature pairs $(\mathbf{V}_\lambda, \Theta_\lambda)$, it is often convenient to use the corresponding velocity-speed pairs $(\mathbf{V}_\lambda, \alpha_\lambda)$ with

$$\alpha_\lambda = (k\Theta_\lambda/m). \tag{9.4}$$

10. Approximating functions

The approximating functions that we propose to use, in conjunction with the procedure outlined in § 7, have the general form of sums of modified Maxwellian functions based on the characteristic velocity-temperature pairs $(\mathbf{V}_\lambda, \Theta_\lambda)$ or associated velocity-speed pairs $(\mathbf{V}_\lambda, \alpha_\lambda)$ ($\lambda = 1, 2 \ldots s$). We thus assign to f_+ and f_- or to f, the general approximate representations

$$f_\pm = \sum_{\lambda=1}^{s} \Phi(\mathbf{v}; \mathbf{V}_\lambda, \alpha_\lambda) P_\lambda^{(\pm)}\left(\frac{\mathbf{v}}{\alpha_\lambda}\right), \tag{10.1a,b}$$

$$f = \sum_{\lambda=1}^{s} \Phi(\mathbf{v}; \mathbf{V}_\lambda, \alpha_\lambda) P_\lambda\left(\frac{\mathbf{v}}{\alpha_\lambda}\right). \tag{10.1c}$$

The modifying polynomials $P_\lambda^{(+)}$, $P_\lambda^{(-)}$ and P_λ contain $N_\lambda^{(+)}$, $N_\lambda^{(-)}$ and N_λ terms, respectively, with coefficients that are regarded as unknown functions of x and t.

The approximation provided by the formulae (10.1 *a*, *b*) is of order $\sum_{\lambda}(N_{\lambda}^{(+)}+N_{\lambda}^{(-)})$, and that provided by (10.1 *c*) is of order $\sum_{\lambda} N_{\lambda}$.

In practice, of course, we would not generally include in the sums (10.1) components corresponding to *all* available velocity-temperature pairs $(\mathbf{V}_{\lambda}, \Theta_{\lambda})$ $(\lambda = 1, 2 \ldots s)$. In most cases, physical considerations suggest that certain components may reasonably be omitted from the representations. Some arguments to justify the representation of distribution functions in terms of *MM* functions will be given in § 14.

We have already noted the desirability of using representations that permit the expression of interaction moments, in sufficiently simple form, as functions of the basic state-variables. This requirement is most stringent when the interaction term $\delta f/\delta t$ has the Maxwell–Boltzmann form (1.5). Complete interaction moments $\mathscr{P}[\phi_j]$ can generally be reduced in a straightforward manner for representations of the form (10.1 *c*). The reduction of the half-space moments $\mathscr{P}_{\pm}[\phi_j]$ with approximating forms (10.1 *a*, *b*) is much more troublesome when $\delta f/\delta t$ has the Maxwell–Boltzmann form.

The reduction of the interaction moments is simpler when the interaction terms have the Fokker–Planck form, as for ionized gases (see Rosenbluth, MacDonald & Judd, 1957). For the class of 'statistical models' discussed in § 11, the reduction of the interaction moments $\mathscr{P}[\phi_j]$, $\mathscr{P}_{\pm}[\phi_j]$ can usually be effected without difficulty.

The use of approximating forms (8.5 *a*, *b*, *c*) may be regarded as constituting a natural generalization of Mott–Smith's method of solution of the Boltzmann equation for a stationary plane shock wave in a simple gas (Mott-Smith 1951). Mott-Smith represents the distribution function f as a sum of two (unmodified) Maxwellian functions

$$f(\mathbf{v}, x) = A(x)\Psi(\mathbf{v};\, Q_1\mathbf{i}, T_1) + B(x)\Psi(\mathbf{v};\, Q_2\mathbf{i}, T_2), \tag{10.2}$$

where $(Q_1\mathbf{i}, T_1)$ and $(Q_2\mathbf{i}, T_2)$ are the (constant) velocity-temperature pairs that correspond to the equilibrium conditions at $x = -\infty$ and $x = +\infty$, respectively. The application of the generalized approximations for this problem will be discussed in § 15.

From another point of view, the approximating forms (10.1 *a*, *b*, *c*) may also be regarded as providing a generalization of Grad's method which is based on a representation of f as a single *MM* function based on the local velocity and temperature, i.e. on $(\mathbf{q}, T)$.

11. Collisional temperatures

The velocities $\mathbf{q}$, $\mathbf{q}_{\pm}$ and temperatures T, $T_{\pm}$, $T'_{\pm}$ defined in § 9, serve to characterize the local velocity distributions f and $f_{\pm}$. We may introduce another type of characteristic velocity $\mathbf{Q}_c(x, t)$ and temperature $T_c(x, t)$ to characterize the velocity distribution of those molecules that have suffered collisions locally.

Let $\sigma(\mathbf{v}, x, t)$ denote the local collision frequency for molecules of velocity $\mathbf{v}$. In the Maxwell–Boltzmann model (for example), we would have

$$\sigma(\mathbf{v}, x, t) = \iiint f(\mathbf{w}, x, t)\, |\mathbf{v}-\mathbf{w}|\, b\, db\, d\epsilon\, d\mathbf{w}. \tag{11.1}$$

A possible, but not unique, definition of $\mathbf{Q}_c(x,t)$ and $T_c(x,t)$ is contained in the following five equations:

$$\left.\begin{aligned} &\nu\int\phi(\mathrm{v})\,\sigma(\mathrm{v},x,t)\Psi(\mathrm{v};\,\mathbf{Q}_c,T_c)\,d\mathrm{v} = \int\phi\sigma f(\mathrm{v},x,t)\,d\mathrm{v},\\ &\phi = 1, v_1, v_2, v_3, \mathrm{v}^2. \end{aligned}\right\} \tag{11.2}$$

(A number density $\nu(x,t)$ is also defined automatically by these equations.)

The basis for the definitions (11.2) is provided by the property that those molecules which have suffered collision at x will, after collision, have an approximately Maxwellian velocity distribution corresponding to an average velocity and a temperature determined by the total momentum and energy of the colliding molecules. Since the collision frequency σ generally depends on v, the 'collisional velocity' $\mathbf{Q}_c(x,t)$ and 'collisional temperature' $T_c(x,t)$ will differ from the local velocity $\mathbf{q}(x,t)$ and local kinetic temperature $T(x,t)$ of the gas.

12. Interaction models

The formal complexity of the Maxwell–Boltzmann collision integrals is a consequence of the fact that they take into account the detailed geometry of all individual kinds of binary collision. In the Fokker–Planck model (for ionized gases), the collision geometry is treated statistically to a certain extent.

In the class of 'statistical' models, the velocity distribution of those molecules that have locally suffered a collision is related purely statistically to their pre-collision velocity distribution. Two characteristic features of these models are: (*a*) the formal simplicity of their interaction terms as compared to those of the Maxwell–Boltzmann and Fokker–Planck models, and (*b*) their flexibility in permitting a representation of many detailed aspects of molecular interactions. A general account of statistical models will be published elsewhere.

In one of the simpler types of statistical model, the interaction term is assumed to have the form

$$\frac{\delta f}{\delta t} = \sigma(\mathrm{v},x,t)\{-f+\nu\Psi(\mathrm{v},\mathbf{Q},\mathscr{T})\}, \tag{12.1}$$

where the collision frequency $\sigma(\mathrm{v},x,t)$ may be prescribed, or may be a functional of f as, for example, in equation (11.1). The macroscopic variables $\nu(x,t)$, $\mathbf{Q}(x,t)$ and $\mathscr{T}(x,t)$ are determined uniquely by the conditions that particle-number, momentum, and energy be conserved in molecular interactions. The defining relations for ν, $\mathbf{Q}$ and $\mathscr{T}$ are then just the five equations (11.2).

For the special case that $\sigma = n.\kappa(x,t)$ is independent of v, the interaction term (12.1) is particularly simple. Here $\nu \equiv n$, $\mathbf{Q} \equiv \mathbf{q}$ and $\mathscr{T} \equiv T$, where $n, \mathbf{q}, T$ are, respectively, the local number density, average velocity, and kinetic temperature (see Bhatnagar, Gross & Krook, 1954). We then have

$$\frac{\delta f}{\delta t} = -n\kappa f + n^2\kappa\Psi(\mathrm{v};\,\mathbf{q},T). \tag{12.2}$$

We note that, with the model (12.2), the interaction moments are obtained directly in terms of moments of f.

Apart from its great intrinsic simplicity, this constant collision-time model is of special formal interest for the reason that numerically exact solutions can be obtained without excessive difficulty for a number of one-dimensional boundary-value problems (Krook 1955*b*). Some insight may then be gained into the accuracy of the present and other approximation methods by comparing approximate solutions with the exact solutions for the same problem. The results of such a comparison in the case of Couette flow with boundary walls at different temperatures, and for various values of Mach numbers, Knudsen number and ratio of wall temperatures, will be reported as soon as exact solutions become available from calculations now in progress on an IBM 704 computer.

13. Integral equations

For one-dimensional, time-independent problems, the kinetic equation (1.5) can be written in the general form

$$v_1 \frac{\partial f(\mathbf{v}, x)}{\partial x} = \sigma(\mathbf{v}, x)\{-f(\mathbf{v}, x) + \mathscr{E}(\mathbf{v}, x)\}, \tag{13.1}$$

where σ and $\sigma\mathscr{E}$ are prescribed functionals of f. The function $\sigma(\mathbf{v}, x)$ may be interpreted formally as a '(collisional) absorption coefficient' for molecules of velocity $\mathbf{v}$ at x. The function $\sigma(\mathbf{v}, x)\,\mathscr{E}(\mathbf{v}, x)$ may then be interpreted as the 'rate of generation' of molecules of velocity $\mathbf{v}$, by collisions at x.

Any boundary-value problem for the equation (13.1) is readily transformable to an integral-equation problem. To this end, we define a function

$$\lambda(\mathbf{v}, x) = \int_{x_1}^{x} \sigma(\mathbf{v}, x')\,dx' \tag{13.2}$$

which will, in general, be a functional of f. Equation (13.1) may then be written in the form:

$$\frac{\partial}{\partial x}\{f \exp[\lambda(\mathbf{v}, x)]\} = \frac{1}{v_1}\sigma(\mathbf{v}, x)\,\mathscr{E}(\mathbf{v}, x)\exp[\lambda(\mathbf{v}, x)]. \tag{13.3}$$

Integrating equation (13.3) over (x_1, x) for $v_1 > 0$, and over (x, x_2) for $v_1 < 0$, we obtain the non-linear integral equations:

$$f_+(\mathbf{v}, x) = f_+(\mathbf{v}, x_1)\exp[-\lambda(\mathbf{v}, x)/v_1] + \frac{1}{v_1}\int_{x_1}^{x} \mathscr{E}(\mathbf{v}, x)\exp[-\{\lambda(\mathbf{v}, x) - \lambda(\mathbf{v}, x')\}/v_1]\,d\lambda', \tag{13.4a}$$

$$f_-(\mathbf{v}, x) = f_-(\mathbf{v}, x_2)\exp[-\{\lambda(\mathbf{v}, x_2) - \lambda(\mathbf{v}, x)\}/|v_1|] + \frac{1}{|v_1|}\int_{x}^{x_2} \mathscr{E}(\mathbf{v}, x')\exp[-\{\lambda(\mathbf{v}, x') - \lambda(\mathbf{v}, x)\}/|v_1|]\,d\lambda', \tag{13.4b}$$

where we have written $d\lambda' \equiv \sigma(\mathbf{v}, x')\,dx'$. The form of these equations is instructive when considered in connexion with the approximation procedures presented in this paper.

We note first that, for a fixed x, the emission function $\sigma(\mathbf{v}, x)\,\mathscr{E}(\mathbf{v}, x)$ is the velocity distribution (after collision) of just those molecules that have suffered collision at x. On general grounds, we may expect $\mathscr{E}(\mathbf{v}, x)$ to be approximately

Maxwellian in $\mathbf{v}$; the average velocity and the temperature appropriate to $\mathscr{E}(\mathbf{v}, x)$ are the collisional velocity $\mathbf{Q}_c(x)$ and the collisional temperature $T_c(x)$ defined in § 11. Further, the function $[\lambda(\mathbf{v}, x) - \lambda(\mathbf{v}, x')]/|v_1|$ is the number of mean free paths between planes perpendicular to $\mathbf{i}$ at x and x', for molecules of velocity $\mathbf{v}$.

Equations (13.4) show that, in general, each of $f_+(\mathbf{v}, x)$ and $f_-(\mathbf{v}, x)$ can be regarded as a superposition of two essentially different types of distribution:

A. A partially-attenuated boundary distribution represented by the first term on the right-hand side of each equation (13.4). The degree of attenuation depends on the position of x relative to the boundary, and depends on the magnitude and direction of the molecular velocity $\mathbf{v}$.

B. A more complex distribution represented by the second term on the right-hand sides of equations (13.4), and made up of weighted contributions from the collisional emission of $\mathbf{v}$-molecules at all points $x' < x$ for $f_+(\mathbf{v}, x)$, and at all points $x' > x$ for $f_-(\mathbf{v}, x)$. In this component, the emission $\sigma\mathscr{E}(\mathbf{v}, x')$ at x' is weighted by the negative exponential of the number of mean free paths of a $\mathbf{v}$-molecule between x' and x.

In subsequent sections, we will refer to these two types of partial distribution as component A and component B, respectively.

One negative conclusion can be drawn immediately from the structure of equations (13.4) and, in particular, from the structure of the terms corresponding to component B: any representation of $f_+(\mathbf{v}, x)$ (or of $f_-(\mathbf{v}, x)$), as a modified Maxwellian function based on a *single* velocity-temperature pair, is liable to have poor accuracy except in certain special limiting cases.

Proceeding rather heuristically, we could approximate the component B by a sum of *MM* functions based on the collisional velocity-temperature pairs $(\mathbf{Q}_c(x'_j), T_c(x'_j))$ at a number of points $x'_1, x'_2 \ldots$ in the interval (x_1, x_2). Such an approximation procedure would itself be rather formidable, and we would of course prefer to use *local* velocity-temperature pairs for the field point x rather than pairs for a sequence of source-points x'_j. By defining a sufficiently wide variety of characteristic local velocity-temperature pairs, and by using *MM* functions based on such local pairs, we may hope to mimic the representation provided by *MM* functions based on collisional pairs in the above way. This argument can in no way be regarded as *justifying* the approximation procedures of the previous sections; it serves only to lend some plausibility to those procedures.

In the subsequent sections of this paper, we shall discuss in a formal way two particular time-independent boundary-value problems: (a) a problem of non-linear heat conduction, and (b) the problem of shock-wave structure.

14. Non-linear heat conduction

We consider a system composed of a simple gas in a steady state between parallel plates $x = x_1$ and $x = x_2$ $(x_2 > x_1)$. The plates are maintained at constant temperatures T_1 and T_2, respectively $(T_1 > T_2)$. We shall suppose that molecules which strike a wall are adsorbed and are subsequently re-emitted into the gas with a Maxwellian distribution appropriate to the wall temperature.

The boundary conditions then have the form

$$f_+(\mathbf{v}, x_1) = a_1\Psi(\mathbf{v};\, 0, T_1), \quad f_-(\mathbf{v}, x_2) = a_2\Psi(\mathbf{v};\, 0, T_2), \qquad (14.1\,a, b)$$

where at most one of the positive constants a_1, a_2 may be specified arbitrarily. In the integral equations (13.4a, b) we have now to substitute the formulae (14.1a, b) for $f_+(\mathbf{v}, x_1)$ and $f_-(\mathbf{v}, x_2)$. (For the simplest statistical models, the exact numerical solution of these equations is then feasible (Krook 1955*b*).)

The system is characterized by two dimensionless ratios, the Knudsen number K and the temperature ratio of the plates, $r = T_2/T_1$. We shall suppose that r is appreciably less than unity, so that the gradients in the gas are steep, unless $K \ll 1$. The Knudsen number can be defined as the reciprocal of some average value of the function $\lambda(v, \mathbf{i}, x)/|v_1|$.

Since the velocity distribution has axial symmetry about a direction parallel to $\mathbf{i}$, we may refer velocity space to the co-ordinates (v, μ, ϕ). The distribution functions $f_\pm(v, \mu, x)$ could be represented generally by a sum of *MM* functions based on T_1, T_2, and on an extensive set of local characteristic velocity-temperature pairs. In the interests of mathematical tractability, we would of course economize as far as possible in the number of *MM* functions to be used in a representation of $f_\pm$. This would generally require the use of different kinds of approximation in different ranges of Knudsen number.

To discuss the formal dependence of the velocity distribution on the value of the Knudsen number, we subdivide the range $(0, \infty)$ of K roughly into five subintervals:

(I) $K \ll 1$;
(II) K an order of magnitude less than unity, say $K \sim 0{\cdot}2$;
(III) $K \sim 1$;
(IV) K an order of magnitude greater than unity, say $K \sim 5$;
(V) $K \gg 1$.

Only in ranges I and V can we make a reasonably unambiguous choice of approximate representations for $f_\pm$. We shall discuss the five ranges of K separately, and shall indicate possible, but by no means unique, approximations for each range.

Range I. ($K \ll 1$)

The distance $x_2 - x_1$ comprises many mean free paths. Equations (13.4) then show that the wall distributions (14.1) are completely attenuated in comparatively thin layers in the immediate vicinity of the respective plates. Further, the component B for the point x is made up of (attenuated) collisional emissions at points x' for which $\mathscr{E}(\mathbf{v}, x')$ differs only slightly from $\mathscr{E}(\mathbf{v}, x)$. The local velocity distribution at x thus differs only slightly from a Maxwellian velocity distribution for a single velocity and temperature, which may therefore be taken to be the local velocity $\mathbf{q}(x)$, and the local kinetic temperature $T(x)$. Moreover, the velocity distribution $f(\mathbf{v}, x)$ at a boundary has only a slight discontinuity on the plane $v_1 = 0$. In this case, departures from local thermodynamic equilibrium are everywhere small, and so the problem for $K \ll 1$ can be treated by the Navier–Stokes formalism.

Range V. ($K \gg 1$)

The distance $(x_2 - x_1)$ is a very small fraction of a mean free path. Nearly all the molecules emitted by a plate (except those emitted practically tangentially) strike the opposite plate before they can collide with another gas molecule. In the formulae (13.4*a*, *b*) for $f_{\pm}(\mathbf{v}, x)$, component A predominates everywhere and component B is comparatively small everywhere.

In this range, the primary requirement is that we should provide representations for the non-uniformly attenuating wall distributions. We could thus use the approximating forms

$$f_{+}(\mathbf{v}, x) = \Psi(\mathbf{v};\, 0, T_1) \sum_{m,n} A^{(+)}_{m,n}(x)\, \mu^m v^n, \tag{14.2a}$$

$$f_{-}(\mathbf{v}, x) = \Psi(\mathbf{v};\, 0, T_2) \sum_{m,n} A^{(-)}_{m,n}(x)\, \mu^m v^n. \tag{14.2b}$$

Component B in f_+ or f_- would by itself be represented rather inaccurately by an *MM* function based on T_1 or T_2. In the derivation of continuum equations from the relations (14.2), the presence of component B gives rise to a slight modification of the coefficients $A^{(\pm)}_{m,n}$ from what would be their pure component A values.

Range IV. ($K \sim 5$)

In this case, most of the molecules emitted from a wall reach the opposite wall before they can collide with other gas molecules. Component A, i.e. the attenuating wall distribution, is still, as in range V, the dominant term in equations (13.4). Component B, however, is by no means negligible and should receive explicit recognition in our approximations for $f_{\pm}$.

In formula (13.4*a*) for $f_{+}(\mathbf{v}, x)$, component B includes significant contributions from the collisional emission $\mathscr{E}(\mathbf{v}, x')$ at all points x' in $(x_1,\, x)$. Similarly, component B in $f_{-}(\mathbf{v}, x)$ includes significant contributions from the collisional emission at all points in (x, x_2). Roughly speaking, the emission $\mathscr{E}(\mathbf{v}, x')$ at any point results from the interaction of two distributions with temperatures T_1 and T_2. We therefore approximate component B as a sum of *MM* functions based on the boundary temperatures T_1 and T_2. We would then represent the complete distributions $f_{\pm}(\mathbf{v}, x)$ (component A + component B) in the form

$$f_{\pm}(\mathbf{v}, x) = \sum_{\lambda=1}^{2} \Psi(\mathbf{v};\, 0, T_\lambda) \sum_{m,n} A^{(\lambda,\pm)}_{m,n}(x)\, \mu^m v^n, \tag{14.3a}$$

$$A^{(\lambda,+)}_{m,n}(x_1) = a_1 \delta_{\lambda,1} \delta_{m,0} \delta_{n,0}, \quad A^{(\lambda,-)}_{m,n}(x_2) = a_2 \delta_{\lambda,2} \delta_{m,0} \delta_{n,0}. \tag{14.4a, b}$$

Range II. ($K \sim 0{\cdot}2$)

Most of the molecules emitted from a plate collide in the gas before they can strike the opposite plate. Component B of equation (13.4) thus predominates, but component A is by no means negligible.

For $v_1 > 0$, the contributions to component B of $f_{+}(v, \mu, x)$ come from collisional emission $\mathscr{E}(\mathbf{v}, x')$ at points $x' < x$ and within about one mean free path of x. In this case we may approximate $f_{\pm}(v, \mu, x)$ by the forms

$$f_{\pm} = \Psi(\mathbf{v};\, 0, T(x)) \sum_{m,n} A^{(\pm)}_{m,n} \mu^m v^n + \Psi(\mathbf{v};\, 0, T_{\pm}(x)) \sum_{m,n} B^{(\pm)}_{m,n} \mu^m v^n, \tag{14.5a, b}$$

where $T(x)$ is the local kinetic temperature and $T_{+}(x)$, $T_{-}(x)$ are the temperatures associated with molecules that have $v_1 > 0$, $v_1 < 0$, respectively.

We note that $T_+(x_1) = T_1$, $T_-(x_2) = T_2$, so that

$$A^{(+)}_{m,n}(x_1) = 0, \quad B^{(+)}_{m,n}(x_1) = a_1 \delta_{m,0}\delta_{n,0};$$

and

$$A^{(-)}_{m,n}(x_2) = 0, \quad B^{(-)}_{m,n}(x_2) = a_2 \delta_{m,0}\delta_{n,0}.$$

Range III. ($K \sim 1$)

In this range, component A and component B of equation (13.4) are of comparable importance. The collisional temperature $T_c(x)$ also varies appreciably with x between x_1 and x_2. It would appear to be desirable to use sums of at least three *MM* functions for this case, e.g.

$$f_\pm = \sum_{\lambda=1}^{2} \Psi(\mathbf{v};\, 0, T_\lambda) \sum_{m,n} A^{(\lambda,\pm)}_{m,n} \mu^m v^n + \Psi(\mathbf{v};\, 0, T_\pm) \sum_{m,n} B^{(\pm)}_{m,n} \mu^m v^n, \qquad (14.6a, b)$$

(or the form with $T(x)$ instead of $T_\pm(x)$).

The types of approximation quoted above for various ranges of K are of course not the only, or even necessarily the best, approximating forms. When *MM* functions based on local characteristic temperatures appear in the representation, the resulting continuum equations are formally complex (see § 15). It may sometimes be desirable to exploit the formal simplicity that results from the use of *constant* velocity-temperature pairs, by using only *MM* functions based on the boundary temperatures T_1, T_2 and on a sequence of constant temperatures intermediate between T_1 and T_2.

15. Choice of basic state-variables

In cases where the approximate representation of the distribution function involves only constant velocity-temperature pairs, the derivation of continuum equations is completely straightforward. The formalism is somewhat more complicated when the approximations include *MM* functions based on local characteristic velocity-temperature pairs. We shall illustrate this point by considering the approximation (14.5) (range II) for the heat transfer problem of the previous section.

Let us define the half-space moments $R^{(\pm)}_{j,l}(x)$ by the equations

$$R^{(\pm)}_{j,l} = \frac{1}{\beta_1^{l+3}} \int_\pm \mu^j v^l f_\pm(v, \mu, x)\, d\mathbf{v} \quad (j, l = 0, 1, 2 \ldots), \qquad (15.1)$$

where $\beta_1^2 = kT_1/m$. The local temperatures $T(x)$, $T_+(x)$, $T_-(x)$ and the corresponding speeds $\beta(x)$, $\beta_+(x)$, $\beta_-(x)$, are defined by the relations

$$\beta^2 = \frac{kT}{m} = \frac{R^{(+)}_{0,2} + R^{(-)}_{0,2}}{3(R^{(+)}_{0,0} + R^{(-)}_{0,0})}, \qquad (15.2)$$

$$\beta_\pm^2 = \frac{kT_\pm}{m} = \frac{R^{(\pm)}_{0,2}}{3R^{(\pm)}_{0,0}}. \qquad (15.3a, b)$$

If we use the approximating forms

$$f_\pm = \Phi(\mathbf{v};\, 0, \beta) \sum_{m,n} A^{(\pm)}_{mn} \mu^m \left(\frac{v}{\beta}\right)^n + \Phi(\mathbf{v};\, 0, \beta_\pm) \sum_{m,n} B^{(\pm)}_{mn} \mu^m \left(\frac{v}{\beta_\pm}\right)^n, \quad (15.4a, b)$$

we obtain, for the moments, the approximations

$$\left.\begin{aligned} R^{(\pm)}_{j,l} = \sum_{m,n} A^{(\pm)}_{mn} \frac{(\pm 1)^{j+m}\, 2^{\frac{1}{2}(l+n)}\, \Gamma\{\frac{1}{2}(l+n+3)\}}{(j+m+1)\sqrt{\pi}} \left(\frac{\beta}{\beta_1}\right)^l \\ + \sum_{m,n} B^{(\pm)}_{mn} \frac{(\pm 1)^{j+m}\, 2^{\frac{1}{2}(l+n)}\, \Gamma\{\frac{1}{2}(l+n+3)\}}{(j+m+1)\sqrt{\pi}} \left(\frac{\beta_\pm}{\beta_1}\right)^l \end{aligned}\right\} \qquad (15.5a,b)$$

The local speeds $\beta(x)$, $\beta_\pm(x)$ that appear in the coefficients on the right-hand side of equations (15.5a, b) are themselves given in terms of the moments $R^{(\pm)}_{0,0}(x)$, $R^{(\pm)}_{0,2}(x)$ by the relations (15.3). It is then convenient to include these four moments $R^{(\pm)}_{0,0}$ and $R^{(\pm)}_{0,2}$ in the set of basic state-variables. The coefficients $A^{(\pm)}_{m,n}$, $B^{(\pm)}_{m,n}$ are then non-linear in $R^{(\pm)}_{0,0}$ and $R^{(\pm)}_{0,2}$, but are linear functions of the remaining basic state-variables.

Examples of continuum equations for such cases will be given in a subsequent paper where the methods of this paper are used, in conjunction with statistical models, to discuss the problem of Couette flow with heat transfer.

16. Structure of shock waves

We consider a plane stationary shock wave in a simple gas. The boundary conditions are

$$\left.\begin{aligned} f(\mathbf{v}, -\infty) &= n_1 \Psi(\mathbf{v}; Q_1\mathbf{i}, T_1), \\ f(\mathbf{v}, +\infty) &= n_2 \Psi(\mathbf{v}; Q_2\mathbf{i}, T_2). \end{aligned}\right\} \qquad (16.1a,b)$$

The number density $n_2 = n(+\infty)$, average velocity $Q_2\mathbf{i} = \mathbf{q}(+\infty)$, and temperature $T_2 = T(+\infty)$ are determined uniquely by n_1, Q_1, T_1, and the Mach number $M = Q_1/(5kT_1/3m)^{\frac{1}{2}}$.

Since the boundaries are at infinity, the integral equations (13.4) reduce to the form

$$f_+(\mathbf{v},x) = \frac{1}{v_1}\int_{-\infty}^{x} \mathscr{E}(\mathbf{v},x)\exp[-\{\lambda(\mathbf{v},x)-\lambda(\mathbf{v},x')\}/v_1]\,d\lambda', \qquad (16.2a)$$

$$f_-(\mathbf{v},x) = \frac{1}{|v_1|}\int_{x}^{\infty} \mathscr{E}(\mathbf{v},x)\exp[-\{\lambda(\mathbf{v},x')-\lambda(\mathbf{v},x)\}/|v_1|]\,d\lambda'. \qquad (16.2b)$$

The Knudsen number $K = 0$, and the distribution function $f(\mathbf{v}, x)$ is continuous in v-space. However, the transition from the supersonic régime to the subsonic régime is practically confined to a layer whose thickness is of the order of a few mean free paths. In this layer, the distribution function exhibits steep gradients (the local Knudsen number is of order unity). In this case

$$\mathscr{E}(\mathbf{v},x) \to \left\{\begin{aligned} &\text{const.}\times f(\mathbf{v}, -\infty) \quad \text{as} \quad x \to -\infty, \\ &\text{const.}\times f(\mathbf{v}, +\infty) \quad \text{as} \quad x \to +\infty. \end{aligned}\right\} \qquad (16.3)$$

The velocity distribution is axially symmetric about the direction **i**. We obtain formally simple continuum equations if we represent the complete distribution as the sum of MM functions based on the constant pairs $(Q_1\mathbf{i}, T_1)$ $(Q_2\mathbf{i}, T_2)$, in the form

$$f = \sum_{\lambda=1}^{2} \Psi(\mathbf{v}; Q_\lambda\mathbf{i}, T_\lambda) \sum_{m,n} A^{(\lambda)}_{m,n} v_1^m v^{2n}. \qquad (16.4)$$

Formally more complicated equations are obtained with the unsymmetrical approximation

$$f = \Psi(\mathbf{v};\, Q_1\mathbf{i}, T_1) \sum_{m,n} A_{mn} v_1^m v^{2n} + \Psi(\mathbf{v};\, \mathbf{q}, T) \sum_{m,n} B_{mn} v_1^m v^{2n}. \qquad (16.5)$$

Even with the Maxwell–Boltzmann model, the representations (15.4) and (15.5) permit the multiple integrals involved in the interaction moments to be evaluated in terms of error functions. Approximations of the form (16.4) have been used to analyse the structure of shock fronts in ionized gases (Krook 1959).

If we use the simpler forms of statistical model for the molecular interactions, it is feasible to use separate representations for $f_+(\mathbf{v}, x)$ and $f_-(\mathbf{v}, x)$, e.g.

$$f_+ = \Psi(\mathbf{v}, Q_1\mathbf{i}, T_1) \sum_{m,n} A^{(+)}_{mn} v_1^m v^{2n} + \Psi(\mathbf{v}, \mathbf{q}, T) \sum_{m,n} B^{(+)}_{mn} v_1^m v^{2n}, \qquad (16.6a)$$

$$f_- = \Psi(\mathbf{v}, Q_2\mathbf{i}, T_2) \sum_{m,n} A^{(-)}_{mn} v_1^m v^{2n} + \Psi(\mathbf{v}, \mathbf{q}, T) \sum_{m,n} B^{(-)}_{mn} v_1^m v^{2n}. \qquad (16.6b)$$

The forms (16.5) and (16.6*a*, *b*) contain a more explicit representation of the collisional emission than does the form (16.4).

17. Conclusion

When the methods of this paper are used to construct continuum equations, the only place in which we may encounter difficulty is in the expression of the interaction moments as functions of the basic state-variables. This process generally involves the evaluation of multiple integrals with products of two *MM* functions as integrands.

If the law of force between molecules is given in analytic form, and if f is not singular on the plane $v_1 = 0$, these integrals can usually be evaluated explicitly, even when the interaction term has the Maxwell–Boltzmann form. If f is singular on the plane $v_1 = 0$, and we therefore use different representations for f_+ and f_-, the evaluation of the relevant integrals for the half-space interaction moments in the Maxwell–Boltzmann model is troublesome. It is for just such cases that the statistical models prove particularly useful; the evaluation of the half-space interaction moments is generally quite straightforward with these models.

In subsequent papers, the methods presented in this paper will be applied to obtain approximate solutions for the problems of shock-wave structure, and Couette flow with heat transfer.

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