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A Spectral Solution of the Boltzmann Equation for the Infinitely Strong Shock

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A SPECTRAL SOLUTION OF THE BOLTZMANN EQUATION FOR THE INFINITELY STRONG SHOCK

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We formulate and implement a new spectral method for the solution of the Boltzmann equation, making extensive use of the theory of irreducible tensors together with the symbolic notation of Dirac. These tools are shown to provide a transparent organization of the algebra of the method and the efficient automation of the associated calculations. The power of the proposed method is demonstrated by application to the highly nonlinear problem of the infinitely strong shock. It is shown that the distribution function can in this limit be decomposed into a singular part corresponding to the molecular beam, which represents the supersonic side of the shock, and a regular part, which provides the evolving 'background' gas and covers the rest of velocity space. Separate governing equations for the singular and regular parts are derived, and solved by an expansion of the latter in an infinite series of orthogonal functions. The basis for this expansion is the same set that was used by Burnett (*Proc. Lond. math. Soc.* **39**, 385–430 (1935)), but is centred around the (fixed) downstream maxwellian. This basis, because of the presence of spherical harmonics which provide an irreducible representation of the group SO(3), lends itself to the utilization of powerful group-theoretic tools. The present expansion, not being about local equilibrium, does not imply any constitutive relations; instead it reduces the Boltzmann equation to an equivalent infinite-order nonlinear dynamical system. A solution with six modes shows encouraging convergence in the density profile, towards a shock thickness of about 6.7 hot-side mean free paths.

1. Introduction

The purpose of this paper is two-fold. The first is to describe a spectral approach to the solution of the Boltzmann equation, and provide enough details of its mechanics to enable application to a variety of problems. The second is to demonstrate the power of the method by applying it to the highly nonlinear problem of the infinitely strong shock.

The central element of a spectral method is an expansion of the unknown (in the present case the distribution function) in a suitable basis, and the formulation of the equations governing the coefficients in the expansion. Expansions have a long (but not always happy) history in kinetic theory: the evaluation of transport coefficients by the classical Chapman–Enskog theory depended on such expansions around local equilibrium. This linear transport theory reached a state of maturity with the work of Burnett (1935, 1936) and Chapman & Cowling (1939), who demonstrated the advantages of using Sonine polynomials and spherical harmonics as the basis for the expansion, the latter having been advocated more than 50 years earlier by Maxwell (1879). The algebra involved in the use of any of these expansions has been heavy (likened by Chapman to 'chewing glass', Brush 1976), and numerous efforts have been made, at intervals, to find suitable bases or formalisms to lighten the burden (see, for example, Grad 1949*a*, *b*; Ikenberry & Truesdell 1956; Waldmann 1958). However, the failure of these expansions to handle problems involving significant departures from equilibrium has led to a certain disenchantment with such series methods in recent decades.

In an interesting analysis of linear transport theory, Kumar (1966*a*, 1967) has confirmed that the associated calculations are most efficiently carried out in the basis proposed by Burnett, especially if use is made of the theory of irreducible tensors (of which spherical harmonics are an example). The concept of irreducibility had played some part in earlier work (see, for example, Wang Chang & Uhlenbeck 1952; Waldmann 1958), but Kumar's extensive analysis demonstrated for the first time the considerable gains that would result from a systematic use of the concept. However, by this time the technology of computing transport

coefficients was under such firm control that no great need appears to have been felt for a new approach.

Our first aim here is to show that these modern tools, with appropriate extensions, are useful also in devising a spectral method to tackle nonlinear problems involving large departures from equilibrium; in particular, the use of related group-theoretic ideas and of Dirac's (1958) concept of bra and ket spaces endow the present method with both conceptual and notational elegance, even in strongly nonlinear problems. However, instead of describing the technique in isolation, we demonstrate its power by implementing it in a special case, partly to emphasize how the success of such methods depends not only on the choice of the right basis but also (supporting a point made earlier by Butler & Anderson (1967)) of the right origin or 'centre' around which the basis is built. The problem we select for this purpose is the infinitely strong shock, which has often played the role of a crucial test case, and is so interesting in its own right that it deserves a brief review (see also Cercignani 1983).

The shock wave is an interface of finite thickness between two different equilibrium states of a gas connected by the Rankine–Hugoniot relations. If the two states are close to each other (as when the upstream Mach number M_1 is not far from unity), the structure of the shock is adequately described by the continuum (Navier–Stokes) equations; for weak shocks there is an extensive theory (Lighthill 1956). For stronger shocks higher-order continuum approximations (like the Burnett equations) have for long been considered unsuccessful, although this view may need to be revised in view of the recent conclusion of Fiskco & Chapman (1988) that the failures were often the result of inadequacies in the numerical algorithms used for solving the equations. A classical investigation by Mott-Smith (1951) postulated the distribution within a strong shock as the weighted sum of upstream and downstream maxwellians, and determined the weighting by a moment procedure. Although the results obtained depend strongly on the moment function adopted (Rode & Tanenbaum 1967), the Mott-Smith ansatz for the distribution certainly appears to give qualitatively correct results. For this reason, other more rational criteria for the determination of the weighting have been investigated (see, for example, Oberai 1967; Narasimha & Deshpande 1969; Hosokawa & Inage 1986). On the other hand none of the numerous attempts at improving the ansatz itself (see, for example, Holway 1965; Lohn & Lundgren 1974) has led to a unique or even demonstrably better solution.

The problem has also been tackled by strictly numerical procedures such as the Monte Carlo method of Bird (1967, 1970). However, there has been just enough doubt about the faithfulness of these procedures to the Boltzmann equation (see, for example, Deshpande *et al.* 1978; Nanbu 1986) that an exact solution, if available, would add a great deal to the stock of current knowledge in rarefied gas dynamics, besides providing the kind of insight into the nature of the shock that cannot come from any strictly numerical solution.

The current approach may be seen as developing a rational expansion scheme in which a Mott-Smith distribution corresponds to the first term (but not, it must be emphasised, either of the two approximate solutions proposed by Mott-Smith). Interestingly, we find that this expansion is best implemented with the same set of polynomials that Burnett used, but centred around the downstream (and not the local) maxwellian, and making no appeal to any linearization. These differences turn out to be crucial for understanding and solving the problem of the infinitely strong shock, as we shall further discuss in §8.

The infinitely strong shock was first specially treated by Sakurai (1957), who showed that

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'if we take a special form of the function $X(M)$ (the shock thickness at Mach number M), the equation

$$f^{(0)} = \nu(-x)f_\alpha + \nu(x)f_\beta$$

(the Mott-Smith ansatz) satisfies directly the Boltzmann equation at large M for a finite, fixed value [$\boldsymbol{u}_1$, the upstream gas velocity] of $\boldsymbol{c}$'. This statement implies that the residual vanishes at a molecular velocity equal to $\boldsymbol{u}_1$. Narasimha & Deshpande (1969) demonstrated that Sakurai's solution was basically a consequence of balancing the delta-functions (corresponding to the upstream maxwellian in the infinite Mach number limit) that appear on either side of the Boltzmann equation; i.e. of removing the singularity from the Mott-Smith residual. It must be emphasized that there is no simple relation between the residual at isolated points and the error (the latter being the difference between the exact and approximate solutions): thus the error does not necessarily vanish where the residual does so (as is clear from an analysis of the well-known collocation method, see, for example, Finlayson (1972)). Furthermore, the requirement that the residual be nonsingular does not determine a solution uniquely; in fact, all the approximate solutions in the scheme we shall describe below also satisfy the requirement. The interpretation sometimes given to Sakurai's result, that it provides an exact solution for the infinitely strong shock, is therefore unjustified.

It was pointed out by Grad (1969) and R. Narasimha (unpublished work) that the solution for the distribution function anywhere in the shock can in the limit be decomposed into the sum of a delta function and a regular function (see figure 1), corresponding respectively to a molecular beam and a 'background' gas. (We can think of the infinitely strong shock layer as a nonlinear fluid-dynamical device that converts the beam into the background gas at a conjugate equilibrium state.) A possible method for computing these components of the distribution was also proposed by Narasimha (1972). We report on the implementation of this method here; a brief preliminary account has appeared in Narasimha & Das (1986).

In §2 we describe the decomposition of the Boltzmann equation and show how it can be reduced to an infinite set of coupled nonlinear ordinary differential equations. It is shown

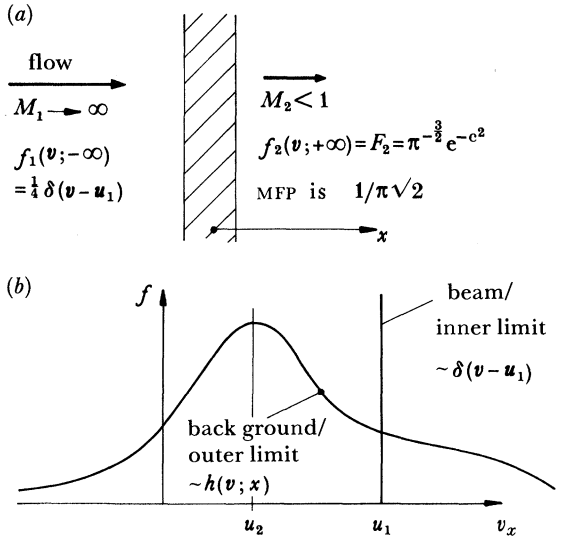

FIGURE 1. (*a*) Notation adopted for the shock layer problem. (*b*) Sketch showing distribution function at any point in the shock layer, decomposed into an inner limit at the upstream gas velocity, and an outer limit over the rest of velocity space.

further that all the coefficients appearing in these equations can be expressed in terms of four basic 'matrix elements'. The irreducible tensor formalism is briefly described in §3, and used in §4 to calculate these matrix elements. The conservation relations to be satisfied by the state variables are also given. Sections 5 and 6 sketch the numerical methods used for computing the basic coefficients and the solutions. Results are presented and discussed in §7 and conclusions are summarized in §8.

2. The governing equations

2.1. *The Boltzmann equation*

We consider a normal shock (figure 1) in a simple gas of rigid spheres in the limit as the upstream Mach number M_1 tends to infinity. The Boltzmann equation for the molecular velocity distribution function $f(\boldsymbol{v}, x)$ is written as

$$v_x \partial f/\partial x = J[f,f] \equiv G[f,f] - \hat{L}[f,f]. \tag{2.1}$$

Here v_x is the component of the molecular velocity $\boldsymbol{v}$ along the mean flow direction x, and, for two arbitrary distributions f_i, f_j the gain and loss operators (whose separation is possible for the assumed molecular model) are respectively given by

$$G[f_i,f_j] \equiv \int f_i(\boldsymbol{v}') f_j(\boldsymbol{w}')\, g\sigma \,\mathrm{d}\Omega\, \mathrm{D}\boldsymbol{w}, \tag{2.2}$$

$$\hat{L}[f_i,f_j] \equiv f_i L[f_j] \equiv f_i \int f_j(\boldsymbol{w})\, g\sigma \,\mathrm{d}\Omega\, \mathrm{D}\boldsymbol{w}, \tag{2.3}$$

where

$$g = |\boldsymbol{g}| = |\boldsymbol{v} - \boldsymbol{w}| = |\boldsymbol{v}' - \boldsymbol{w}'| \tag{2.4}$$

is the relative velocity between two colliding molecules, σ is the differential collision cross section for scattering into the elementary solid angle $\mathrm{d}\Omega$, and primes denote post-collision values of the molecular velocities $\boldsymbol{v}, \boldsymbol{w}$ of two collision partners. (For rigid spheres of diameter b_0 we have $\sigma = \frac{1}{4}b_0^2$.) It is sometimes convenient to replace $\mathrm{d}\Omega$ by $b\,\mathrm{d}b\,\mathrm{d}\epsilon$, where b is the impact parameter and ϵ the azimuthal angle around a polar axis parallel to $\boldsymbol{g}$ and passing through the 'struck' molecule $\boldsymbol{w}$ considered at rest (Chapman & Cowling 1939). The collision integral $J[f_i,f_j]$ is the difference between (2.2) and (2.3).

The boundary conditions for the shock problem are

$$\left.\begin{aligned} f(\boldsymbol{v}; x = -\infty) &= n_1\, \delta(\boldsymbol{v} - \boldsymbol{u}_1) = n_1\, \delta(\boldsymbol{c} - \boldsymbol{U}), \\ f(\boldsymbol{v}; x = +\infty) &= n_2 (\tfrac{1}{2}\alpha_2^2/\pi)^{\frac{3}{2}} \exp(-\tfrac{1}{2}\alpha_2^2 c^2), \end{aligned}\right\} \tag{2.5}$$

where

$$\boldsymbol{c} = \boldsymbol{v} - \boldsymbol{u}_2, \quad \boldsymbol{U} = \boldsymbol{u}_1 - \boldsymbol{u}_2, \tag{2.6}$$

n is the number density, $\boldsymbol{u}$ is the gas velocity, α_2 is the scale parameter for molecular velocity and δ is the Dirac delta function; subscripts 1 and 2 indicate upstream and downstream conditions respectively.

We now adopt the following non-dimensionalization: all velocities are scaled by $\sqrt{2}/\alpha_2$, all distributions by $n_2(\frac{1}{2}\alpha_2^2)^{\frac{3}{2}}$, b by b_0, x by $(n_2 b_0^2)^{-1}$. The Boltzmann equation in the scaled variables has the same form as (2.1) because all the extra factors are absorbed.

In the new variables, the maxwellian distributions on the cold and hot ends of the shock are

$$F_1 = \tfrac{1}{4}\delta(\boldsymbol{c} - \boldsymbol{U}), \quad F_2 = \pi^{-\frac{3}{2}} \exp(-c^2), \tag{2.7}$$

and the Maxwell mean free path on the hot side is $\Lambda_2 = [\sqrt{2}\pi]^{-1}$.

2.2. *Inner and outer limits*

The distribution function may in general be expected to be singular within the infinitely strong shock, as it is a delta function on the cold side. However, the collision integrals can only smear or weaken the singularity, in the manner described in detail by Narasimha & Deshpande (1969). Thus the strongest singularity in f can only be the remnant of the delta function advected from upstream; we can therefore write

$$f(\boldsymbol{v};x) = \tfrac{1}{4}\nu_0(x)\,\delta(\boldsymbol{v}-\boldsymbol{u}_1) + h(\boldsymbol{v};x), \tag{2.8}$$

where h is a non-singular function of $\boldsymbol{v}$. It is immediately clear that it will be convenient to study this distribution in two parts: the first at the upstream velocity $\boldsymbol{u}_1$, corresponding to the beam, and the second, consisting of the rest of velocity space, constituting the background. Following Narasimha & Deshpande (1969), it is convenient to refer to these as the inner and outer limits. No matching, however, is involved, and (2.8) may be thought of as the composite expansion to the lowest order as $M_1 \to \infty$.

2.3. *Ordering of collision terms*

By using (2.8) in the Boltzmann equation (2.1), and noting the bilinearity of the gain and the loss operators, the collision term (with $a = \frac{1}{4}\nu_0$) expands as

$$J[a\delta+h, a\delta+h] = a^2G[\delta,\delta] + aG[\delta,h] + aG[h,\delta] + G[h,h] - a^2\delta L[\delta] - a\delta L[h] - ahL[\delta] - hL[h]. \tag{2.9}$$

We first consider the inner limit. This involves the product of delta functions, which cannot in general be defined uniquely. In the present situation there is, however, no ambiguity, because it is the limit of a maxwellian; thus

$$J[\delta,\delta] = G[\delta,\delta] - \delta L[\delta] = 0. \tag{2.10}$$

Consider now $L[\delta]$. By using (2.3),

$$L[\delta] = \int (\boldsymbol{w}-\boldsymbol{u}_1)\,|\boldsymbol{w}-\boldsymbol{v}|\,\sigma\,\mathrm{D}\boldsymbol{w}\,\mathrm{d}\Omega = \sigma_0|\boldsymbol{v}-\boldsymbol{u}_1|, \tag{2.11}$$

where

$$\sigma_0 = \int \sigma\,\mathrm{d}\Omega. \tag{2.12}$$

Therefore

$$G[\delta,\delta] = \delta L[\delta] = \sigma_0|\boldsymbol{v}-\boldsymbol{u}_1|\,\delta(\boldsymbol{v}-\boldsymbol{u}_1). \tag{2.13}$$

This says that although the gain at $\boldsymbol{u}_1$ is infinite, its integral is zero; in the limit, therefore, there is no net loss or gain at any velocity when two molecular beams interact.

As h is not singular, $L[h]$ is in general non-zero and finite. Therefore

$$\delta L[h] = (\ )\,\delta, \tag{2.14}$$

which, from (2.13), dominates the term $\delta L(\delta)$. Consider now

$$G[\delta,h] = \int \delta(\boldsymbol{v}'-\boldsymbol{u}_1)\,h(\boldsymbol{w}')\,g\sigma\,\mathrm{d}\Omega\,\mathrm{D}\boldsymbol{w}.$$

The contribution to this integral can obviously come only from $\boldsymbol{v}' = \boldsymbol{u}_1$. In the inner limit, $\boldsymbol{v} = \boldsymbol{u}_1$ also; therefore $\boldsymbol{v} = \boldsymbol{v}'\,(= \boldsymbol{u}_1)$; necessarily $\boldsymbol{w} = \boldsymbol{w}'$ as well. There is therefore no collision that contributes; hence

$$G[\delta,h] = 0 \quad \text{at} \quad \boldsymbol{v} = \boldsymbol{u}_1, \tag{2.15}$$

similarly $G[h,\delta]$. So in the inner limit we can write

$$J[a\delta+h,a\delta+h] = -a\delta L[h]. \tag{2.16}$$

In the outer limit the term $a\delta L[h]$ makes no contribution, so we have

$$J[a\delta+h,a\delta+h] = aG[\delta,h]+aJ[h,\delta]+J[h,h]. \tag{2.17}$$

2.4. *The inner and outer equations*

Using the form (2.8), the left-hand side of the Boltzmann equation (2.1) becomes, in the inner and the outer limits respectively,

$$v_x\frac{\partial f}{\partial x} = v_x n_1 \dot{\nu}_0\,\delta(\boldsymbol{c}-\boldsymbol{U}), \quad v_x\frac{\partial f}{\partial x} = v_x\frac{\partial h}{\partial x}, \tag{2.18}$$

where the dot denotes differentiation with respect to x.

Keeping in view the spectral method we shall propose, it is now convenient to adopt the Dirac notation (see, for example, Dirac 1958), and rewrite the Boltzmann equation (2.1) as

$$\frac{\partial}{\partial x}|v_x f\rangle = J|f,f\rangle \equiv G|f,f\rangle - \hat{L}|f,f\rangle, \tag{2.19}$$

where each term is a Dirac ket vector identified by the labels inside the ket, and the collision integrals (2.2) and (2.3) have the 'coordinate' representations given by the brackets $\langle\boldsymbol{v}|G|f_i,f_j\rangle$, $\langle\boldsymbol{v}|\hat{L}|f_i,f_j\rangle$, $\langle\boldsymbol{v}|L|f_j\rangle$, to be thought of as the 'components' at $\boldsymbol{v}$ of the corresponding kets. Using (2.16) and (2.17), we can similarly write the inner and outer equations as

$$u_1\dot{\nu}_0 = -\nu_0\langle\boldsymbol{U}|L|h\rangle, \tag{2.20}$$

$$\frac{\partial}{\partial x}|v_x h\rangle = \tfrac{1}{4}\nu_0[G|\delta,h\rangle + J|h,\delta\rangle] + J|h,h\rangle, \tag{2.21}$$

where $\langle\boldsymbol{U}|L|h\rangle$ is the value of $L[h]$ at $\boldsymbol{c}=\boldsymbol{U}$ (or $\boldsymbol{v}=\boldsymbol{u}_1$). Note that the inner equation (2.20), which describes a decaying molecular beam, has been formed by balancing the delta-functions on both sides, i.e. we ensure a non-singular residual, as in Narasimha & Deshpande's (1969) interpretation of Sakurai's solution.

The coefficient $\langle\boldsymbol{U}|L|h\rangle$ in (2.20) is really the local absorption rate of the beam molecules in the evolving background gas; the corresponding free path is $u_1/\langle\boldsymbol{U}|L|h\rangle$, whose value on the hot side (F_2 replacing h) would be the mean absorption length of a weak beam in the background gas F_2. Within the shock the beam is gradually transformed to the background, so the beam attenuation rate varies correspondingly with position.

The equations (2.20) and (2.21) are a transformed version of the Boltzmann equation (2.1), equivalent to it. Grad (1969) has arrived at a similar form, assuming that the gain operator is symmetric, i.e. that $G[f_i,f_j] = G[f_j,f_i]$. We prove in §4 that this symmetry is valid for hard-sphere molecules but is not more generally true. (The proof will turn out to be very simple in the irreducible tensor formalism that we are going to use.)

At first sight, the outer equation (2.21) appears even more formidable than the Boltzmann equation. However the background distribution $h(\boldsymbol{v};x)$, which eventually relaxes to the hot-side maxwellian F_2, may be expected to be not too far from it at any point in the shock, especially as fast molecules from the hot side have a tendency to 'leak' to the cold side (Narasimha 1968).

Equation (2.21) therefore lends itself to solution through an expansion scheme. Based on this expectation we expand h around F_2, in a complete set of three-dimensional polynomials $\phi^{[\alpha]}$ centred at $\boldsymbol{u}_2$ and orthogonal with the weight $F_2(\boldsymbol{c})$, so that we can write (2.8) as

$$f(\boldsymbol{v};\boldsymbol{x}) = \tfrac{1}{4}\nu_0(x)\,\delta(\boldsymbol{c}-\boldsymbol{U}) + \nu_\alpha(x)\,F_2(c)\,\phi^{[\alpha]}(\boldsymbol{c}). \tag{2.22}$$

We shall call ν_0 the 'beam intensity', the $\phi^{[\alpha]}$ 'modes', and the $\nu_\alpha(x)$ in (2.22) 'modal amplitudes'.

Alternatively, using the Dirac notation, we write the modes in coordinate representation as $\langle \boldsymbol{c}\,|\,\alpha\rangle$, where α is any suitable label for the mode, obeying the orthonormality relation

$$\langle \alpha\,|\,\beta\rangle = \delta_{\alpha\beta}. \tag{2.23}$$

The expansion of h in terms of these modes is now written as

$$|h\rangle = |\alpha\rangle\langle\alpha\,|\,h\rangle = \nu_\alpha(x)\,|\,\alpha\rangle, \tag{2.24}$$

where the ν_α are the modal amplitudes. Utilizing an expansion of the delta function in the same basis,

$$\delta(\boldsymbol{c}-\boldsymbol{U}) = F_2(\boldsymbol{c})\langle \boldsymbol{c}\,|\,\boldsymbol{U}\rangle = F_2(\boldsymbol{c})\langle \boldsymbol{c}\,|\,\alpha\rangle\langle\alpha\,|\,\boldsymbol{U}\rangle \equiv \langle \boldsymbol{c}\,|\,\alpha\rangle\langle\alpha\,|\,\delta\rangle, \tag{2.25}$$

and using the operator $|\alpha\rangle\langle\alpha|$ in the equations (2.20) and (2.21), we obtain

$$u_1\,\dot{\nu}_0 = -\nu_0\langle \boldsymbol{U}|L|\,\alpha\rangle\langle\alpha\,|\,h\rangle, \tag{2.26}$$

and

$$\frac{\partial}{\partial x}|\gamma\rangle\langle\gamma|v_x|\,\alpha\rangle\langle\alpha\,|\,h\rangle = \tfrac{1}{4}\nu_0[|\gamma\rangle\langle\gamma|G|\,\beta,\alpha\rangle\langle\beta\,|\,\delta\rangle\langle\alpha\,|\,h\rangle + |\gamma\rangle\langle\gamma|J|\,\alpha,\beta\rangle\langle\alpha\,|\,h\rangle\langle\beta\,|\,\delta\rangle] + |\gamma\rangle\langle\gamma|J|\,\alpha,\beta\rangle\langle\alpha\,|\,h\rangle\langle\beta\,|\,h\rangle. \tag{2.27}$$

It is convenient to rewrite these equations as

$$\dot{\nu}_0 = -C_\alpha\,\nu_0\,\nu_\alpha, \tag{2.28}$$

$$A^\gamma_\alpha\,\dot{\nu}_\alpha = B^\gamma_\alpha\,\nu_0\,\nu_\alpha + J^\gamma_{\alpha\beta}\,\nu_\alpha\,\nu_\beta, \tag{2.29}$$

where

$$C_\alpha = \langle \boldsymbol{U}|L|\,\alpha\rangle/u_1, \quad A^\gamma_\alpha = \langle\gamma|v_x|\,\alpha\rangle,$$

$$B^\gamma_\alpha = \tfrac{1}{4}[\langle\gamma|G|\beta,\alpha\rangle + \langle\gamma|J|\,\alpha,\beta\rangle]\langle\beta\,|\,\boldsymbol{U}\rangle,$$

and

$$J^\gamma_{\alpha\beta} = \langle\gamma|J|\,\alpha,\beta\rangle. \tag{2.30}$$

If the expansion in (2.22) is truncated after N terms, the running indices α, β, and γ in (2.27) and (2.28) take values in the range $1, 2, \ldots, N$. We then have a set of $(N+1)$ equations to be solved. Inverting the truncated matrix A and pre-multiplying by it on both sides of (2.28), we finally have

$$\dot{\nu}_0 = C_\alpha\,\nu_0\,\nu_\alpha \quad (\alpha = 1, \ldots, N), \tag{2.31}$$

$$\dot{\nu}_\gamma = P^\gamma_\alpha(N)\,\nu_0\,\nu_\alpha + Q^\gamma_{\alpha\beta}(N)\,\nu_\alpha\,\nu_\beta \quad (\alpha,\beta,\gamma = 1, \ldots, N). \tag{2.32}$$

We denote the solution to (2.29) and (2.30) by $\nu_\alpha(x;N)$ $(\alpha = 0, 1, \ldots, N)$. Our strategy is to solve (2.29) and (2.30) for increasing values of N till convergence is obtained.

All the basic coefficients in the equations (2.28) and (2.29) can be expressed in terms of the four basic matrix elements $\langle \boldsymbol{U}|L|\,\alpha\rangle$, $\langle\gamma|v_x|\,\alpha\rangle$, $\langle\gamma|G|\,\alpha,\beta\rangle$ and $\langle\gamma|\hat{L}|\,\alpha,\beta\rangle$, whose evaluation we consider after a brief introduction to the irreducible tensor formalism.

3. The irreducible-tensor approach

The Boltzmann collision integrals involve three operations: transformation of velocities through collision, multiplication of the distributions because of the quadratic nonlinearity, and integration over velocities and the encounter variables. An appropriate formalism for the treatment of the Boltzmann equation must handle these operations effectively, and we consider these in turn (see Kumar (1966*a*) for a somewhat different treatment).

3.1. *General remarks*

To start with, integration in velocity space clearly calls for orthogonal functions, with a gaussian weight if the expansion is around a maxwellian (local or otherwise). An example of such functions is the set of Hermite polynomials devised by Grad (1949*a*, *b*),

$$\left.\begin{aligned} H(\boldsymbol{c}) = 1, \quad H_i(\boldsymbol{c}) = c_i, \quad H_{ij}(\boldsymbol{c}) = c_i c_j - \delta_{ij}, \\ H_{ijk}(\boldsymbol{c}) = c_i c_j c_k - c_i \delta_{jk} - c_j \delta_{ki} - c_k \delta_{ij}, \text{ etc.} \end{aligned}\right\} \tag{3.1}$$

Here the number of functions of any given degree n (which may be defined as equal to the largest exponent of $\boldsymbol{c}$ and also to the number of subscripts on H) is 3^n, although (because of symmetry) only $\frac{1}{2}(n+1)(n+2)$ of these are effectively used. It is clearly desirable to build in such symmetry considerations right from the beginning, to avoid undue proliferation of redundant functions and indices; the use of irreducible tensors enables one to do this, but in addition confers many advantages in the other operations as well, as we shall show below.

We begin by noting that a tensorial set of order n may be defined (Fano & Racah 1959) as 'any set of n quantities which are defined in connection with a system of space (velocity in our case) coordinates and which experience a linear transformation when this system rotates'. Such a set is more general than the tensors that are widely familiar, in that it could be made up of vectors, tensors, or even operators. Given two tensorial sets a_α and b_α of the same order, their sum is a set whose elements are $a_\alpha + b_\alpha$. Two sets a_α, b_β of order n and m respectively have a 'direct' product whose nm elements are $a_\alpha b_\beta$, which could indicate either ordinary algebraic multiplication or other forms of combination, such as, for example, the action of an operator $\mathbf{a}$ on a vector $\boldsymbol{b}$, or the dyadic product of two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$.

When subjected to a rotation of the coordinate axes, the a_α are transformed to (say) $a''_\alpha = D_{\alpha\beta} a_\beta$ (sum over β), where $D_{\alpha\beta}$ is the matrix of transformation. Note that in general this sum is over all members of the set a_α; thus, if the set were the products $c_i c_j c_k$, the number of terms would be 27. However, it often happens that the set a_α can be replaced by another transformed set

$$a'_\alpha = A_{\alpha\beta} a_\beta, \tag{3.2}$$

where $A_{\alpha\beta}$ is a unitary matrix, such that a rotation of coordinates transforms certain subsets of the a'_α separately, i.e. among themselves, without involving members of other subsets. In this case the transformed matrix $D' = ADA^{-1}$ would have a block diagonal form as shown in figure 2, with vanishing elements outside the blocks; each block operates on a subset of the a'_α, each element of which transforms into a linear combination of members of the same subset. The procedure by which such subsets are formed, called reduction, has an ultimate limit in which we are left with 'irreducible tensorial sets', on which no further reduction is possible.

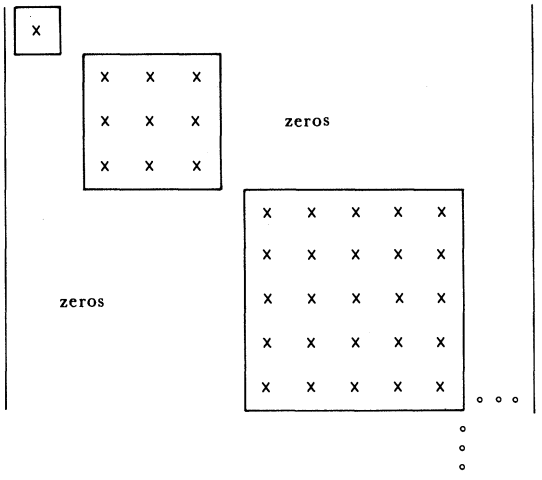

FIGURE 2. Block-diagonal structure of the transformation matrix D', when a tensorial set is expressed in a privileged basis.

The need for such a decomposition of tensorial sets into irreducible parts has indeed been earlier felt in kinetic theory, but the efforts made have usually fallen short of reaching their logical conclusion. Thus Chapman & Cowling (1970) introduce, for a second rank tensor $\mathbf{T}$ in a cartesian frame $(x\ y\ z)$, its divergence $(T_{xx}+T_{yy}+T_{zz})$, its antisymmetrical or skew part and the symmetric non-divergent tensor,

$$\overset{\times}{\mathbf{T}} \quad \text{and} \quad \overset{0}{\underline{\mathbf{T}}}$$

respectively. The difference, however, is that $\overset{0}{\underline{\mathbf{T}}}$ has been thought of as a 3×3 array, and there is no automatic or explicit recognition of the fact that the third component on the diagonal is not independent of the other two (because of the trace already identified). The corresponding irreducible tensorial sets are, in cartesian dyadic notation with $\boldsymbol{i},\boldsymbol{j},\boldsymbol{k}$ as unit vectors,

$$\mathbf{T}^{(0)} = \tfrac{1}{3}(\boldsymbol{ii}+\boldsymbol{jj}+\boldsymbol{kk})\,(T_{xx}+T_{yy}+T_{zz}),$$

$$\mathbf{T}^{(1)} = \tfrac{1}{2}[(\boldsymbol{jk}-\boldsymbol{kj})\,(T_{yz}-T_{zy})+(\boldsymbol{ki}-\boldsymbol{ik})\,(T_{zx}-T_{xz})+(\boldsymbol{ij}-\boldsymbol{ji})\,(T_{xy}-T_{yx})],$$

$$\mathbf{T}^{(2)} = \tfrac{1}{2}[\tfrac{1}{3}(2\boldsymbol{kk}-\boldsymbol{ii}-\boldsymbol{jj})\,(2T_{zz}-T_{xx}-T_{yy})+(\boldsymbol{ii}-\boldsymbol{jj})\,(T_{xx}-T_{yy})$$
$$+(\boldsymbol{jk}+\boldsymbol{kj})\,(T_{yz}+T_{zy})+(\boldsymbol{ki}+\boldsymbol{ik})\,(T_{zx}+T_{xz})+(\boldsymbol{ij}+\boldsymbol{ji})\,(T_{xy}+T_{yx})],$$

whose direct sum is the tensor $\mathbf{T}$:

$$\mathbf{T} = \mathbf{T}^{(0)}+\mathbf{T}^{(1)}+\mathbf{T}^{(2)}.$$

Note that these three tensors contain respectively one, three and five elements (so accounting for the nine independent components of $\mathbf{T}$); although at first sight the above irreducible sets may appear clumsy, their virtues become apparent as the order of the tensor $\mathbf{T}$ increases, and will include elegance when the right basis is adopted.

3.2. *The Burnett basis*

In three-dimensional space, such irreducible tensors (which we shall for brevity call i-tensors) can provide a basis for an irreducible representation of the group of proper rotations, known commonly as SO(3) (for special orthogonal in three dimensions); this fact immediately

makes available many powerful group-theoretic tools in further analysis. For example, it is well known that the complex spherical harmonics $Y_m^l(\hat{\boldsymbol{c}})$ (the same functions as in Edmonds 1957), where $\hat{\boldsymbol{c}}$ is the unit vector along $\boldsymbol{c}$, are a special case of and provide a basis for 'irreducible' representations of this group (see, for example, Wigner 1959). This means that after a proper rotation of the coordinates in $\boldsymbol{c}$-space, any given member of the set Y_m^l is transformed to a linear combination of members of the set belonging to the same value of l (which we shall call the polar index; m will be called the azimuthal index). There are $2l+1$ of these partners, corresponding to $m=-l, -l+1, \ldots +l$, in the irreducible representation of rank l or dimension $(2l+1)$. Thus, let $R(\boldsymbol{\omega}), \boldsymbol{\omega}=\omega\hat{\boldsymbol{\omega}}$, represent rotation of the coordinates by the angle ω around an axis defined by the unit vector $\hat{\boldsymbol{\omega}}$; the effect of such a rotation on the function Y_m^l, denoted by P_{R}, is

$$P_{\mathrm{R}}(\boldsymbol{\omega})\, Y_m^l(\theta,\varphi) = \sum_{m'=-l}^{+l} Y_{m'}^l(\theta,\varphi)\, D_{m'm}^l(\boldsymbol{\omega}), \tag{3.3}$$

where $\hat{\boldsymbol{c}}$ is indicated by the polar angle θ and azimuthal angle φ relative to some chosen polar axis; $D_{m'm}^l(\boldsymbol{\omega})$ is a matrix 'representation' of the group, defined for every element of the group (i.e. any rotation $\boldsymbol{\omega}$) such that the product of any two elements is represented by the product of the corresponding representatives: i.e. if

$$\boldsymbol{\omega}_3 = \boldsymbol{\omega}_2 \boldsymbol{\omega}_1, \quad \text{then} \quad D[\boldsymbol{\omega}_3] = D[\boldsymbol{\omega}_2]\, D[\boldsymbol{\omega}_1] \tag{3.4}$$

(the latter product being conventional matrix multiplication). A group may have many representations, but the set that is called irreducible has (again) the property that products among members of any given irreducible representation remain within that representation. As rotations are described by continuous variables, they form a continuous (or 'Lie') group, and representatives (like $D_{m'm}$ for example) are actually functions of the polar and azimuthal angles corresponding to $\boldsymbol{\omega}$. Furthermore, these functions may be shown to obey partial differential equations whose solutions include spherical harmonics (Fano & Racah 1959, Appendix E; Talman 1968, §9.6).

Clearly it would be most convenient if the polynomials in $\boldsymbol{c}$ that we use should be orthogonal with a weight corresponding to the downstream maxwellian, which in our normalization is the isotropic function $\exp(-c^2)$. We may therefore separate the angular dependence (to be contained in the spherical harmonics) from that on the magnitude, and associate polynomials of different degree in $\boldsymbol{c}$ with each value of l. Noting that the spherical harmonics are orthogonal to each other over the solid angle $\mathrm{D}\hat{\boldsymbol{c}} = \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\varphi$,

$$\int Y_m^l(\hat{\boldsymbol{c}})\, Y_{m'}^{l'}(\hat{\boldsymbol{c}})\, \mathrm{D}\hat{\boldsymbol{c}} = \delta_{ll'}\delta_{mm'}, \tag{3.5}$$

we are led to consider functions of the type

$$\phi_m^{rl}(\boldsymbol{c}) = R_{rl}(c)\, Y_m^l(\hat{\boldsymbol{c}}), \tag{3.6}$$

where the radial functions R_{rl} are proportional to the Sonine polynomials (as defined by Chapman & Cowling (1970)) of index l and degree r in c^2,

$$R_{rl}(c) \equiv N(r,l)\, c^l S_r^{(l)}(c^2), \tag{3.7}$$

and obey the orthogonality relation

$$\int_0^\infty F_2(c)\, R_{rl}(c)\, R_{r'l}(c)\, c^2\, \mathrm{d}c = \delta_{rr'} \tag{3.8}$$

$N(r,l)$ being the normalization factor $[2\pi^{\frac{3}{2}}r!/\Gamma(r+l+\frac{3}{2})]^{\frac{1}{2}}$. (The subscript on the Sonine polynomial appears more commonly as $l+\frac{1}{2}$, for example in Chapman & Cowling (1970).) The functions (3.6) were introduced into kinetic theory by Burnett (1935), who demonstrated their advantages in calculation; it therefore seems appropriate to call them the Burnett functions.

3.3. *Some useful results*

We now list here some of the major results that we shall need for our later work, taking the opportunity to introduce the notations and normalizations we shall henceforth adopt. First of all, we note that the Burnett functions are themselves orthonormal in the sense that

$$\int F_2(c)\,\phi^{(i)}(\boldsymbol{c})\,\phi^{[j]}(\boldsymbol{c})\,\mathrm{D}\boldsymbol{c} = \delta(\boldsymbol{i},\boldsymbol{j}), \tag{3.9}$$

where $\boldsymbol{i}$ represents the triplet (rlm) (r being the 'radial' index), $\phi^{(i)} = \phi^{[i]*}$ (the star standing for complex conjugation) and indices enclosed in round and square brackets indicate respectively the 'standard' and 'contrastandard' forms of the function, in the notation of Fano & Racah (1959). The Burnett functions provide a complete expansion for $h(\boldsymbol{v})$ in velocity space,

$$h(\boldsymbol{v},x) = F_2(c)\,\psi(\boldsymbol{c}) = F_2(c)\,\nu_i(x)\,\phi^{[i]}(\boldsymbol{c}), \tag{3.10}$$

summed over $\boldsymbol{i}$, these $\phi^{[i]}$ and ν_i being the 'modes' and 'modal amplitudes' of (2.22).

When it is unnecessary to indicate explicitly the dependence of the functions on the independent variable, we shall again find the Dirac notation very convenient: the mode $\phi^{[i]}(\boldsymbol{c})$ is expressed as the 'ket' $|\boldsymbol{i}\rangle$ ($\equiv|rlm\rangle$) with a dual 'bra' denoted by $\langle\boldsymbol{i}|$ which in our case would just be $\phi^{(i)} = \phi^{[i]*}$. (The radial and angular parts of $\phi^{[i]}$ will be denoted by $\langle c\,|\,rl\rangle$ and $\langle\hat{\boldsymbol{c}}\,|\,lm\rangle$ respectively.) An inner product is defined by the bracket

$$\langle\boldsymbol{i}|\boldsymbol{j}\rangle = \int F_2(c)\,\phi^{[i]*}(\boldsymbol{c})\,\phi^{(j)}(\boldsymbol{c})\,\mathrm{D}\boldsymbol{c} = \delta(\boldsymbol{i},\boldsymbol{j}), \tag{3.11}$$

as we have already seen. This is equivalent to taking $F_2(c)\,\mathrm{D}\boldsymbol{c}$ as the elementary measure for integration in velocity space; a consequence is that the basic vector at $\boldsymbol{c}'$ in the coordinate representation is

$$\langle\boldsymbol{c}'\,|\,\boldsymbol{c}\rangle = \delta(\boldsymbol{c}-\boldsymbol{c}')/F_2(c),$$

and we can consistently write

$$\langle\boldsymbol{c}\,|\,\alpha\rangle = \langle\boldsymbol{c}\,|\,\boldsymbol{i}\rangle\langle\boldsymbol{i}\,|\,\alpha\rangle,$$

with the inner product (3.11). (Note that $f(\boldsymbol{c}) \equiv F_2(\boldsymbol{c})\langle\boldsymbol{c}|f\rangle$.)

Any operator O acting on the ket $|\boldsymbol{j}\rangle$ yields a vector $O|\boldsymbol{j}\rangle$, whose component along $|\boldsymbol{i}\rangle$ is given by the 'matrix element'

$$\langle\boldsymbol{i}|O|\boldsymbol{j}\rangle = \int F_2(c)\,\phi^{[i]*}(\boldsymbol{c})\,(O\phi^{[j]}(\boldsymbol{c}))\,\mathrm{D}\boldsymbol{c}. \tag{3.12}$$

An irreducible tensorial operator $T^{(k)}$ of rank k is a quantity with $2k+1$ components $T^{(k)}_q$, $q=-k,-k+1,\ldots,+k$, each of which, under a coordinate rotation $\boldsymbol{c}' = R(\boldsymbol{\omega})\,\boldsymbol{c}$, satisfies the relation

$$T'^{(k)}_q = P_{\mathrm{R}}\,T^{(k)}_q P^{-1}_{\mathrm{R}} = \sum_{q'} T^{(k)}_{q'} D^{(k)}_{q'q}(R), \quad k=0,1,2,\ldots, q'=-k,-k+1,\ldots,+k, \tag{3.13}$$

where $D^{(k)}_{q'q}(R)$ are matrix elements associated with the irreducible representation $D^{(k)}$ of the group SO(3). It is clear that the spherical harmonics Y^l_m can therefore be interpreted as

irreducible tensorial operators; equally, any set of operators $T^{(k)}$ can provide a basis for an irreducible representation D^k of SO(3). Entities like $T^{(k)}$ are often called 'spherical' tensors, to distinguish them from the more familiar cartesian tensors.

Note also that for any given value of r, the kets $|rlm\rangle$ constitute an irreducible tensorial set of rank l and dimension $(2l+1)$ with m ranging over the values $-l$ to $+l$.

Two i-tensors of rank l_1, l_2 may be 'coupled' to produce another i-tensor of rank l with components $|lm, l_1 l_2\rangle$ given by

$$|lm, l_1 l_2\rangle = \sum_{m_1 m_2} |l_1 m_1\rangle |l_2 m_2\rangle (l_1 m_1 l_2 m_2 | lm) \tag{3.14}$$

where the parentheses indicate the well-known Clebsch–Gordan (or Wigner) coefficients (see, for example, Edmonds 1957). These coefficients have been extensively studied and tabulated; in the Condon–Shortley convention which we adopt here, they are real, unitary, and orthogonal in the sense that

$$\sum_{m_1 m_2} (l_1 m_1 l_2 m_2 | lm) (l_1 m_1 l_2 m_2 | l'm') = \delta_{ll'} \delta_{mm'}, \tag{3.15a}$$

$$\sum_{l, m} (l_1 m_1 l_2 m_2 | lm) (l_1 m_1' l_2 m_2' | lm) = \delta_{m_1 m_1'} \delta_{m_2 m_2'}. \tag{3.15b}$$

They further obey the selection rules

$$(l_1 m_1 l_2 m_2 | lm) = 0,$$

unless
$$m = m_1 + m_2, \quad |l_1 - l_2| \leqslant l \leqslant l_1 + l_2, \tag{3.16}$$

the latter being called the 'betweenness' or triangle condition. One consequence of their orthogonality is a rule for decomposition of products,

$$|l_1 m_1\rangle |l_2 m_2\rangle = \sum_{lm} |lm\rangle (lm | l_1 m_1 l_2 m_2). \tag{3.17}$$

A product of Burnett functions therefore has the decomposition

$$|r_1 l_1 m_1\rangle |r_2 l_2 m_2\rangle = \sum_{rlm} |rlm\rangle (lm | l_1 m_1 l_2 m_2), \tag{3.18}$$

where the sum extends over all l, m for which the Clebsch–Gordan coefficient does not vanish, and r is determined for each l from the condition that the largest exponent of c on both sides be the same, i.e. that

$$2r_1 + l_1 + 2r_2 + l_2 = 2r + l.$$

An important property of i-tensors is that they obey the Wigner–Eckart theorem, which splits the matrix element of an i-tensor operator $T_q^{(k)}$ into two factors,

$$\langle rlm | T_q^{(k)} | r'l'm' \rangle = (2l+1)^{\frac{1}{2}} (l'm'kq | lm) \langle rl \| T^{(k)} \| r'l' \rangle, \tag{3.19}$$

where the first bracket on the right is a Clebsch–Gordan coefficient, and the second, called the 'reduced' matrix element (identified by the double bar and independent of the azimuthal indices m, m' and q) is a scalar. As the Clebsch–Gordan coefficients can be computed independently once and for all, the theorem enables a drastic reduction of effort in computing integrals over products of the Burnett functions, especially when the rank of the tensors involved is high.

3.4. *Transformation to central and relative modes*

The remaining problem of transformation between pre- and post-collision velocities in handling the collision integrals is tackled through the Talmi transformation for the Burnett functions (Talmi 1952; Kumar 1966*a*). These coefficients are the elements of a matrix of transformation from a basis consisting of products of Burnett functions in the $\boldsymbol{c}$-space for two particles to those in the centre-of-mass and relative-velocity coordinates. The defining relation is

$$\langle \boldsymbol{c}_1 | \boldsymbol{i} \rangle \langle \boldsymbol{c}_2 | \boldsymbol{j} \rangle = \langle \boldsymbol{c}_+ | \boldsymbol{n}_+ \rangle \langle \boldsymbol{c}_- | \boldsymbol{n}_- \rangle \left\langle \begin{matrix} \boldsymbol{n}_+ \\ \boldsymbol{n}_- \end{matrix} \middle| \begin{matrix} \boldsymbol{i} \\ \boldsymbol{j} \end{matrix} \right\rangle, \tag{3.20}$$

where

$$\boldsymbol{c}_+ = \frac{1}{\sqrt{2}}(\boldsymbol{c}_1 + \boldsymbol{c}_2), \quad \boldsymbol{c}_- = \frac{1}{\sqrt{2}}(\boldsymbol{c}_1 - \boldsymbol{c}_2),$$

and the subscripts + and − denote respectively indices and velocities in the centre-of-mass and relative coordinates; the third angular bracket on the right-hand side denotes the Talmi coefficients. Our definition of these coefficients differs from that of Kumar (1966*a*) by a phase factor of $(-)^{\frac{1}{2}}(l_+ + l_- - l_i - l_j)$, owing to the difference in the definition of the Burnett function by a factor i^l.

Balashov & Eltekov (1960) have shown how the dependence of the Talmi coefficients on the azimuthal indices can be extracted out through the appropriate Clebsch–Gordan coefficients, leading to the expression

$$\left\langle \begin{matrix} r_+ \, l_+ \, m_+ \\ r_- \, l_- \, m_- \end{matrix} \middle| \begin{matrix} r_i \, l_i \, m_i \\ r_j \, l_j \, m_j \end{matrix} \right\rangle = (l_- \, m_- \, l_+ \, m_+ \, | \, \lambda\mu) \left\langle \begin{matrix} r_+ \, l_+ \\ r_- \, l_- \end{matrix} \middle| (\lambda) \middle| \begin{matrix} r_i \, l_i \\ r_j \, l_j \end{matrix} \right\rangle (\lambda\mu \, | \, l_i \, m_i \, l_j \, m_j) \tag{3.21}$$

where the angular brackets on the right-hand side are the coefficients named after Brody & Moshinsky (1960) (also called the 'oscillator brackets').

A fact of great value is that for given values of the indices $\boldsymbol{i}$ and $\boldsymbol{j}$, the sum in (3.20) is finite, i.e. that only a limited range of values for the indices $\boldsymbol{n}_+$ and $\boldsymbol{n}_-$ lead to non-vanishing Talmi coefficients. The actual range is given by the selection rules:

$$\left.\begin{aligned} &(a)\ \ m_+ + m_- = m_i + m_j, \\ &(b)\ \ l_+ + l_- \geqslant |l_i - l_j|, \\ &(c)\ \ (l_i + l_j) \geqslant |l_+ - l_-|, \\ &(d)\ \ 2(r_+ + r_-) + l_+ + l_- = 2(r_i + r_j) + l_i + l_j. \end{aligned}\right\} \tag{3.22}$$

The first three of these rules follow from those for the Clebsch–Gordan coefficients (3.16), and the last is necessary to ensure that the degrees of the polynomials on both sides of (3.20) are the same. The Brody–Moshinsky coefficients follow only the selection rule (3.22*d*) above.

It is clear that the transformation (3.20) enables products of Burnett functions in a specified frame of reference to modes in centre-of-mass and relative-velocity coordinates. The inverse transformation enables us to return to the original frame when necessary.

4. The matrix elements

In the present section we now derive closed-form expressions for the four basic elements of §2.4, namely $\langle \boldsymbol{U}|L|\boldsymbol{i}\rangle$, $\langle \boldsymbol{k}|v_x|\boldsymbol{j}\rangle$, $\langle \boldsymbol{k}|G|\boldsymbol{i},\boldsymbol{j}\rangle$ and $\langle \boldsymbol{k}|L|\boldsymbol{i},\boldsymbol{j}\rangle$, and for the modal amplitude of the beam $\langle \boldsymbol{i}\,|\,\boldsymbol{U}\rangle$ (note that here we are using triplets instead of single indices).

4.1. *The streaming operator*

The matrix elements of the streaming operator are given by

$$\langle \boldsymbol{i}|v_x|\boldsymbol{j}\rangle = \int \mathrm{d}\boldsymbol{c}\, F_2(c)\,\langle \boldsymbol{i}\,|\,\boldsymbol{c}\rangle\, v_x \langle \boldsymbol{c}\,|\,\boldsymbol{j}\rangle, \tag{4.1}$$

where $\boldsymbol{i} = (r_i, l_i, m_i)$ and $\boldsymbol{j} = (r_j, l_j, m_j)$. As we have chosen u_2 as the reference velocity (see (2.6)), we write $v_x = c_x + u_2$ and note that c_x, the streamwise component of the molecular velocity c, is proportional to a Burnett function,

$$c_x = \tfrac{1}{\sqrt{2}}\langle 010\,|\,\boldsymbol{c}\rangle = \sqrt{(\tfrac{4}{3}\pi)}\, c\langle 10\,|\,c\rangle = \sqrt{(\tfrac{4}{3}\pi)}\, cY_0^1, \tag{4.2}$$

where $c = |\boldsymbol{c}|$ (choosing the polar axis along the x-direction). Using (4.2) in (4.1) and noting that

$$\langle \boldsymbol{i}|u_2|\boldsymbol{j}\rangle = u_2\,\delta(\boldsymbol{i},\boldsymbol{j}),$$

we get

$$\langle \boldsymbol{i}|v_x|\boldsymbol{j}\rangle = \sqrt{(4\pi/3)}\,\langle \boldsymbol{i}|cY_0^1|\boldsymbol{j}\rangle + u_2\,\delta(\boldsymbol{i},\boldsymbol{j}). \tag{4.3}$$

As the Burnett function here is a polynomial of degree l, the first term on the right will be non-zero only if $p_i\,(=2r_i+l_i) \leqslant p_j+1$ and $p_j \leqslant p_i+1$. But the integral is zero for $p_i = p_j$, as in that case the integrand is odd. So we are led to the following selection rule for $\langle \boldsymbol{i}|c_x|\boldsymbol{j}\rangle$:

$$p_i = p_j \pm 1. \tag{4.4}$$

Separating the integral in (4.3) into its radial and angular parts, we can write

$$\langle \boldsymbol{i}|cY_0^1|\boldsymbol{j}\rangle = \langle r_i\, l_i \| c \| r_j\, l_j\rangle \langle l_i\, m_i|Y_0^1|\, l_j\, m_j\rangle, \tag{4.5}$$

where we have introduced the radial integral

$$\langle r_i\, l_i \| f(c) \,\|\, r_j\, l_j\rangle \equiv \int_0^\infty \langle r_i\, l_i\,|\,c\rangle f(c)\,\langle c\,|\,r_j\, l_j\rangle\, c^2\,\mathrm{d}c. \tag{4.6}$$

By using the Wigner–Eckart theorem, the angular integral in (4.5) is

$$\begin{aligned}\langle l_i\, m_i|Y_0^1|\, l_j\, m_j\rangle &\equiv \int \langle l_i\, m_i\,|\,\hat{\boldsymbol{c}}\rangle\langle \hat{\boldsymbol{c}}\,|\,10\rangle\langle \hat{\boldsymbol{c}}\,|\,l_j\, m_j\rangle\,\mathrm{d}\hat{\boldsymbol{c}}\\ &= \langle l_i \| 1 \| l_j\rangle\,(l_i\, m_i\,|\,10 l_j\, m_j),\end{aligned} \tag{4.7}$$

where

$$\langle l_i \| 1 \| l_j\rangle = \left(\frac{3(2l_j+1)}{4\pi(2l_i+1)}\right)^{\frac{1}{2}} (l_i\, 0\,|\,10 l_j\, 0). \tag{4.8}$$

The selection rules (3.16) for the Clebsch–Gordan coefficients imply the following selection rules for the matrix elements in (4.5):

$$l_i - 1 \leqslant l_j \leqslant l_i + 1,\ m_i = m_i, \quad \text{and} \quad (l_i + l_j + 1) \quad \text{even};$$

i.e.

$$l_j = l_i \pm 1. \tag{4.9}$$

Consider first the case $l_j = l_i - 1$. The radial integral (4.6) now simplifies enormously, for, using the definition (3.7) of the radial functions, we have

$$\langle r_i\, l_i \| c \| r_j\, l_j \rangle = \left(\frac{r_i!\, r_j!}{(r_i+s)!\, r_j+s')!} \right)^{\frac{1}{2}} \int_0^\infty \mathrm{e}^{-t} t^{k+s} S_{r_i}^{(l_i)}(t)\, S_{r_j}^{(l_j)}(t)\, \mathrm{d}t, \tag{4.10}$$

where $$s = l_i + \tfrac{1}{2}, s' = l_j + \tfrac{1}{2},$$

and $$k = \tfrac{1}{2}(l_i + l_j + 2) - s = \tfrac{1}{2}(l_j - l_i + 1) = 0.$$

Now we use the well-known result (Erdelyi *et al.* 1953, vol. 2)

$$\int_0^\infty \mathrm{e}^{-t} t^s S_{r_i}^{(l_i)}(t)\, S_{r_j}^{(l_j)}(t)\, \mathrm{d}t = \frac{(s+r_i)!\, (s'-s, r_j-r_i)}{r_i!\, (r_j-r_i)!}, \tag{4.11}$$

where $(x, r) = \Gamma(r+x)/\Gamma(x)$. As $s'-s = -1$, we have $(s'-s, r_j-r_i) = 0$ unless $r_j - r_i \leqslant 1$, and $1/(r_j-r_i)! = 0$ unless $r_j - r_i \geqslant 0$. This gives us the selection rule for the radial integral,

$$0 \leqslant r_j - r_i \leqslant 1. \tag{4.12}$$

By using (4.11) and (4.12) and the fact that $l_j = l_i - 1$, (4.10) simplifies to

$$\langle r_i\, l_i \| c \| r_j\, l_j \rangle = \delta(l_j, l_i - 1)\, [\delta(r_j, r_i) \sqrt{(r_i + s_i)} - \delta(r_j, r_i + 1) \sqrt{r_j}]. \tag{4.13}$$

In addition in the present problem we have the azimuthal indices zero. Putting $l_j = l_i - 1$ in (4.7) and using the explicit expression for the Clebsch–Gordan coefficients (see Edmonds 1957), the angular part of the matrix element becomes

$$\langle l_i\, 0 | \sqrt{(4\pi/3)}\, Y_0^1 | l_j\, 0 \rangle = [(2l_i + 1)\, (2l_j + 1)]^{\frac{1}{2}} l_i.$$

Therefore

$$\langle r_i\, l_i\, 0 | c_x | r_j\, l_j\, 0 \rangle = \delta(l_j, l_i - 1)\, [(2l_i + 1)\, (2l_j + 1)]^{-\frac{1}{2}} l_i\, [\delta(r_j, r_i) \sqrt{(r_i + l_i + \tfrac{1}{2})} - \delta(r_j, r_i + 1) \sqrt{r_j}]. \tag{4.14}$$

When $l_j = l_i + 1$ the argument is similar, with r_i replacing r_j and l_i replacing l_j.
So finally we can write for all r_i, l_i, r_j, l_j

$$\begin{aligned} \langle r_i\, l_i\, 0 | v_x | r_j\, l_j\, 0 \rangle = {} & \boldsymbol{u}_2\, \delta(r_i, r_j)\, \delta(l_i, l_j) + [(2l_i + 1)\, (2l_j + 1)]^{-\frac{1}{2}} \\ & \times [\delta(l_j, l_i - 1)\, l_i \{\delta(r_j, r_i) \sqrt{(r_i + l_i + \tfrac{1}{2})} - \delta(r_j, r_i + 1) \sqrt{r_j}\} \\ & \times \delta(l_i, l_j - 1)\, l_j \{\delta(r_i, r_j) \sqrt{(r_j + l_j + \tfrac{1}{2})} - \delta(r_i, r_j + 1)\, r_i\}. \end{aligned} \tag{4.15}$$

It is clear from this expression that the streaming operator acting on any mode produces four neighbouring new modes, all of the same parity (see figure 3). The streaming matrix $[A]$ has only five non-zero diagonals, including the principal.

An expression similar to (4.15) has been derived by Mott-Smith (1954) (see Sirovich 1963) without using the irreducible tensor formalism. Kumar (1967) has given an equivalent expression, which he derived using a generating function for the Burnett functions.

4.2. *Matrix elements of the collision operator*

Expressions for the full collision matrix elements have been derived by Kumar (1966*a*); for our use we need separate expressions for the gain and loss elements. It will be convenient to

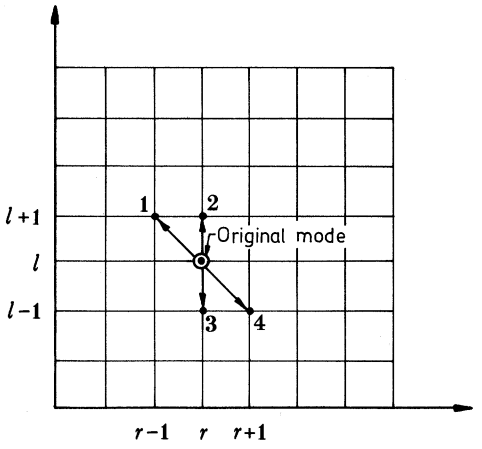

FIGURE 3. Sketch showing the new modes produced from the mode $|rl0\rangle$ by streaming.

quote results for spherically symmetric molecules with a cut-off in the potential, specializing to hard spheres when necessary. The main steps in the derivation will be described as an illustration of the technique we adopt.

Consider the gain matrix elements, which are given by the integral

$$\langle \boldsymbol{k}|G|\boldsymbol{i},\boldsymbol{j}\rangle = \int \langle \boldsymbol{k}\,|\,\boldsymbol{c}\rangle\, G(F_2(\boldsymbol{c})\langle \boldsymbol{c}\,|\,\boldsymbol{i}\rangle, F_2(\boldsymbol{c})\langle \boldsymbol{c}\,|\,\boldsymbol{j}\rangle)\,\mathrm{D}\boldsymbol{c}$$

$$= \int \langle \boldsymbol{k}\,|\,\boldsymbol{c}\rangle\, F_2(\boldsymbol{c}_1')\, F_2(\boldsymbol{c}_1)\langle \boldsymbol{c}'\,|\,\boldsymbol{i}\rangle\langle \boldsymbol{c}_1'|\boldsymbol{j}\rangle\, g\sigma(g,\chi)\,\mathrm{D}\boldsymbol{c}\,\mathrm{D}\boldsymbol{c}_1\,\mathrm{d}\Omega. \tag{4.16}$$

The crucial step is to express the integrand completely in terms of Burnett functions in centre-of-mass and relative-velocity coordinates (or in 'central' and 'relative' modes, as we shall say). This resolution is achieved by the Talmi transformation (3.20):

$$\langle \boldsymbol{c}_1'\,|\,\boldsymbol{i}\rangle\langle \boldsymbol{c}_2'|\boldsymbol{j}\rangle = \langle \boldsymbol{c}_+\,|\,\boldsymbol{n}_+\rangle\langle \boldsymbol{c}_-\,|\,\boldsymbol{n}_-\rangle \left\langle \begin{matrix}\boldsymbol{n}_+ \\ \boldsymbol{n}_-\end{matrix}\middle|\begin{matrix}\boldsymbol{i} \\ \boldsymbol{j}\end{matrix}\right\rangle$$

$$= \langle \boldsymbol{c}_+\,|\,\boldsymbol{n}_+\rangle\langle c_-\,|\,r_-\,l_-\rangle\langle \hat{\boldsymbol{c}}_-\,|\,l_-\,m_-\rangle \left\langle \begin{matrix}\boldsymbol{n}_+ \\ \boldsymbol{n}_-\end{matrix}\middle|\begin{matrix}\boldsymbol{i} \\ \boldsymbol{j}\end{matrix}\right\rangle, \tag{4.17}$$

$$\langle \boldsymbol{k}\,|\,\boldsymbol{c}_1\rangle = \langle \boldsymbol{k}\,|\,\boldsymbol{c}_1\rangle\langle \boldsymbol{0}\,|\,\boldsymbol{c}_2\rangle$$

$$= \left\langle \begin{matrix}\boldsymbol{k} \\ \boldsymbol{0}\end{matrix}\middle|\begin{matrix}\boldsymbol{n}_+' \\ \boldsymbol{n}_-'\end{matrix}\right\rangle \langle \boldsymbol{n}_+\,|\,\boldsymbol{c}_+\rangle\langle r_-'\,l_-'\,|\,c_-\rangle\langle l_-'\,m_-'\,|\,\hat{\boldsymbol{c}}_-\rangle, \tag{4.18}$$

where we have split the relative Burnett modes $\langle \boldsymbol{c}_-\,|\,\boldsymbol{n}_-\rangle$ and $\langle \boldsymbol{n}_-'\,|\,\boldsymbol{c}_-\rangle$ into their radial and angular parts.

For spherically symmetric molecules the differential cross section can also be expanded as

$$\begin{aligned}\sigma(g,\chi) &= \sigma_p(g)\,[(2l+1)/4\pi]^{\frac{1}{2}} P_p(\cos\chi) \\ &= \sigma_p(g)\,\langle \hat{\boldsymbol{g}}\,|\,pq\rangle\langle pq\,|\,\hat{\boldsymbol{g}}'\rangle,\end{aligned} \tag{4.19}$$

where $|pq\rangle$ are the spherical harmonics $Y_q^p(\chi,\epsilon)$ and

$$\sigma_p(g) = 2\pi \int_{-1}^{1} \sigma(g,\chi)\, P_p(\cos\chi)\,\mathrm{d}(\cos\chi). \tag{4.20}$$

Substituting (4.17) and (4.19) in the integral (4.16), and recalling that $g = c_- \sqrt{2}$, the latter becomes

$$\langle \boldsymbol{k} \,|\, G \,|\, \boldsymbol{ij} \rangle = \sqrt{2} \left\langle \begin{matrix} \boldsymbol{k} \\ \boldsymbol{0} \end{matrix} \middle| \begin{matrix} \boldsymbol{n}'_+ \\ \boldsymbol{n}'_- \end{matrix} \right\rangle \left\langle \begin{matrix} \boldsymbol{n}_+ \\ \boldsymbol{n}_- \end{matrix} \middle| \begin{matrix} \boldsymbol{i} \\ \boldsymbol{j} \end{matrix} \right\rangle$$

$$\int \langle r'_- l'_- \,|\, c_- \rangle\, c_- \sigma_p(c_- \sqrt{2}, \chi) \langle c_- \,|\, r_- l_- \rangle F_2(c_-)\, c_-^2 \mathrm{d}c_- \int \langle l'm' \,|\, \hat{\boldsymbol{c}}_- \rangle \langle \hat{\boldsymbol{c}}_- \,|\, pq \rangle \, \mathrm{d}\hat{\boldsymbol{c}}_-$$

$$\times \int \langle pq \,|\, \hat{\boldsymbol{c}}'_- \rangle \langle \hat{\boldsymbol{c}}'_- \,|\, lm \rangle \, \mathrm{d}\hat{c}'_- \int \langle \boldsymbol{n}_+ \,|\, \boldsymbol{c}_+ \rangle \langle \boldsymbol{c}_+ \,|\, \boldsymbol{n}'_+ \rangle \, \mathrm{D}\boldsymbol{c}_+. \quad (4.21)$$

The integrals in (4.21) are respectively $\langle r'l' \| c_- \sigma_p(c_- \sqrt{2}) \| rl \rangle$, $\langle l'm' \,|\, pq \rangle$, $\langle pq \,|\, lm \rangle$, and $\langle \boldsymbol{n}_+ \,|\, \boldsymbol{n}' \rangle$ (excepting the first, all of these are Krönecker deltas owing to the orthogonality of the Burnett functions and the spherical harmonics). Using these values (4.21) simplifies to

$$\langle \boldsymbol{k} | G | \boldsymbol{i},\boldsymbol{j} \rangle = \sqrt{2} \left\langle \begin{matrix} k \\ \boldsymbol{0} \end{matrix} \middle| \begin{matrix} \boldsymbol{n}_+ \\ r'_- l_- m_- \end{matrix} \right\rangle \langle r'_- l_- \| c_- \sigma_{l_-}(c_- \sqrt{2}) \| r_- l_- \rangle \left\langle \begin{matrix} \boldsymbol{n}_+ \\ r_- l_- m_- \end{matrix} \middle| \begin{matrix} \boldsymbol{i} \\ \boldsymbol{j} \end{matrix} \right\rangle \quad (4.22)$$

Similarly, we can arrive at the corresponding expression for the loss operator,

$$\begin{aligned} \langle \boldsymbol{k} | \hat{L} | \boldsymbol{i},\boldsymbol{j} \rangle &= \sqrt{2} \langle \boldsymbol{k} \,|\, \boldsymbol{n}_+ \rangle \langle r'_- l_- \| c_- \sigma_0(c_- \sqrt{2}) \| r_- l_- \rangle \langle \boldsymbol{n}_+ \,|\, \boldsymbol{i} \rangle \\ \langle \boldsymbol{k} | \hat{L} | \boldsymbol{i},\boldsymbol{j} \rangle &= \sqrt{2} \langle \boldsymbol{0} \,|\, r'_- l_- m_- \rangle \langle r'_- l_- \| c_- \sigma_0(c_- \sqrt{2} \| r_- l_- \rangle \langle \boldsymbol{n}_- \,|\, \boldsymbol{j} \rangle \quad . \end{aligned} \quad (4.23)$$

The structure of the expressions (4.22) and (4.23) suggests the following physical picture (see figure 4). The modes $|\boldsymbol{i}\rangle$ and $|\boldsymbol{j}\rangle$ are transformed to the central and relative modes $|\boldsymbol{n}_+\rangle$ and $|\boldsymbol{n}_-\rangle$ through the Talmi coefficients. The central modes $|\boldsymbol{n}_+\rangle$ are unaffected by collision, and, due to the assumed spherical symmetry of the molecular model, the angular parts of the relative modes $|\boldsymbol{n}_-\rangle$ are also unaffected. So what changes in collision is only the radial part of the relative modes. The outcoming modes are anti-transformed back to the original modes in the usual coordinates through a further set of Talmi coefficients.

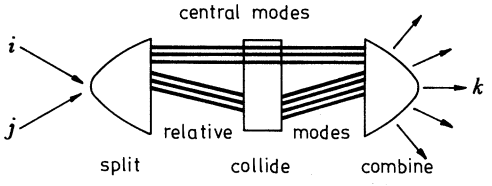

FIGURE 4. Diagram to illustrate the computation of collision matrix elements. To compute the interaction of modes $\boldsymbol{i},\boldsymbol{j}$, they are first split into central and relative modes through a Talmi transformation. Only the latter change by collision: the resultant relative modes are recombined with the unaffected central modes through Talmi transformations to calculate the amplitude of mode $\boldsymbol{k}$.

For hard-sphere molecules, $\sigma = \frac{1}{4}$ and $\sigma_0 = \pi$ in the scales we have chosen; therefore,

$$\sigma_{l_-} = 2\pi \int_{-1}^{+1} \tfrac{1}{4} P_{l_-}(\cos\chi)\, \mathrm{d}(\cos\chi) = \sigma_0\, \delta(l_-, 0). \quad (4.24)$$

Thus only $l_- = 0$ contributes to the sum in (4.22). However, all possible values of l_- contribute to the loss matrix elements; otherwise there is no difference in the evaluation of the two matrix elements for hard-sphere molecules. In fact, if (4.22) is written as a sum over the index l_-, then the first term in the sum is the gain matrix element.

The expressions (4.22) and (4.23) can be simplified by writing the two Talmi coefficients in an expanded form using (3.21):

$$\langle \boldsymbol{k}|G|\boldsymbol{i},\boldsymbol{j}\rangle = \sqrt{2}(l_k m_k 0\,0\,|\,\lambda_1\mu_1)\left\langle \begin{matrix} r_k l_k \\ 0\,0 \end{matrix} (\lambda_1) \begin{matrix} r_+ l_+ \\ r'_- l_- \end{matrix}\right\rangle \times (\lambda_1\mu_1\,|\,l_- m_- l_+ m_+)\langle r'_- l_-\|\, c_-\sigma_{l_-}(c_-\sqrt{2})\,\|\, r_- l_-\rangle \times (l_- m_- l_+ m_+\,|\,\lambda_2\mu_2)\left\langle \begin{matrix} r_+ l_+ \\ r_- l_- \end{matrix} (\lambda_2) \begin{matrix} r_i l_i \\ r_j l_j \end{matrix}\right\rangle (\lambda_2\mu_2\,|\,l_i m_i l_j m_j). \tag{4.25}$$

From the properties of the Clebsch–Gordan coefficients (Rose 1957),

$$(l_k m_k 0\,0\,|\,\lambda_1\mu_1) = \delta(l_k,\lambda_1)\,\delta(m_k,\mu_1). \tag{4.26}$$

By using (4.26), and (3.15*a*) in (4.25), the latter simplifies to

$$\langle \boldsymbol{k}|G|\boldsymbol{i},\boldsymbol{j}\rangle = \sqrt{2}\left\langle \begin{matrix} r_k l_k \\ 0\,0 \end{matrix} (l_k) \begin{matrix} r_+ l_+ \\ r'_- l_- \end{matrix}\right\rangle \langle r'_- l_-\|\, c_-\sigma_{l_-}(c_-\sqrt{2})\,\|\, r_- l_-\rangle \times \left\langle \begin{matrix} r_+ l_+ \\ r'_- l_- \end{matrix} (l_k) \begin{matrix} r_i l_i \\ r_j l_j \end{matrix}\right\rangle (l_k m_k\,|\,l_i m_i l_j m_j). \tag{4.27}$$

Similarly, the matrix elements of the loss operator simplify to

$$\langle \boldsymbol{k}|\hat{L}|\boldsymbol{i},\boldsymbol{j}\rangle = \sqrt{2}\left\langle \begin{matrix} r_k l_k \\ 0\,0 \end{matrix} (l_k) \begin{matrix} r_+ l_+ \\ r'_- l_- \end{matrix}\right\rangle \langle r'_- l_-\|\, c_-\sigma_0(c_-\sqrt{2})\,\|\, r_- l_-\rangle \times \left\langle \begin{matrix} r_+ l_+ \\ r_- l_- \end{matrix} (l_k) \begin{matrix} r_i l_i \\ r_j l_j \end{matrix}\right\rangle (l_k m_k\,|\,l_i m_i l_j m_j). \tag{4.28}$$

After deriving the simplified expressions (4.27) and (4.28) we have learnt that essentially the same derivation was carried out by Ness & Robson (1985). In §4.4 we will provide a group-theoretic interpretation of these results.

The expressions (4.27) and (4.28) have a rather neat structure. For example, we can write them as

$$\left.\begin{aligned} \langle \boldsymbol{k}|G|\boldsymbol{i},\boldsymbol{j}\rangle &= \langle r_k l_k\|\, G\,\|\, r_i l_i, r_j l_j\rangle\,(l_k m_k\,|\,l_i m_i l_j m_j), \\ \text{and}\qquad \langle \boldsymbol{k}|\hat{L}|\boldsymbol{i},\boldsymbol{j}\rangle &= \langle r_k l_k\|\hat{L}\|\, r_i l_i, r_j l_j\rangle\,(l_k m_k\,|\,l_i m_i l_j m_j). \end{aligned}\right\} \tag{4.29}$$

The brackets on the right here are free of azimuthal indices and so are scalars, and, by comparison with the Wigner–Eckart theorem (3.19), may be interpreted as reduced matrix elements. These quantities (which are much less numerous than the gain and loss matrix elements) alone contain the 'physics' of the collisional interactions.

The expressions (4.27) and (4.28) afford great economy in terms of computation. For example, for hard-sphere molecules, when $\boldsymbol{k} = (4,5,2)$, $\boldsymbol{i} = (3,5,1)$, and $\boldsymbol{j} = (4,4,1)$, the computation of collisional matrix elements using (4.22) and (4.23) involves a sum over 505 terms and takes 62 seconds on a DEC-10, whereas the use of (4.27) and (4.28) leads to a sum involving only 110 terms and takes less than three seconds.

We see that for spherically symmetric molecules the Brody–Moshinsky coefficients are all that are needed to compute the matrix elements, and one can do away with the relatively complicated Talmi coefficients. Further, it is only the radial integrals that depend on the molecular model, the Brody–Moshinsky (or Talmi) coefficients and the Clebsch–Gordan coefficients being 'geometric' or model-independent. Conceptually, this helps us distinguish

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the effects of the particular molecular model from those arising from geometric considerations. Algebraically, because explicit formulae are available for all the 'geometric' coefficients mentioned above, we only have to worry about evaluating the radial integrals. (For the hard-sphere molecule here considered, analytical expressions for these integrals are available, as we shall see in the next section.) This alone is a matter of great importance to kinetic theory, because workers have often been forced to use Maxwell molecules not so much because it is superior for physical reasons but purely to reduce the prohibitive algebra. (Also, contrast the present method with classical methods, for example Chapman & Cowling (1939) and especially Burnett (1936), who used almost the same polynomials as we do.) Computationally, the geometric coefficients, being problem independent, may be computed and stored once and for all for use with any molecular model. In addition, the selection rules for these coefficients ensure that we do not compute those terms that vanish by symmetry. (We will see in §4.4 that these selection rules lead to selection rules for the collision matrix elements themselves!) By using Brody–Moshinsky (or Talmi) coefficients one can compute the collision matrix elements to at least nine significant figures in a matter of minutes on a computer like the DEC-10, and for a given molecular model this has to be done only once. The significance of this facility can be understood in the light of the fact that time-consuming Monte Carlo procedures (see, for example, Hicks *et al.* 1972) have been used to evaluate the collision integral approximately.

4.3. *The beam-loss coefficients*

We now derive an analytical expression for the integral

$$\langle \boldsymbol{c}|L|\boldsymbol{i}\rangle = \pi \int F_2(\boldsymbol{c}_1)\,\langle \boldsymbol{c}_1|\boldsymbol{i}\rangle\, g\mathrm{D}\boldsymbol{c}_1, \tag{4.30}$$

where we have again put $\sigma_0 = \pi$. The strategy is now to expand g in central and relative modes, and use the Talmi coefficients to transform to Burnett functions in the usual coordinates, at which stage integration becomes automatic.

Putting

$$g = g\phi^{(0)}(\boldsymbol{c}_+), \tag{4.31}$$

we write

$$\left.\begin{aligned} \langle g|\langle \mathbf{0}_+| &= \langle g|\boldsymbol{n}_-\rangle\langle \boldsymbol{n}_-|\langle \mathbf{0}_+| \\ &= \langle g|\boldsymbol{n}_-\rangle \left\langle \begin{matrix}\mathbf{0}_+ \\ \boldsymbol{n}_-\end{matrix}\middle|\begin{matrix}\boldsymbol{k} \\ \boldsymbol{j}\end{matrix}\right\rangle \langle \boldsymbol{k}|\boldsymbol{c}\rangle\langle \boldsymbol{j}|\boldsymbol{c}_1\rangle \end{aligned}\right\} \tag{4.32}$$

where the bra $\langle \mathbf{0}_+|$ corresponds to the dual Burnett mode $\phi^{[0]}(\boldsymbol{c}_+)$, and the bra $\langle g|$ corresponds to the function g.

Using (4.32) in (4.30) and using the orthogonality of the modes $\boldsymbol{i}, \boldsymbol{j}$, we have

$$\langle \boldsymbol{c}|L|\boldsymbol{i}\rangle = \pi\langle g|\boldsymbol{n}_-\rangle \left\langle \begin{matrix}\mathbf{0}_+ \\ \boldsymbol{n}_-\end{matrix}\middle|\begin{matrix}\boldsymbol{k} \\ \boldsymbol{l}\end{matrix}\right\rangle \langle \boldsymbol{k}|\boldsymbol{c}\rangle \tag{4.33}$$

But

$$\left.\begin{aligned} \langle g|\boldsymbol{n}_-\rangle &\equiv \pi\sqrt{2}\int_0^\infty F_2(c_-)\,\langle c_-|r_-\,l_-\rangle\, c_-\, c_-^2\,\mathrm{d}c_- \int \langle \hat{\boldsymbol{c}}_-|\,l_-\,m_-\rangle\,\mathrm{d}\hat{\boldsymbol{c}}_- \\ &= \pi\sqrt{2}\,\langle r_-\,l_-\|\,c_-\|\,0\,0\rangle\,\delta(l_-,0)\,\delta(m_-,0), \end{aligned}\right\} \tag{4.34}$$

so only $l_- = 0, m_- = 0$ contribute; we encounter again the radial integral introduced in (4.6). The expression (4.33) is formally an infinite sum over the index triplet $\boldsymbol{k} = (r_k, l_k, m_k)$ and $\boldsymbol{n}_-$.

However, because only $l_- = 0$ and $m_- = 0$ contribute to the sum, using the selection rules (3.22) for the Talmi coefficients, we have

$$l_k = l_i, \quad m_k = -m_i, \quad r_- = r_k + r_i + l_i. \tag{4.35}$$

Incorporating these rules we obtain

$$\langle \boldsymbol{c}|L|\boldsymbol{i}\rangle = \pi\sqrt{2}\langle 00\|c_-\|r_-0\rangle \left\langle \begin{matrix} 000 \\ r_-00 \end{matrix} \middle| \begin{matrix} r_k\, l_i - m_i \\ r_i\, l_i\, m_i \end{matrix} \right\rangle \langle r_k\, l_i - m_i|\, \boldsymbol{c}\rangle, \tag{4.36}$$

with summation over r_k which can take values from 0 to ∞. The presence of zero indices here leads to further simplification. To achieve this we first note that the radial integral $\langle rl\|g^k\|r'l'\rangle$, which is proportional to an expression of Exton (1978, p. 106), is

$$\langle rl\|g^k\|r'l'\rangle = \Gamma(a)\,\frac{(s+1,r)\,(s'+1-a,r')}{r!\,r'!}\left[\frac{r!\,r'!}{(r+s)!\,(r'+s')!}\right]^{\frac{1}{2}} {}_3F_2\left[\frac{a,\,-r,\,a-s'}{s+1,\,a-s'-r};1\right], \tag{4.37}$$

where $s_2 = l+0.5$, $s' = l'+0.5$, $a = \frac{1}{2}(l+l'+k+3)$, and ${}_3F_2$ is a generalized hypergeometric function. A special case of (4.37) is

$$\langle r_-0\|c_-\|00\rangle = \langle 00\|c_-\|r_-0\rangle = (-\tfrac{1}{2}, r_-)\,[r_-!\,(r_-+\tfrac{1}{2})!\,(\tfrac{1}{2})!]^{-\frac{1}{2}}. \tag{4.38}$$

Using the explicit expression for the Talmi coefficients as given by Kumar (1966*b*) for the indices as in (4.36), applying the phase correction mentioned in §3.4, and using the special values of the Clebsch–Gordan coefficients (see Brink & Satchler 1968, p. 140)

$$(00\,00\,|\,\lambda\mu) = \delta(\lambda,0)\,\delta(\mu,0), \tag{4.39}$$

$$(l_i - m_i\, l_i\, m_i\,|\,00) = (-)^{l_i-m_i}(2l_i+1)^{-\frac{1}{2}}, \tag{4.40}$$

we obtain the following simplified expression for the Talmi coefficient in (4.36):

$$\left\langle \begin{matrix} 000 \\ r_-00 \end{matrix} \middle| \begin{matrix} r_k\, l_i - m_i \\ r_i\, l_i\, m_i \end{matrix} \right\rangle = (-)^{r_k+r_i+r_-+l_i-m_i}(\tfrac{1}{2})^{r_-}\left[\frac{\frac{1}{2}!\,r_-!\,(r_-+\frac{1}{2})!}{r_i!\,(r_i+s_i)!\,r_k!\,(r_k+s_i)!}\right]^{\frac{1}{2}}, \tag{4.41}$$

where $s_i = l_i + \frac{1}{2}$.

Splitting the Burnett functions in (4.36) into their radial and angular parts as in §3.3 and noting that the angular part

$$\langle \hat{\boldsymbol{c}}\,|\,l_i\, m_i\rangle = (-)^{m_i}\langle \hat{\boldsymbol{c}}\,|\,l_i - m_i\rangle, \tag{4.42}$$

we have

$$\langle \boldsymbol{c}|L|\boldsymbol{i}\rangle = \pi\sqrt{2}(\tfrac{1}{2})^{2(r_i+l_i)}N(r_i,l_i)\,\{\Gamma(p)/(\Gamma(-\tfrac{1}{2})\,\Gamma(1+s_i)\,r_i!)\}$$
$$\times\langle \hat{\boldsymbol{c}}\,|\,l_i\, m_i\rangle\, c^{l_i}\sum_{r_k=0}^{\infty}(\tfrac{1}{2})^{r_k}\frac{(p,r_k)}{(1+s_i,r_k)}S_{r_k}^{(l_i)}(c^2), \tag{4.43}$$

where $p = r_i + l_i - \frac{1}{2}$, and (x,n) is the Pochammer symbol defined in §4.1.

We can express the summation in (4.43) in terms of hypergeometric functions using the result (Erdelyi *et al.* 1953, vol. 3)

$$(1-t)^{-p}\,{}_1F_1\left[\frac{p}{1+s};-\frac{xt}{1-t}\right] = \sum_{n=0}^{\infty}\frac{(p,n)\,S_n^{(1)}(x)}{(1+s,n)}\,t^n. \tag{4.44}$$

With $t = \frac{1}{2}$, $-xt/(1-t) = -x$, $p = r_i + l_i - \frac{1}{2}$ and $s = s_i$, and applying Kummer's transformation (Erdelyi *et al.* 1953, vol. 1) the left-hand side of (4.44) becomes

$$(\tfrac{1}{2})^{-p} \exp(-c^2)\, {}_1F_1[(2-r_i)/(1+s_i); c^2]. \tag{4.45}$$

Making use of (4.45) in (4.43) and simplifying, we finally have

$$\langle \boldsymbol{c}|L|\boldsymbol{i}\rangle = \pi^{\frac{5}{2}} N(r_i, l_i)\{\Gamma(p)/(\Gamma(-\tfrac{1}{2})\,\Gamma(1+s_i)\,r_i!)\} F_2(\boldsymbol{c})\, c^{l_i} \langle \hat{\boldsymbol{c}}|l_i m_i\rangle\, {}_1F_1[(2-r_i)/(1+s_i); c^2]. \tag{4.46}$$

The above expression is new. For $r_i = 0 = l_i$, we recover from it the expression of Deshpande & Narasimha (1969) for the loss integral of a maxwellian. The hypergeometric function here is an infinite series for $r_i < 2$, but is proportional to a Sonine polynomial otherwise: thus, for $r_i \geqslant 2$,

$$\langle \boldsymbol{c}|L|\boldsymbol{i}\rangle = \pi^{\frac{5}{2}}\{\Gamma(p)/(\Gamma(-\tfrac{1}{2})\,\Gamma(1+s_i)\}\left[\frac{(r_i-2+s_i)!}{r_i!\,(r_i+s_i)!\,(r_i-2)!}\right]^{\frac{1}{2}} \langle \boldsymbol{c}|r_i-2, l_i, m_i\rangle. \tag{4.47}$$

4.4. *Structure of the collision operator*

An application of the selection rules that govern the purely group-theoretic Clebsch–Gordan and Brody–Moshinsky coefficients gives us considerable insight into the structure of the collision operator.

1. The selection rules (3.16) for the Clebsch–Gordan coefficient in (4.27) and (4.28) imply that the gain and the loss matrix elements vanish unless the indices $\boldsymbol{k}$, $\boldsymbol{i}$, and $\boldsymbol{j}$ satisfy the conditions

$$|l_i - l_j| \leqslant l_k \leqslant l_i + l_j \tag{4.48a}$$

and

$$m_k = m_i + m_j. \tag{4.48b}$$

Similarly, the selection rules (3.22) for the Brody–Moshinsky coefficients in (4.27) and (4.28) require that

$$(-)^{l_k} = (-)^{L+l} \quad \text{and} \quad (-)^{L+l} = (-)^{l_i+l_j},$$

implying

$$(l_k + l_i + l_j) \quad \text{is even.} \tag{4.48c}$$

Stated in words, if two 'input' modes $|\boldsymbol{i}\rangle$ and $|\boldsymbol{j}\rangle$ interact by collision, then their polar and azimuthal indices constrain those of the resulting 'output' modes $|\boldsymbol{k}\rangle$. For example, if the interacting modes are $|121\rangle$ and $|121\rangle$, the resulting modes are only $|r_k 42\rangle$ and $|r_k 22\rangle$ ($r_k = 0, 1, 2, \ldots$); symmetry rules out the production of all other modes. From (4.48*c*) the parity of any output mode is the product of that of the input modes. Thus, in the above example, all output modes are even.

An interpretation of the above result is possible by noting that the selection rules (4.48*a*–*c*) are identical to those governing the well-known Gaunt integral (see, for example, Rose 1957)

$$\int \langle l_k m_k|\hat{\boldsymbol{c}}\rangle \langle \hat{\boldsymbol{c}}|l_i m_i\rangle \langle \hat{\boldsymbol{c}}|l_j m_j\rangle \, \mathrm{d}\hat{\boldsymbol{c}}.$$

Because the spherical harmonics appearing in the integrand above are the angular parts of the modes $\langle \boldsymbol{k}|\boldsymbol{c}\rangle$, $\langle \boldsymbol{c}|\boldsymbol{i}\rangle$, and $\langle \boldsymbol{c}|\boldsymbol{j}\rangle$, we conclude that the angular dependence of the collision integral $\langle \boldsymbol{c}|J|\boldsymbol{i},\boldsymbol{j}\rangle$ (as also of $\langle \boldsymbol{c}|G|\boldsymbol{i},\boldsymbol{j}\rangle$ and $\langle c|\hat{L}|\boldsymbol{i},\boldsymbol{j}\rangle$ separately) must be the same as that of $\langle \hat{\boldsymbol{c}}|l_i m_i\rangle\langle \hat{\boldsymbol{c}}|l_j m_j\rangle$. (That this is so for the loss part was already explicit in (4.46).) This is a simple consequence of the scalar nature of the collision operator (i.e. it is an i-tensor operator of rank 0) for spherically symmetric molecules.

The radial part of $\langle \boldsymbol{c}|J|\boldsymbol{i},\boldsymbol{j}\rangle$ is of course not identical to that of the product $F_2 F_2 \langle \boldsymbol{c}|\boldsymbol{i}\rangle \langle \boldsymbol{c}|\boldsymbol{j}\rangle$, as the collisions produce new radial modes. However, as is clear from (4.46), the loss integral of a Burnett mode has a maxwellian factor. The results of Deshpande & Narasimha (1969) show that even the gain integral has maxwellian factors when the input distributions are maxwellians. Therefore, we may expect the following form for the full collision integral:

$$\langle \boldsymbol{c}|J|\boldsymbol{i},\boldsymbol{j}\rangle = \text{const.} \times F_2(\boldsymbol{c})\, F_2(\boldsymbol{c})\, \langle \hat{\boldsymbol{c}}|\, l_i m_i\rangle \langle \hat{\boldsymbol{c}}|\, l_j m_j\rangle \times (\text{radial function}). \tag{4.49}$$

For $r_i \geqslant 2$, the expression $L|\boldsymbol{i}\rangle$ is proportional to a Burnett mode as seen in (4.47), so that

$$L|\boldsymbol{i},\boldsymbol{j}\rangle = \text{const.}\, |\boldsymbol{i}\rangle |r_j - 2, l_j, m_j\rangle. \tag{4.50}$$

2. The Talmi coefficients have the property

$$\left\langle \begin{matrix} \boldsymbol{n}_+ \\ r_- l_- m_- \end{matrix} \middle| \begin{matrix} \boldsymbol{j} \\ \boldsymbol{i} \end{matrix} \right\rangle = (-)^{l_-} \left\langle \begin{matrix} \boldsymbol{n}_+ \\ r_- l_- m_- \end{matrix} \middle| \begin{matrix} \boldsymbol{i} \\ \boldsymbol{j} \end{matrix} \right\rangle. \tag{4.51}$$

Using this in (4.22), we get for the transposed gain operator

$$\langle \boldsymbol{k}|G|\boldsymbol{j},\boldsymbol{i}\rangle = (-)^l \sqrt{2} \left\langle \begin{matrix} \boldsymbol{k} \\ \boldsymbol{0} \end{matrix} \middle| \begin{matrix} \boldsymbol{n}_+ \\ r' l_- m_- \end{matrix} \right\rangle \langle r' l_- \| c_- \sigma_{l_-}(c_- \sqrt{2}) \| r_- l_- \rangle \left\langle \begin{matrix} \boldsymbol{n}_+ \\ r_- l_- m_- \end{matrix} \middle| \begin{matrix} \boldsymbol{i} \\ \boldsymbol{j} \end{matrix} \right\rangle. \tag{4.52}$$

It is clear from comparison with (4.22) that this sum has the same terms as $\langle \boldsymbol{k}|G|\boldsymbol{i},\boldsymbol{j}\rangle$, but with alternating signs. In general, therefore, the gain matrix element is not symmetric in $\boldsymbol{i},\boldsymbol{j}$: the order in which the input modes interact must be specified, and $|\boldsymbol{i}\rangle$ hitting $|\boldsymbol{j}\rangle$ is different from $|\boldsymbol{j}\rangle$ hitting $|\boldsymbol{i}\rangle$. But for hard-sphere molecules (4.24) implies that only $l_- = 0$ contributes to the sum in (4.22) and (4.52), and therefore that the gain elements are indeed symmetric,

$$\langle \boldsymbol{k}|G|\boldsymbol{i},\boldsymbol{j}\rangle = \langle \boldsymbol{k}|G|\boldsymbol{j},\boldsymbol{i}\rangle, \tag{4.53}$$

equivalently,

$$G|\boldsymbol{i},\boldsymbol{j}\rangle = G|\boldsymbol{j},\boldsymbol{i}\rangle, G|f,h\rangle = G|h,f\rangle, \tag{4.54}$$

a result used earlier by Grad (1969) without explicit restriction to hard-sphere molecules.

3. From (4.23) we see that for spherically symmetric molecules the loss operator depends only on $\sigma_0(g)$. So it is independent of the variation of the cross-section with scattering angle χ. In other words, two molecular models having the same σ_0 but different σ_1, σ_2, etc., will result in the same loss integral.

4. Following Kumar (1967) we may define the symmetric sum

$$\langle \boldsymbol{k}|\bar{J}|\boldsymbol{i},\boldsymbol{j}\rangle = \tfrac{1}{2}[\langle \boldsymbol{k}|J|\boldsymbol{i},\boldsymbol{j}\rangle + \langle \boldsymbol{k}|J|\boldsymbol{j},\boldsymbol{i}\rangle]. \tag{4.55}$$

Linear transport theory involves the matrix elements

$$\langle \boldsymbol{k}|\bar{J}|r1m,\boldsymbol{0}\rangle, \quad \langle \boldsymbol{k}|\bar{J}|r2m,\boldsymbol{0}\rangle,$$

respectively for the thermal conductivity and the viscosity; indeed the 'Chapman brackets' [,] (see Chapman & Cowling 1939) and the B-coefficients of Sirovich & Thurber (1965) are special cases of the Kumar bracket (4.55),

$$-[\phi^{[k]}, \phi^{[i]}] = B(r_k l_k; r_i l_i) = \langle \boldsymbol{k}|\bar{J}|\boldsymbol{i},\boldsymbol{0}\rangle. \tag{4.56}$$

Chapman & Cowling actually use in (4.56) only certain linear combinations of the brackets, the most complex of them being (in their notation)

$$[S_{\frac{5}{2}}^{(3)}(c^2)\, \boldsymbol{c}\overset{0}{\circ}\boldsymbol{c}, S_{\frac{5}{2}}^{(3)}(c^2)\, \boldsymbol{c}\overset{0}{\circ}\boldsymbol{c}], \tag{4.57}$$

which is related to our $\langle 32m|\bar{J}|32m,000\rangle$: i.e. the highest polar and radial indices used are 2 and 3 respectively.

Using classical methods Mott-Smith (1954) derived an analytical formula for (4.56). From this formula Sirovich & Thurber have computed (to six significant figures) many blocks of these coefficients normalized with respect to $B(02;02)$. Our computed values for

$$\langle \boldsymbol{k}|\bar{J}|\boldsymbol{i},\boldsymbol{0}\rangle/\langle 020|\bar{J}|020,\boldsymbol{0}\rangle$$

agree with the tabulation of Sirovich & Thurber (1965). Mott-Smith also showed that the B-coefficients were zero unless $l_k = l_i$, which is a special case of the selection rule (4.48) for the collision matrix elements.

Kumar (1967, eq. 116) has shown that

$$\langle \boldsymbol{n}^*|\bar{J}|\boldsymbol{i},\boldsymbol{j}\rangle = 0, \langle \boldsymbol{k}|\bar{J}|\boldsymbol{0},\boldsymbol{n}^*\rangle = 0, \tag{4.58}$$

where $\boldsymbol{n}^*$ is any one of the five triplets, 000, $01m$, $(m = 0, \pm 1)$, 100. Because (4.58) implies that the modes $|\boldsymbol{n}^*\rangle$ can neither produce other modes nor be produced by them, the relations (4.58) reflect the existence of collisional invariants and the conservation of particle number, momentum and energy respectively.

In actual computation it is convenient to use a singlet label for the modes instead of the triplets $\boldsymbol{i}, \boldsymbol{j}$, etc. A systematic procedure for identifying a unique α with any $\boldsymbol{i}$ is described in Appendix A. Using this identification we can derive, from (4.58), the conservation laws that are followed by the first six modes ν_α $(\alpha = 0\text{–}5)$ in the case of the normal shock. These laws are described next.

4.5. *The conservation laws*

We now show that equations (2.28) and (2.29) automatically satisfy all the three conservation laws at any stage of truncation. For the one-dimensional shock problem these laws can be stated as

$$\frac{\partial}{\partial x}\langle \gamma|v_x|f\rangle = \langle \gamma|J|f,f\rangle = 0, \quad \gamma = 1,2,3, \tag{4.59}$$

where $\langle\gamma|$ are the first three Burnett functions in the order described in Appendix A.

Using (2.9) we rewrite the collision term in (4.59) as

$$-\langle \gamma|\delta(\boldsymbol{c}-\boldsymbol{U})|L[h]\rangle a + \langle \gamma|J[h,h] + aG[\delta,h] + aJ[h,\delta]\rangle = 0. \tag{4.60}$$

From (2.26) the first term here is

$$-a\langle \gamma|\boldsymbol{U}\rangle\langle \boldsymbol{U}|L|h\rangle = -n_1\nu_0\nu_\alpha\langle \gamma|\boldsymbol{U}\rangle\langle \boldsymbol{U}|L|\alpha\rangle; \tag{4.61}$$

and from (2.30), the rest of the terms are

$$\langle \gamma|J[h,h] + aG[\delta,h] + aJ[h,\delta]\rangle = J^\gamma_{\alpha\beta}\nu_\alpha\nu_\beta + B^\gamma_\alpha\nu_0\nu_\alpha. \tag{4.62}$$

Putting (4.61) and (4.62) in (4.59) and collecting like terms we have

$$0 = [-n_1\langle \gamma|\boldsymbol{U}\rangle\langle \boldsymbol{U}|L|\alpha\rangle + B^\gamma_\alpha]\nu_0\nu_\alpha + J^\gamma_{\alpha\beta}\nu_\alpha\nu_\beta. \tag{4.63}$$

This implies that $$(J^{\gamma}_{\alpha\beta}+J^{\gamma}_{\beta\alpha})=0, \tag{4.64}$$

which is the same as (4.58), and

$$B^1_{\alpha}=n_1\langle \boldsymbol{U}|L|\alpha\rangle, \quad B^2_{\alpha}=n_1\sqrt{3}\,\langle \boldsymbol{u}|L|\alpha\rangle, \quad B^3_{\alpha}=0. \tag{4.65}$$

The relations (4.64) and (4.65) are valid for all α and β and must hold for all molecular models incorporating elastic collisions. Therefore, the coefficients appearing in any truncated version of (4.28) and (4.29) also obviously satisfy them, and hence the corresponding solutions $\nu_{\alpha}(x;N)$ automatically satisfy the conservation laws. This feature is common to all moment expansions where the coefficients are combinations of a finite number of moments (for example, when an alternate polynomial set with the same weight is used).

We now proceed to express the conservation laws in terms of the basic unknowns in our formulation, namely the beam intensity ν_0 and the modal amplitudes ν_{α}. By using the form (2.8) of f the left-hand side of (4.59) can be written as

$$\frac{\partial}{\partial x}\langle\gamma|v_x|\,\delta(\boldsymbol{c}-\boldsymbol{U})\rangle\,\dot{a}+\frac{\partial}{\partial x}\langle\gamma|v_x|\,\alpha\rangle\langle\alpha\,|\,h\rangle=n_1\,u_1\,\langle\gamma\,|\,\boldsymbol{U}\rangle\,\dot{\nu}_0+\langle\gamma|v_x|\,\alpha\rangle\,\dot{\nu}_{\alpha}, \tag{4.66}$$

where $\langle\gamma|v_x|\,\alpha\rangle$ are given by (4.15), and the first three terms $\langle\gamma\,|\,\boldsymbol{U}\rangle$ are

$$\langle 1\,|\,\boldsymbol{U}\rangle=1, \quad \langle 2\,|\,\boldsymbol{U}\rangle=\sqrt{2}U=\sqrt{3}, \quad \langle 3\,|\,\boldsymbol{U}\rangle=0. \tag{4.67}$$

Using (4.67) and the explicit expression (4.15) in (4.66) we have

$$[S]\{\dot{\hat{\nu}}\}=0, \tag{4.68}$$

where
$$[S]=\begin{bmatrix} \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{2}} & 0 & 0 & 0 \\ \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{3}} & \sqrt{\frac{2}{3}} & 0 \\ 0 & 0 & -\sqrt{\frac{1}{3}} & \sqrt{\frac{1}{6}} & 0 & \sqrt{\frac{5}{6}} \end{bmatrix}$$

and
$$\{\hat{\nu}\}=\{\nu_0,\nu_1,\nu_2,\ldots,\nu_5\}^t. \tag{4.69}$$

Integrating (4.68) and evaluating the constants of integration from the upstream conditions,

$$[S]\{\hat{\nu}\}=\{\tfrac{1}{6},\tfrac{1}{2},0\}^t. \tag{4.70}$$

We can use (4.70) to express the amplitudes ν_2, ν_3, ν_4 in terms of ν_0, ν_1, ν_5 as follows:

$$\begin{Bmatrix}\nu_2\\ \nu_3\\ \nu_4\end{Bmatrix}=\begin{bmatrix} -\sqrt{\frac{1}{3}} & -\sqrt{\frac{1}{3}} & 0 \\ -\sqrt{\frac{2}{3}} & -\sqrt{\frac{2}{3}} & \sqrt{\frac{15}{2}} \\ -\frac{2}{\sqrt{3}} & -\frac{2}{\sqrt{3}} & \sqrt{\frac{15}{8}} \end{bmatrix}\begin{Bmatrix}\nu_0\\ \nu_1\\ \nu_5\end{Bmatrix}+\begin{Bmatrix}\sqrt{\frac{1}{3}}\\ \sqrt{\frac{2}{3}}\\ \frac{2}{\sqrt{3}}\end{Bmatrix}. \tag{4.71}$$

Thus the three equations (4.59) translate to the three linear algebraic equations (4.71) for the ν_{α}, by virtue of which three of the infinite set of differential equations (4.28) and (4.29) are redundant.

4.6. *The fluid-dynamical variables*

The Burnett functions are polynomials and hence the ν_{α} are linear combinations of the moments of the distribution function. Expressions for the fluid-dynamical variables in terms of the ν_{α} are given below (in table 1).

TABLE 1. EXPRESSIONS FOR THE FLUID-DYNAMICAL VARIABLES IN TERMS OF THE ν_α

expression in terms of the ν_α	upstream value	downstream value
density: $n = n_1 \nu_0 + \nu_1$	n_1	1
velocity: $u = u_2/n$	u_1	u_2
temperature: $T = (\frac{1}{2}n)\,[n_1(u^\sim - U)^2\nu_0 + (u^{\sim 2} + \frac{3}{2})\,\nu_1 - 2u^\sim \nu_2 - \frac{3}{2}\nu_3]\; u^\sim = u - u_2$	0	$\frac{3}{4}$
hydrostatic pressure: $p = (\frac{2}{3}n)\;T$	0	$\frac{1}{2}$
stress $\sigma_{xx} = p + \tau_{xx}$: $\sigma_{xx} = [n_1(u^\sim - U)^2\nu_0 + (u^{\sim 2} + \frac{1}{2})\,\nu_1 - 2u^\sim \nu_2 - \sqrt{\frac{1}{6}}\nu_3 + \sqrt{\frac{1}{3}}\nu_4]$	0	$\frac{1}{2}$
stress $\sigma_{yy} = p + \tau_{yy}$: $\tau_{yy} = \frac{1}{2}[\nu_1 - \sqrt{\frac{2}{3}}\nu_3 - \sqrt{\frac{1}{3}}\nu_4]$	0	$\frac{1}{2}$
heat flux: $q = \frac{1}{2}[n_1(u^\sim - U)^3\nu_0 - u^\sim(u^{\sim 2} + \frac{5}{2})\,\nu_1 + \sqrt{\frac{1}{2}}(3u^{\sim 2} + \frac{5}{2})\,\nu_2 + (\frac{5}{\sqrt{6}})\,u^\sim \nu_3 - (\frac{2}{\sqrt{3}})\,u^\sim \nu_4 - \frac{5}{2}\nu_5]$.	0	0

5. COMPUTATION OF THE COEFFICIENTS

We present in this section a brief summary of the way we compute the Clebsch–Gordan and Brody–Moshinsky coefficients as well as the radial integrals, which appear in the expressions for the basic matrix elements derived in §4. Although analytical expressions are available for all of these, their computer evaluation presents special difficulties. These difficulties are critical in the context of nonlinear kinetic theory, where some of the coefficients are required for indices much larger than in earlier work (for example the Brody–Moshinsky coefficients are needed in nuclear physics only up to $r \approx 8$, whereas we go up to $r \approx 40$). The existing methods of computing do not seem to be widely known and appreciated, and it is not unusual, in computations of this kind, to spend considerable effort in trial and error for want of appropriate algorithms. So we hope this short guide may help avoid duplication of effort.

Most of the expressions to be evaluated involve sums over terms of alternating signs, and hence there is a possibility of loss of significance by subtraction. So, as a safety measure, we have written alternative programs for all the coefficients we compute and have used double precision throughout. The expressions used, together with the associated computer programs, are available in Das (1989).

The Clebsch–Gordan coefficients are computed using an explicit formula given by Edmonds (1957, p. 45), using the scheme of Wills (1971). In this scheme the expression is recast in terms of hypergeometric polynomials expressed in nested brackets, and evaluated by Horner's rule. For large values of the polar indices the factorials in Edmonds's expression become very large, leading to overflow–underflow problems; this difficulty is avoided (Tamura 1970) by taking logarithms of the terms containing factorials (the logarithms being conveniently stored in a look-up table) and exponentiating the result before summing. However, because the sum involves terms of alternating sign, errors due to series cancellation appear for large l. Wills showed that in single precision his method fails at $l = 30$.

We have programmed Wills's method in double precision arithmetic. As even this does not guarantee immunity from series cancellation errors when the indices are sufficiently large, we have, for cross-checking the results, written an alternative program using an equivalent hypergeometric expression given by Biedenharn & Louck (1981, p. 432).

The Brody–Moshinsky coefficients are computed by the method of Dobes (1979), using Wills's approach for the hypergeometric polynomials and Tamura's technique for handling

factorials. We are thus able to compute the Brody–Moshinsky coefficients up to values of r as high as 40.

The expressions used for the Brody–Moshinsky coefficients involve the 9-j and 6-j coefficients, which are evaluated respectively by using a formula of Edmonds (1957, p. 101), and a hypergeometric expression given by Biedenharn & Louck (1981, p. 430).

Various equivalent analytical expressions are available for the radial integral $\langle rl\|c^k\|r'l'\rangle$. We use here the hypergeometric expression (4.37), which is evaluated using Horner's rule, and works well when $l = l'$, as in the present problem. However, when $l \neq l'$ the hypergeometric function can have negative integers in the denominator larger than those in the numerator. To be able to compute the integral for these cases, and to validate the results in others, a second program has been written using an alternative expression given by Exton (1978, p. 106).

Finally, the Sonine polynomials in the Burnett function are best computed using the expression (Exton 1978)

$$S_r^{(l)}(x) = [(r+s)!/s!\,r!]\,{}_1F_1[-r/(s+1);x], \tag{5.1}$$

or, alternatively, by using the recursion relation (Abramowitz & Stegun 1964, p. 782)

$$(r+1)\,S_{r+1}^{(l)}(x) = (2r+s+1-x)\,S_r^{(l)}(x) - (n+s)\,S_{r-1}^{(l)}(x) \tag{5.2}$$

with $S_0^{(l)}(x) = 1$ and $S_1^{(l)}(x) = 1+s-x$.

6. Solution of nonlinear system

6.1. *The system*

We have seen in §2.4 that retaining N terms in the expansion (2.21) results in the set of $(N+1)$ equations

$$\dot{\nu}_0 = C_\alpha \nu_0 \nu_\alpha \quad (\alpha = 1, \ldots, N), \tag{6.1}$$

$$\dot{\nu}_\alpha = P_\alpha^\gamma \nu_0 \nu_\alpha + Q_{\alpha\beta}^\gamma \nu_\alpha \nu_\beta \quad (\gamma, \alpha, \beta = 1, \ldots, N), \tag{6.2}$$

subject to the boundary conditions

$$\{\nu_\alpha(-\infty; N)\} = \{1, 0, 0, \ldots, 0\}^t,$$

$$\{\nu_\alpha(+\infty; N)\} = \{0, 1, 0, \ldots, 0\}^t \quad (\alpha = 0, 1, 2, \ldots, N). \tag{6.3}$$

The set (6.1) and (6.2) belongs to the class of generalized matrix Ricatti equations (see, for example, Kerner 1981), about which very little analytical information is available. Such equations have been encountered outside kinetic theory (for example, when the Navier–Stokes equations are Fourier-discretized), but the conditions (6.3) are unusual, as they imply that the two vectors in (6.3) are equilibrium points in the $(N+1)$-dimensional phase space corresponding to the equations (6.1) and (6.2). The solution $\nu_\alpha(x; N)$ is represented by a phase orbit that joins the cold- and hot-side equilibrium points, i.e. is heteroclinic (see, for example, Smoller 1983).

For the purpose of numerical solution the system (6.1) and (6.2) cannot be considered as an initial value problem because the data are given only at equilibrium points, where all the derivatives vanish, so one cannot numerically 'march' out of them. The problem cannot be considered as a boundary value problem either, because there are $2(N+1)$ boundary

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conditions for only $(N+1)$ equations! In the next section we discuss our method of solution in the presence of these peculiarities.

A major part of the computational effort is spent in evaluating the right-hand side of (6.1) and (6.2). Some economy can be effected by exploiting the fact that $\nu_\alpha \nu_\beta = \nu_\beta \nu_\alpha$. For example, for $N = 2$,

$$Q^2_\alpha \nu_\alpha \nu_\beta = Q_{11}\nu_1^2 + (Q_{12}+Q_{21})\nu_1\nu_2 + Q_{22}\nu_2^2$$
$$= \bar{Q}^2_\mu \sigma_\mu \quad (\mu = 1,2,3), \tag{6.4}$$

where $\sigma_\mu = \nu_{\alpha(\mu)}\nu_{\beta(\mu)}$ and $\bar{Q}$ is a (2×3) matrix. The N^2 terms corresponding to $\alpha = 1$ to N, $\beta = 1$ to N have been replaced by the $\frac{1}{2}N(N+1)$ terms corresponding to $\mu = 1$ to $\frac{1}{2}N(N+1)$. (A similar process done on the matrix $J^\gamma_{\alpha\beta}$ would result in a matrix $\bar{J}^\gamma_{\mu\cdot}$.) The latter terms have been relabelled by a single index μ. Given the $(N+1)$-vector ν_α we first evaluate the $\frac{1}{2}N(N+1)$-vector σ_μ, and premultiply it by the matrix $\bar{Q}$, which is $\frac{1}{2}N \times N(N+1)$.

6.2. *Method of solution*

The strategy we have adopted is to start close to one of the equilibrium points, say the cold side, and march in x until the hot-side equilibrium point is nearly reached, using, say, a Runge–Kutta integrator. The success of this simple method depends crucially on the topological nature of the target equilibrium point in phase space (see Arrowsmith & Place (1982) for a good discussion of phase space geometry). If the point happens to be a sink ('stable node'), then the orbits approaching it converge, any initial error is attenuated, and the method obviously succeeds. If the point is a saddle even very small initial errors grow and the orbit eventually diverges away from the equilibrium point; the situation is 'unstable' and the method fails. The topological nature of the equilibrium points easily follows from the eigenvalues of the jacobians of the equations (6.1) and (6.2) at these points. If all the eigenvalues are of the same sign, the point is a sink (or a source); it is a saddle-point otherwise.

For $N = 1$, the equations are

$$\dot{\nu}_0 = C_1 \nu_0 \nu_1, \quad \dot{\nu}_1 = P^1_1(1)\,\nu_0\nu_1, \tag{6.5}$$

where $C_1 = -3.122\,195 = -P^1_1(1)$. The solution to this set is the familiar tanh profile

$$\nu_0 = \tfrac{1}{2}[1-\tanh(\tfrac{1}{2}C_1 x)], \quad \nu_1 = \tfrac{1}{2}[1+\tanh(\tfrac{1}{2}C_1 x)]. \tag{6.6}$$

By virtue of the conservation laws $\nu_\alpha(x;1) = \nu_\alpha(x;2)\,\nu_\alpha = (x;3)$, i.e. the $N = 1$ solutions are as good as those for $N = 2$ and $N = 3$.

For $N = 4$, the hot-side equilibrium point is a sink as the jacobian there has the eigenvalues

$$\{\lambda(N)\} = \{-3.1222, -4.9120, 0, 0, 0\}^+. \tag{6.7}$$

(Notice that the zero eigenvalues are a consequence of the redundancy in the equation set owing to the conservation laws as discussed in §4.5.) We choose $\{\nu_\alpha\} = \{1-e, e, 0, 0, 0\}^+$ ($e = 10^{-8}$) as the initial condition and march forward in x.

The eigenvalues for $N = 6$ are

$$\{\lambda(N)\} = \{7.8207, 5.0460, 0.7838, 0.1369, 0, 0, 0\}^+. \tag{6.8}$$

Different initial conditions now lead to slightly different solutions, so after trial and error we retain the one that keeps the beam-intensity positive, which is physically necessary.

The solutions for $N = 1$, 4, and 6 are shown in figure 5.

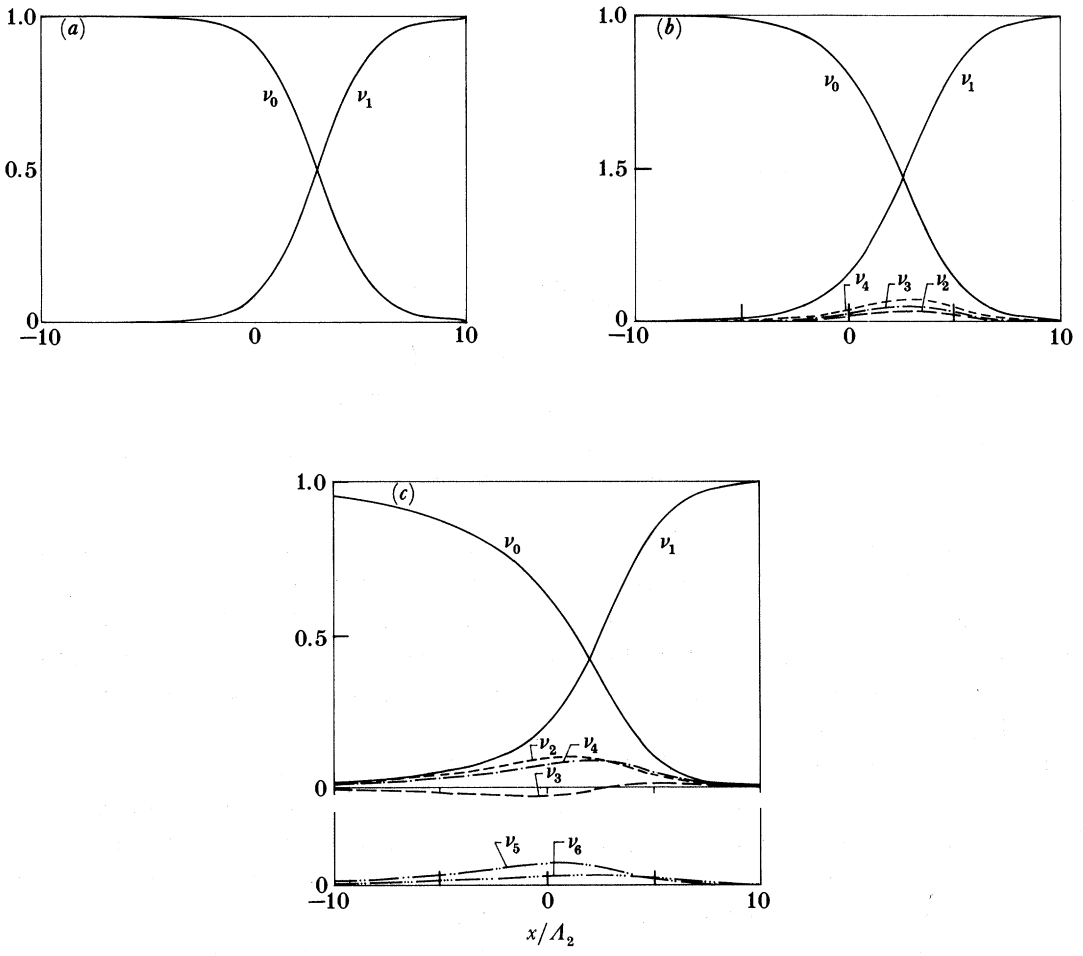

FIGURE 5. (*a*) Plots of the computed solutions with single mode. (*b*) Plots of the computed solutions with four modes. (*c*) Plots of the computed solutions with six modes.

All higher truncations (we have tried up to $N = 12$) lead to saddle-points on both sides of the shock, and hence cannot be solved by an initial value technique.

7. RESULTS AND DISCUSSION

We now discuss in turn the results obtained on the shock structure, the shock thickness and the distribution function.

7.1. *The shock structure*

The lowest-order solution $\nu_\alpha(x; 1)$ is known analytically as the tanh profile (6.6) and is identical with that suggested by Sakurai (1957) and that determined by Narasimha & Deshpande (1969) as the least-squares solution for the Mott-Smith ansatz. Figure 6 shows the number density profile with inclusion of more modes. It is seen that with six modes the profile has converged over almost the whole shock, the exception being the tail on the cold side: the present solutions (with more than one mode) show a distinct asymmetry in the form of such a tail, in contrast to the Mott-Smith solutions which are always symmetric in x. The asymmetry coefficient, which may be defined as the departure from unity of the ratio of the areas from the

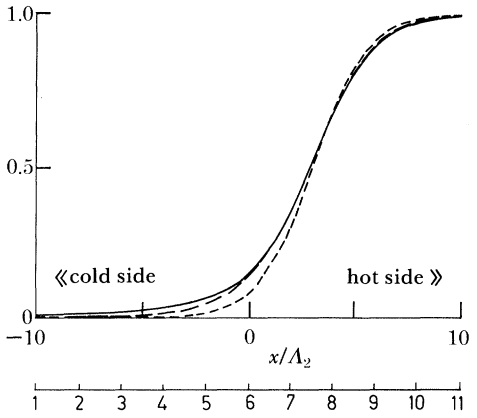

FIGURE 6. Profiles of the reduced density $\hat{n} = (n-n_1)/(n_2-n_1)$ obtained from the three computed solutions. ----------, one mode; ————, four modes; ——, six modes.

midpoint of the density profile to the respective asymptotic state on either side, is 0, 0.14 and 0.28 for one, four and six modes respectively. The tail is not as pronounced as in the BGK solutions of Liepmann *et al.* (1962), but this is understandable in the light of the analysis of Narasimha (1968), who showed that the tails are more pronounced for softer molecular potentials. We also note that with the inclusion of more modes the shock is distinctly thicker than the single-mode profile.

A Monte Carlo simulation at a Mach number of 100, kindly carried out by G. A. Bird (personal communication), leads to results 'in reasonably good agreement' with the present theory. However, an explicit comparison between the present results and Monte Carlo calculations is not given here, as (for reasons not yet understood) all Monte Carlo codes do not give the same results (D. Chapman, personal communication).

The temperature profile is shown in figure 7*a*. The cold side now has a more pronounced tail than the density profile, as seen in other solutions, but there is no sign of a temperature overshoot on the hot side, as reported, for example, by Lohn & Lundgren (1974). However, the temperature profile has not yet converged with six modes: the separation between the midpoints of the normalized density and temperature profiles is 3.2, 3.9 and 5.2 hot-side mean free paths with 1, 4 and 6 modes respectively.

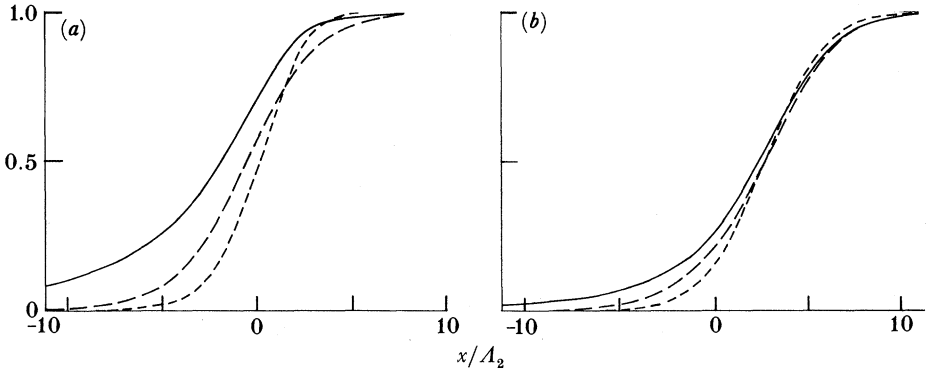

FIGURE 7. (*a*) Profiles of the normalized temperature $\hat{T} = T/T_2$. ----------, one mode; ————, four modes; ——, six modes. (*b*) Profiles of the normalized hydrostatic pressure $\hat{p} = (p-p_1)/(p_2-p_1)$. ----------, one mode; ————, four modes; ——, six modes.

The hydrostatic pressure (see figure 7*b*), which is not so sensitive as the temperature, has converged over a region close to the hot side.

The normal stress σ_{xx}, being linearly related to the velocity, provides no new information.

The deviatoric stresses τ_{xx} and τ_{yy} (figure 8) have converged only over a region on the hot side of the shock. So also the heat flux (figure 9), which shows a peak at the middle of the shock and a marked tail on the cold side.

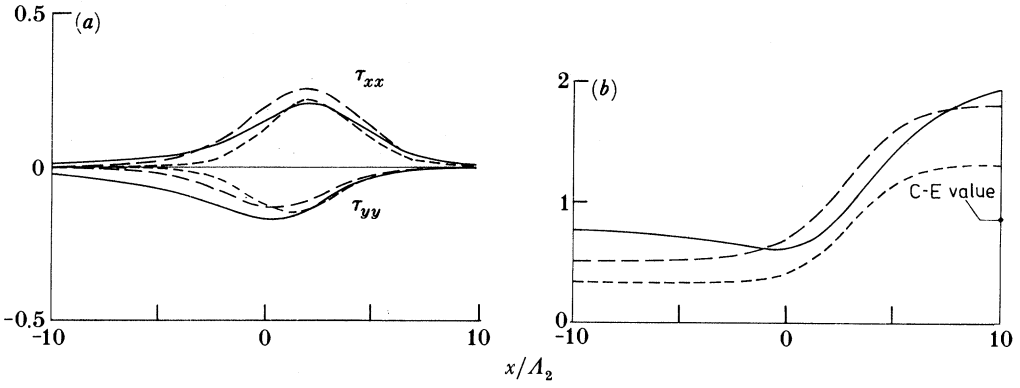

FIGURE 8. (*a*) Profiles of the stresses (positive value stands for compression). (*b*) Profiles of the effective viscosity scaled by the Chapman–Enskog value on the hot side.

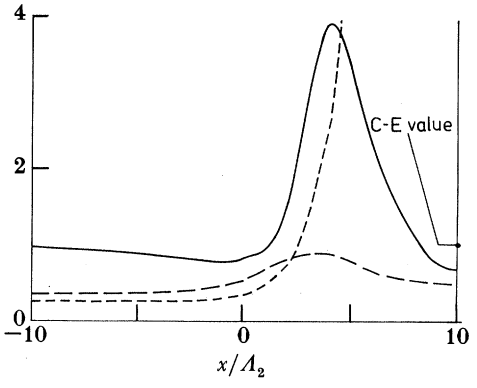

FIGURE 9. Profiles of effective heat-conductivity scaled by the Chapman–Enskog value on the hot side.

The Chapman–Enskog theory for hard-spheres gives the following expressions for the heat-conductivity and viscosity (see Chapman & Cowling 1939) in the scales chosen in §2:

$$\mu = 1.01600\,(5/16)\,[T/\pi]^{\frac{1}{2}},$$

$$k = 1.025\,13\,(75/64)\,[T/\pi]^{\frac{1}{2}}.$$

As a matter of possible interest, we show in figure 8*b* and figure 9*b* the effective viscosity and conductivity implied by the present six-mode solution. Although there is no satisfactory convergence yet in the ratio of the flux to the corresponding gradient, it is interesting that the heat conductivity from the present four- and six-mode solutions is always finite, unlike the Mott-Smith solution which makes it infinite on the hot side. Neither the conductivity nor the viscosity shows any trend of convergence towards the Chapman–Enskog values anywhere in the shock, including the hot and cold sides.

7.2. *The shock thickness*

As the number density profile has converged over the whole shock excepting the cold-side tail, the density slope shock-thickness from the present solutions is of interest. This has the value of $5.692\Lambda_2$ in the lowest-order solution, rises to $6.671\Lambda_2$ with four modes and falls to $6.662\Lambda_2$ with six modes (a rise of 18% and a fall of 2%). There is therefore reason to believe that we have a converged value of the density-slope shock thickness, of about $6.7\Lambda_2$. This value is compared with experimental determinations and other theories in figure 10 taken from Narasimha & Deshpande (1969), who showed that if the hot-side mean free path is taken as the scaling length the thickness is not very sensitive to the molecular model. The agreement with experiment can be considered good, although (because of uncertainties in the molecular model for a given gas) the hot-side mean free path cannot always be satisfactorily determined.

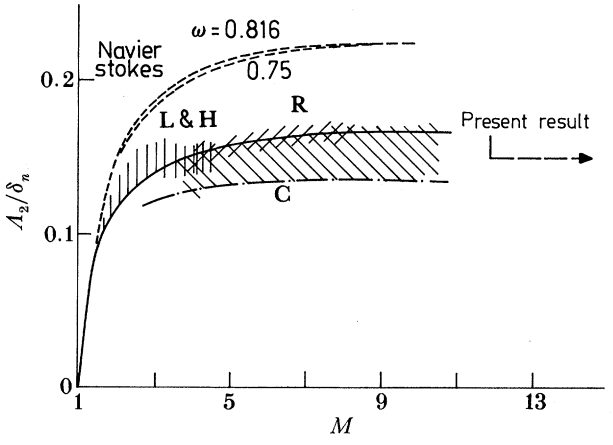

FIGURE 10. Present prediction of shock thickness compared with the experimental values and prediction by other theories; ——, minimum total error solution of Narasimha & Deshpande (1969); —·—·—, Mott-Smith v_x^2 moment value with $\omega = 0.816$ ($\mu \sim T^{\omega}$). Hatched areas represent experimental data; L & H, Linzer & Hornig (1963); C, Camac (1965); R, Russel (1965).

7.3. *The distribution function*

We finally present, in figure 11, some cross sections at $c_\perp = 0$ (component of molecular velocity perpendicular to the flow) of the distribution function at the x-stations marked 10, 7 and 4 in figure 6. At station 10, the regular part h of the distribution function coincides for all

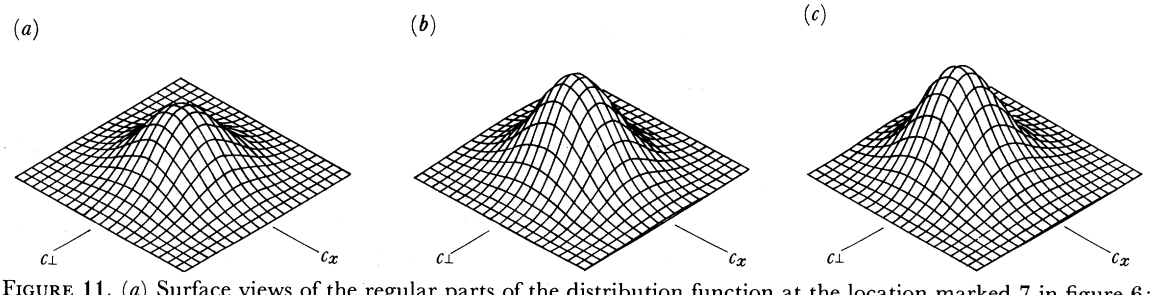

FIGURE 11. (*a*) Surface views of the regular parts of the distribution function at the location marked 7 in figure 6; single mode. (*b*) Surface views of the regular parts of the distribution function at the location marked 7 in figure 6; four modes. (*c*) Surface views of the regular parts of the distribution function at the location marked 7 in figure 6; six modes.

the three truncations (one, four and six modes). At station 7, differences are noticeable, but the regular part always resembles a maxwellian. This is clearly seen in figure 12 which shows isometric views of the 'background' distribution at this station. The deviation from the hot-side maxwellian, which has been absorbed in the polynomial expansion, remains small. At station 4, which is in the cold tail, there are small regions of velocity space where the distribution becomes slightly negative.

Contrary to previous speculation (see, for example, Grad 1969), solutions with up to six modes show no double peak in the regular part of the distribution function, hence f remains essentially bimodal.

8. Conclusion

We have endeavoured to show in this paper that a spectral technique for handling the nonlinear Boltzmann equation is entirely feasible even when the nonlinearity is extreme, provided the basis of the spectral expansion and its centre are properly chosen. A 'proper' choice appears to have been found for the infinitely strong shock, if we may go by the fact that the shock thickness with six modes is only about 17% higher than with only one mode; this may be contrasted with reported differences of +45% and −20% respectively when modifications of the Mott-Smith distribution were attempted in the earlier studies of Holway (1965) and Lohn & Lundgren (1974). Nevertheless, more conclusive evidence of the convergence of the present scheme is desirable, especially for higher moments of the distribution. This demands at the present stage more effective methods of handling high-dimensional nonlinear dynamical systems subject to the unusual boundary conditions of the shock problem.

It is expected that the powerful tools developed here for computing the collision integrals can be exploited for handling other problems in hypersonic rarefied gas dynamics, and in those involving less severe departures from equilibrium. These are now the subject of further investigation by the authors.

It needs to be emphasized that in spite of the use of the Burnett basis, the present scheme is totally different in spirit from that of the classical Burnett expansion, and not only because the centre of expansion is not local equilibrium. Thus, no constitutive relations are inherent in the present work. Table 1 shows that while the first three modal amplitudes determine density, velocity and temperature, the stresses and the heat flux involve the first four and five amplitudes respectively, and can therefore never be expressed entirely in terms of the first three (or their derivatives). Furthermore, the present work does not involve proceeding from an Euler-dominated equation of change in a first approximation as the classical Chapman–Enskog–Burnett procedure does.

Indeed, the present method is best seen as replacing the Boltzmann equation by an equivalent nonlinear dynamical system. This provides an alternative picture of molecular gas dynamics, in which inter-particle collisions are replaced by modal interactions. The modal picture has several attractive features: it replaces the infinitely many particles with a non-denumerable triple infinity in argument (namely the molecular velocity) by a denumerable triple infinity of modes. An apparent disadvantage is that when two modes interact there result (in general) an infinity of modes, whereas two colliding particles remain two after (elastic) collision. What is conserved in modal interaction is not number, but symmetry; it is for this reason that group theory plays a key role in the modal picture. At first sight the proliferation

of modes after interaction may seem disturbing, but two factors limit the proliferation: first the selection rules required for symmetry conservation, and second the rapid decrease in modal interaction coefficients for 'distant modes', which therefore do not make a significant contribution to the solution. Indeed, there is the distinct possibility that reasonable solutions may be obtained for low-order moments considering only a relatively small number of modes.

This work was begun during a visit by R.N. to the University of Strathclyde in 1971–72, its completion was helped by short visits to Caltech during 1986 and 1987. He thanks his hosts, Professor D. C. Pack and Professor D. S. Butler at Glasgow and Professor H. W. Liepmann and Professor A. Roshko at Pasadena, for their encouragement and hospitality. The authors are grateful to Professor Graeme Bird and Professor Dean Chapman for sharing with them the results of their unpublished Monte Carlo calculations.

Appendix A. Ordering of the Burnett functions

Although the Burnett functions are naturally labelled by a triplet of indices $\boldsymbol{i} = (r, l, m)$, it is convenient to associate the triplet with a unique singlet α that corresponds to the order in which we wish to include more terms in the expansion (2.22). Because it is natural to exhaust polynomials of a given degree $p = 2r + l$ before introducing those of a higher degree, we choose to order these functions first according to the value of p. For each p we suborder them in increasing l, and in m for each l from $-l$ to $+l$. In the plane shock problem we are considering the azimuthal indices m are zero owing to the symmetry around the x-axis. Table 2 indicates the correspondence for the first five indices with $m = 0$. A general expression for α, again with $m = 0$, is

$$\alpha = p + \tfrac{1}{2}\{(p+1)\,\tfrac{1}{2}(p-2) + \tfrac{1}{2}[\tfrac{1}{2}(p-1)]\,(3+(-)^{p-1})\} + [\tfrac{1}{2}l] + 1,$$

where the $[x]$ stands for the integer part of x.

Table 2. Correspondence for the first five indices with $m = 0$

triplet	degree	single index
rlm	p	—
(0 0 0)	0	1
(0 1 0)	1	2
(1 0 0)	2	3
(0 2 0)	2	4
(1 1 0)	3	5

The inverse transformation (Sirovich & Thurber 1965) is

$$p(\alpha) = 2[(-1+(4j+1))^{\frac{1}{2}}] + \tfrac{1}{2}(1+(-)^q),$$

$$r(\alpha) = -j + [\tfrac{1}{2}p]\,([\tfrac{1}{2}p]+2) + \{\tfrac{1}{2}(1+(-)^q)\}\,|\tfrac{1}{2}(p+1)|,$$

$$l(\alpha) = p(\alpha) - 2r(\alpha),$$

where

$$q(\alpha) = \tfrac{1}{2}(1+\operatorname{sgn}\{j-[\sqrt{j}]^2-[\sqrt{j}]\}), \quad j = \alpha - 1;$$

q is zero when the function is odd, and one when it is even.

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