A NUMERICAL SOLUTION OF BOLTZMANN'S EQUATION

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April, 1976

ABSTRACT

We consider the numerical solution of Boltzmann's equation for a gas model consisting of rigid spheres by means of Hilbert's expansion. If we retain only the first two terms of the expansion, Boltzmann's equation reduces to the Boltzmann-Hilbert integral equation. Successive terms in the Hilbert expansion are obtained by solving the same integral equation with a different source term. The Boltzmann-Hilbert integral equation is solved by a new very fast numerical method. The success of the method rests upon the simultaneous use of four judiciously chosen expansions; Hilbert's expansion for the distribution function, another expansion of the distribution function in terms of Hermite polynomials, the expansion of the kernel in terms of the eigenvalues and eigenfunctions of the Hilbert operator, and an expansion involved in solving a system of linear equations through a singular value decomposition.

The numerical method is applied to the study of the shock structure in one space dimension. Numerical results are presented for Mach numbers of 1.1 and 1.6.

ACKNOWLEDGMENTS

I would like to thank my dissertation advisor Professor Alexandre Chorin for his unselfish guidance, patience, and friendship. He was always willing to listen and give advice; without this support I would never have been able to complete this work.

My thanks are given to Dr. Paul Concus and Lawrence Berkeley Laboratory for the financial support and the provision of computing facilities. I would also like to thank Drs. Berni Alder and Julius Chang and Lawrence Livermore Laboratory for providing me with alternate computing facilities during the last six months of my work.

Two colleagues, friends, and co-students were invaluable during the course of my work. Michel McCoy was always available for discussions concerning the work on the dissertation as well as general philosophy. Robert Miller offered stimulating discussions on Boltzmann's equation.

I would like to thank my wife Lorraine, who typed the rough draft from my illegible notes, for her patience and encouragement; without which this dissertation would not be possible.

CONTENTS

I. INTRODUCTION

The perfect gas is characterized by the fact that the state of any of its molecules is independent of that of all the others except at the instant of collision. We can describe the gas completely by specifying the position and the velocity of every molecule at a given time. We shall restrict our attention to a gas model consisting of monatomic rigid sphere molecules with diameter σ.

Boltzmann's equation describes the evolution of the one particle distribution function $f = f(\underline{x},\underline{u},t)$, where $\underline{x}$, with components (x_1,x_2,x_3), is the position vector, $\underline{u}$, with components (u_1,u_2,u_3), is the velocity *vector, and t is time. In the case of a gas consisting of rigid spheres* it has the form

$$\mathscr{D}f \equiv \frac{\partial f}{\partial t} + (\underline{u}\cdot\underline{\nabla}_x)\, f + \frac{1}{m}\,(\underline{F}\cdot\underline{\nabla}_u)\, f = \frac{\sigma^2}{2}\iint |\underline{V}.\underline{e}|\ (f'f_1'-ff_1)d\underline{u},d\omega \qquad (I.1)$$

where m is the mass of the particle, $\underline{\nabla}_x$ denotes the gradient operator with respect to the $\underline{x}$ variables, $\underline{\nabla}_u$ denotes the gradient operator with respect to the $\underline{u}$ variables, $\underline{F}$ is the external force, $\underline{e}$ is a unit vector pointing in the direction of the solid angle element $d\omega$, $\underline{V} = \underline{u}' - \underline{u}$, a bar under a symbol denotes a vector quantity, and

$$f = f(\underline{x},\underline{u},t),$$
$$f_1 = f(\underline{x},\underline{u}_1,t),$$
$$f' = f(\underline{x},\underline{u}',t),$$
$$f_1' = f(\underline{x},\underline{u}_1',t),$$

where

$$\underline{u}' = \underline{u} + (\underline{V}\cdot\underline{e})\underline{e},$$
$$\underline{u}_1' = \underline{u}_1 - (\underline{V}\cdot\underline{e})\underline{e}.$$

$\underline{u}'$, $\underline{u}_1'$ are the velocities before collision of those rigid spheres which after collision have the velocities $\underline{u}$ and $\underline{u}_1$. For an intuitive discussion of the equation see [51] and [78], for a thorough discussion see [9], [24], [25], [33], [42], [43], [44], [45], and [51].

The average $\overline{\Phi}(\underline{x},t)$ of any property $\phi(\underline{x},\underline{u},t)$ of the flow, taken over the entire velocity space is

$$\overline{\Phi}(\underline{x},t) = \int \phi(\underline{x},\underline{u},t)f(\underline{x},\underline{u},t)d\underline{u}.$$

Some quantities of interest in the solution of equation (I.19) use the following moments of f: the density $\rho(x,t) = \overline{1}$, the mean velocity $\overline{\underline{u}}$, the pressure $P = \frac{1}{2}\ \overline{\rho v^2}$, where $\underline{v} = \underline{u}-\overline{\underline{u}}$, and the temperature $T = P/\rho\mathscr{R}$, where $\mathscr{R}$ is the universal gas constant. One other quantity that requires mention is the Boltzman H - function, defined by

$$H = \overline{\log f} = \int f(\underline{x},\underline{u},t)\ \log f(\underline{x},\underline{u},t)du.$$

In a rigid sphere gas in equilibrium, the rate at which in individual molecules collides with another molecule is given by

$$\Theta = 2\ \sqrt{2\pi}\ \sigma^2\rho C,$$

where C is the thermal velocity (defined in Chapter V) and the mean peculiar velocity is

$$\overline{C} = 2c/\sqrt{\pi}\ .$$

Maxwell's mean free path is then defined as

$$\ell = \overline{C}/\mathcal{A} = (\sqrt{2}\pi\rho\sigma^2)^{-1} .$$

The purpose of this paper is to present a fast (over 200 times faster than Chorin's method described in Chapter II) numerical algorithm for solving equation (I.1) and to apply it to the study of the structure of a shock wave in one dimension. Our method (described below) is similar to Chorin's method in that the distribution function f is assumed to be an expansion around the Maxwellian distribution function f_0; and f is expressed as an expansion in Hermite polynomials. One advantage (other than speed) of our method over Chorin's method is that it does not have the compatibility problem which arises in evaluating numerically the five-fold collision integral in (I.1), i.e. the numerical integration over velocity and angular variables. See Chapter III, section 1. Our method has no integration over angular varialbes.

The method consists of replacing f by Hilbert's expansion (defined in Chapter III) of f. This is the step which removes the angular integration. As is well known, its subsequent development leads to an ill-posed problem. As we shall show later, this ill-posedness is remedied through an appropriate algebraic procedure without changing the solution of the original problem and without losing the advantages of Hilbert's expansion. Substituting this expansion for f into equation (I.1) and retaining only the first two terms we obtain the Boltzmann-Hilbert integral equation (a Fredholm integral equation of the second kind). The unknown function in this integral equation is ϕ, where $f = f_0(1 + \phi)$. The Boltzmann-Hilbert equation is then transformed into a Fredholm integral equation of the first kind. The kernel of the later integral equation is represented by a bilinear expansion of eigenvalues and eigenfunctions of the Hilbert operator (defined in Chapter III), where the eigenfunctions of the Hilbert operator are represented by an expansion in terms of the eigenfunctions for the linearized Boltzmann collision operator for a Maxwellian gas (see Appendix A). The step-by-step procedure for solving the later integral equation is: divide the time into intervals of length Δt; assume that at time $t=n\Delta t$, where n is a nonnegative integer; f is given by an expansion in Hermite polynomials. The moments of f: the density, the mean velocity, and the temperature are then computed at $t=n\Delta t$. Our aim is to evaluate $f(\underline{x},\underline{u},(n+1)\Delta t)$ knowing $f(\underline{x},\underline{u},n\Delta t)$ and the moments at time $t=n\ t$ are used to compute the source term (see Chapter III) of the integral for ϕ at time $t=(n+1)\Delta t$. The integral equation is solved for $\phi(\underline{x},\underline{u},(n+1)\Delta t)$ by expressing it as a system of algebraic equations and solving by using singular-value decomposition and computing the corresponding pseudo-inverse. Successive terms in the Hilbert expansion can be obtained by solving the same integral equation with a different source term (which depends only upon the previous terms in the Hilbert expansion). The two expansions of f are compatable and are useful in different facets of the computation.

It is worth noting that our numerical procedure automatically guarantees that the distribution function f will be nonnegative. This follows from the definition of the Hilbert expansion.

Let N denote the number of points for each velocity component and M denote the number of points for each of the two angular variables in Chorin's quadrature scheme for evaluating the collision integral. Let LA denote the number of points in each velocity component for function evaluation of f (or f_i in our method). The operation count per space point in the evaluation of the collision integral using Chorin's method is $LA^2((6LA^2+41)M+2)MN^3$ $+2LA^2+10)$ multiplications $(LA^2((3LA^2+17)M^2N^3+LA^2+2)$ additions). The operation count using our method (given the right hand side of the Fredholm integral equation of the <u>second</u> kind) for the solution of the Fredholm integral equation of the <u>first</u> kind per space point is $LA^2(6LA^2+7)$ multiplications $(2LA^2$ additions). From the great difference in the order of magnitude of the operation count of the two methods, it can readily be seen that round off error will greatly affect Chorin's evaluation of the collision integral if the integrand is small (corresponding to small Mach numbers, for example) whereas our method does not suffer from this disadvantage.

A major disadvantage of our method is the great amount of computing time needed to generate the eigenvalues and eigenfunctions for the expansion of the kernel. See Appendix A. However, this is a one time computation and the result can thereafter be treated as given.

A partial list of applications of Boltzmann's equation includes plane Poiseuille flow [16],[17], and[94]; cylindrical Poiseuille flow [19]; Poiseuille flow in annular tubes [4]; heat transfer between parallel plates [5],[18], and[90]; heat transfer between concentric cylinders [3]; cylindrical Couette flow [20]; and shock wave structure (for a detailed discussion and list of references see Chapter V). Two other major applications are in the closure problem in turbulence, in which Boltzmann's equation serves as a model, and in combustion theory and chemical kinetics.

What follows is: In Chapter II, a brief historical survey of kinetic theory and various numerical methods; In Chapter III, a detailed discussion of the mathematical formulation of the Boltzmann-Hilbert equation and the model equation to be solved; In Chapter IV, a description of the numerical algorithm; and Chapter V, the numerical method is applied to the study of the structure of a shock wave in one space dimension, for Mach numbers of 1.1 and 1.6.

II. HISTORICAL SURVEY

1. Historical Sketch of Boltzmann's Equation

There is no intention here of describing more than a small part of the effort directed to the development of Boltzmann's equation.

The foundation of the modern theory of transport was laid by Maxwell in his memoirs of 1866 (see [65]); it is essentially this theory which Boltzmann used to make his discoveries. In 1972, Boltzmann,(see [9]), published a paper which for the first time provided a precise mathematical basis for a discussion of the approach to equilibrium. The paper dealt with the approach to equilibrium of a dilute gas and was based on an equation - Boltzmann's equation, as it is called now - for the velocity distribution function of such a gas. Boltzmann's equation still forms the basis of the kinetic theory of gases and has proved fruitful not only for classical gases Boltzmann had in mind, but also - if properly generalized - for the electron gas in a solid and the excitation gas in a superfluid.

Much of modern research in statistical mechanics is based on attempts to solve either Boltzmann's equation or similar equations for other kinds of distribution functions. Two such ways of developing transport theory are based on the solutions of Maxwell's equations or Boltzmann's equation; and these two approaches were followed by Chapman [21] and Enskog [33] respectively, the final result being essentially identical. Previously, Hilbert [53] had investigated Boltzmann's equation for the special case of rigid spheres. See Chapter III.

Hilbert's theory, except for an investigation by Boguslawski [8] of the longitudinal oscillations of a gas, the work of Pidduck [75] on self-diffusion, and the work of Pekeris et al. [71] on the computation of transport coefficients, has not been taken up by subsequent investigators. It forms the basis for this investigation.

For a more detailed historical survey of kinetic theory of gases see [3], [7], [10], [11], [12], [26], [32], [39], [47], [55], [56], [59], [60], [61], [66], [69], [79], [82], and [92].

2. Survey of Numerical Methods

The most direct method of computer simulation is the molecular dynamics technique introduced by Alder and Wainwright [1]. In this approach the evolution of a system of molecules interacting through some prescribed interparticle potential is followed in a deterministic fashion by explicitly solving the equation of motion on the computer. Reduction of computing requirements can be effected by computing the collision in a probabilistic rather than deterministic manner, and this is the basis for Monte-Carlo methods of direct simulation. See Bird [6] and Haviland [50] and [51]. Other Monte-Carlo techniques were developed by Nordsieck and Hicks [70]. Grad attempted to derive general macroscopic equations from Boltzmann's equation with the hope that the results will be valid for these phenomena with which neither Maxwell's equations of transfer nor the Chapman-Enskog theory are valid. This is the basis of Grad's thirteen moment method proposed in [42]. Also see [43], [44], [45], and [46]. Half-range approximation have been proposed by Lees in [63] . The use of the multi model procedure based on more than one Maxwellian distribution was introduced by Mott-Smith [67] . Pekeris et al (see [71]) determine the transport coefficients of viscosity, heat conduction, and diffusion. The method of solution consists of reducing the Boltzmann-Hilbert integral equation to an ordinary differential equation. Chorin's method ([24] and [25]) directly solves Boltzmann's equations where the distribution function is represented by a Hermite expansion and Gaussian quadrature is used to evaluate the five-fold collision integral.

The method of Alder and Wainwright is among the earliest numerical methods; despite its intuitive appeal, it is agonizingly slow (on the order of days in order to reach any meaningful real time). A substantial savings in computing time is achieved by the methods of Bird and Haviland. However, neither of these methods can be considered accurate. The method of Nordsieck and Hicks splits the collision integral into the gain and loss terms and evaluates each separately using Monte-Carlo quadrature.
This use of Hermite series was suggested by Grad. However, the number of polynomials is fixed and cannot be changed in the course of the computation as is allowed by Chorin's method [25] and ours. Also, since Grad's method operates in a finite dimensional polynomial space the boundary conditions are difficult to satisfy. Grad's method does not guarantee that f will be nonnegative; it is this fact which leads to the break down of the method at a Mach number of 1.65. Chorin's method has many advantages, among them: it is quite general and easily used, and it guarantees that $f \geq 0$. However, it possesses the one disadvantage common to most of the existing methods - it is quite slow.

III. MATHEMATICAL FORMULATION

1. *Introduction*

There are several major difficulties in the solution of Boltzmann's equation (I.19). The function f depends on a large number of independent variables - six plus time in the general case - so that if (I.19) is replaced by a system of algebraic equations, their number will be large. The presence of a fivefold nonlinear integral insures that the algebraic equations will not only be numerous, but also very cumbersome. One other difficulty is due to the nature of the collision term, that is, from the integration over the angular variables. If f is represented by a discrete set of values assumed on a discrete set Γ of points in phase space, the integration over $\underline{u}_1$, becomes a sum over the values assumed by f on Γ. The integration with respect to the θ and χ becomes a sum over a discrete set Φ of values θ and χ. For any reasonable choice of Γ and Φ, the argument of f' and f_1', will include points not in Γ.

Elimination of the integration over the angular variables serves two purposes; it reduces the order of the integrals to be evaluated by two and removes the problem introduced by summing over the incommensurable discrete sets Γ and Φ, thus inducing a substantial savings in computer time and an increase in accuracy.

2. Hilbert's Theory

In this section, a derivation of the Boltzmann-Hilbert integral equation is presented along with some of its properties.

Let ξ,η,ρ be the coordinates of a point on the unit sphere

$$\xi^2 + n^2 + \zeta^2 = 1. \qquad \text{(III.1)}$$

Let $\underline{e} = (\xi,\eta,\zeta)$ and $d\underline{e} = d\xi d\eta d\zeta$; define the transformation W of six variables $\underline{u},\underline{u}_1$ by

$$W = \underline{V} \cdot \underline{e} \qquad \text{(III.2)}$$

Also we define the following integral operator (collision operator)

$$Q(f,f) = \frac{\sigma^2}{2m}\iint |V\cdot e|(f'f_1' - ff_1)d\omega d\underline{u}_1 \qquad \text{(III.3)}$$

and the more general, bilinear quantity

$$Q(f,g) = \frac{\sigma^2}{4m}\iint |\underline{V}\cdot\underline{e}| \; (f'g_1' + f_1'g' - fg_1 - f_1g)d\omega d\underline{u}_1 . \qquad \text{(III.4)}$$

Clearly if $f = g$ then (III.4) reduces to (III.3); in addition,

$$Q(f,g) = Q(g,f). \qquad \text{(III.5)}$$

Introduce a small positive parameter ε (representing a scale factor) and write

$$\varepsilon \mathscr{D} f = Q(f,f). \qquad \text{(III.6)}$$

The singular nature of the perturbation procedure in the limit as ε tends to zero is emphasized by the fact that ε multiplies all the derivatives which appear in Boltzmann's equation. Consider a series expansion in powers of ε (called Hilbert's expansion, see [53])

$$f = \sum_{n=0}^{\infty} \varepsilon^n f_n . \qquad (III.7)$$

This postulates the regularity of the solution in ε. Upon substituting (III.7) into (III.6) we obtain

$$\sum_{n=1}^{\infty} \varepsilon^n \frac{\partial f_{n-1}}{\partial t} + (\underline{u}\cdot\underline{\nabla}_x)f_{n-1} + \frac{1}{m}(\underline{F}\cdot\underline{\nabla}_u)f_{n-1}) = \sum_{n=0}^{\infty} \varepsilon^n Q_n , \qquad (III.8)$$

where

$$Q_n = \sum_{k=0}^{n} Q(f_k, f_{n-k}) \quad (n \geq 0). \qquad (III.9)$$

Accordingly,

$$Q_0 = 0, \qquad (III.10)$$

$$\mathcal{D} f_{n-1} = Q_n \quad (n \geq 1). \qquad (III.11)$$

Equation (III.10) ensures that f_0 is Maxwellian, i.e.

$$\phi \equiv f_0 = a \exp \{-b((n_1-\alpha_1)^2+(u_2-\alpha_2)^2+(u_3-\alpha_3)^2)\} . \qquad (III.12)$$

Notice that ϕ satisfies

$$\phi\phi_1 = \phi'\phi_1' , \qquad (III.13)$$

using the notation of equation (I.1).

Consider the case where $n = 1$,

$$Q_1 = \mathcal{D} f_0 , \qquad (III.14)$$

or using (III.9)

$$Q(\phi, f_1) = \frac{1}{2} \mathcal{D}\phi . \qquad (III.15)$$

Write $f_1 = \psi f_0$ where ψ is a new function to be determined. With ψ

and expression (III.13) equation (III.15) assumes the form

$$\frac{\sigma^2}{4}\iint |W|\ \phi\phi_1(\psi_1'+\psi'-\psi_1-\psi)d\underline{u}_1 d\omega \quad = \frac{1}{2}\ \mathscr{D}\phi \tag{III.16}$$

If instead of $\underline{u},\underline{u}_1$ we introduce into the new expression the respective arguments

$$\underline{\alpha} + \underline{u}/\sqrt{b}, \qquad \underline{\alpha} + \underline{u}_1/\sqrt{b}$$

where $\underline{\alpha} = (\alpha_1,\alpha_2,\alpha_3)$ then the expression becomes

$$-\frac{\sigma^2}{4}\ \frac{a^2}{b^2}\mathscr{J}, \tag{III.17}$$

where

$$\mathscr{J} = \iint |W| \exp(-u^2-u_1^2)\ \ (\phi+\phi_1-\phi'-\phi_1')d\underline{u}_1 d\omega \tag{III.18}$$

when ϕ is defined by

$$\phi(\underline{u}) = \psi(\underline{\alpha}+\underline{u}/\sqrt{b}).$$

Expression (III.18) can be decomposed into singular and regular parts,

$$\mathscr{J} = k(\underline{u})\phi \ + \int K(\underline{u},\underline{u}_1)\phi_1 d\underline{u}_1 \tag{III.19}$$

and equation (III.16), which serves to determine ψ, can thus be represented as a Fredholm integral equation of the second kind, called the Boltzmann-Hilbert integral equation. Here $k(\underline{u})$ is the collision frequency of a molecule with velocity $\underline{u}$. It is bounded away from zero, i.e. $k(u) \geq k_0$.

The following derivation is due to Hilbert [53] . For other derivations see [33] , [75] , and [84] . In [3] Enskog's expression is a generalization of the form obtained by Hilbert for the special case of rigid spheres.

In order to establish equation (III.19), note that

$$\int |W| d\omega = 2\pi V,$$

where $V = \| \underline{V} \|$, $\| \cdot \|$ the Euclidean norm, and

$$\iint |W| \exp(-u^2-u_1^2)\phi d\underline{u}, d\omega = \phi e^{-u^2} \iint |W| e^{-u_1^2} d\underline{u}_1 d\omega$$
$$= 2\pi\phi e^{-u^2} \int V e^{-u_1^2} d\underline{u}_1 . \qquad \text{(III.20)}$$

Changing to polar coordinates in (III.20) we obtain

$$= 2\pi^2 \phi e^{-u^2} \left[e^{-u^2} + (2u+\frac{1}{u}) \int_0^u e^{-c^2} dc \right] \qquad \text{(III.21)}$$

$$= k(\underline{u})\phi, \qquad \text{(III.22)}$$

so that k will be a positive function which only depends on u^2.

Further, the surface integral over the unit sphere

$$\mathscr{F}^* = \iint |W| e^{-u_1^2} \phi' d\underline{u}_1 d\omega \qquad \text{(III.23)}$$

is transformed to one over the volume of the volume of the unit sphere by setting

$$\mathscr{F}^* = 3 \int_0^1 \mathscr{F}^* r^2 dr$$

and using independent orthogonal coordinates instead of r and the direction cosines. From the relation

$$r^2 dr d\omega = d\underline{e}$$

it follows that

$$\mathscr{F}^* = 3 \iint_{0 \le e^2 \le 1} \left| \frac{\underline{V} \cdot \underline{e}}{e} \right| e^{-u_1^2} \phi' du_1 d\omega \qquad \text{(III.24)}$$

where ϕ' now must be taken to be

$$\phi' = \phi(\underline{u}') = \phi(\underline{u} + \underline{e}\, W/e^2).$$

If instead of $\underline{u}_1$ we introduce new integration variables

$$\underline{\beta}_1 = (\lambda_1, \mu_1, \nu_1) = \underline{u}_1 - \underline{u}/e^2$$

in the integral $\mathscr{I}^*$, we obtain

$$\mathscr{I}^* = 3 \iint\limits_{0 \le e^2 \le 1} |\underline{\beta}_1 \cdot \underline{e}\,| (\xi^2 + \eta^2 + \zeta^2)^{7/2} \exp(-\|\underline{\beta}_1 e^2 + \underline{u}\,\|^2)\ {}^1 d\underline{\beta}_1 d\underline{e}$$

where $\|\cdot\|$ denotes the Euclidean norm, and

$$\phi' = \phi(\underline{u}_1 + \underline{e}(\underline{\beta}_1 \cdot \underline{e})).$$

Instead of $\underline{e} = (\xi, \eta, \zeta)$ we choose the new integration variable

$$\underline{\beta} = (\lambda, \mu, \nu) = \underline{e}(\underline{\beta}_1 \cdot \underline{e}).$$

In view of the fact that

$$\underline{\beta} \cdot \underline{\beta}_1 = (\underline{\beta}_1 \cdot \underline{e})^2$$

$$\beta^2 = e^2 \underline{\beta} \cdot \underline{\beta}_1$$

and the functional determinant

$$\begin{vmatrix} 2\xi\lambda_1 + \eta\mu_1 + \zeta\nu_1 & \xi\mu_1 & \xi\nu_1 \\ \eta\lambda_1 & \xi\lambda_1 + 2\eta\mu_1 + \zeta\nu_1 & \eta\nu_1 \\ \xi\lambda_1 & \zeta\mu_1 & \xi\lambda_1 + \eta\mu_1 + 2\zeta\nu_1 \end{vmatrix} = 2(\underline{\beta} \cdot \underline{\beta}_1)^{3/2}$$

we obtain

$$\mathscr{F}^* = 3\iint\limits_{0\leq\beta^2\leq\underline{\beta}\cdot\underline{\beta}} \frac{|\beta^2|^{7/2}}{(\underline{\beta}\cdot\underline{\beta}_1)^{9/2}} \exp(-\|\underline{\beta}_1\beta^2/(\underline{\beta}\cdot\underline{\beta}_1)+\underline{u}\|^2)\phi(\underline{e}+\underline{\beta})d\underline{\beta}d\underline{\beta}_1 \qquad \text{(III.26)}$$

In order to carry out the integration here with respect to β_1, we keep in mind that

$$\int(\underline{\beta}\cdot\underline{\beta}_1)^{-9/2}\exp(-\|\underline{\beta}\cdot\beta^2/(\underline{\beta}\cdot\underline{\beta}_1)+\underline{u}\|^2)d\underline{\beta}_1 \qquad \text{(III.27)}$$

is an orthogonal invariant of the two systems of variables $\underline{\beta}$ and $\underline{e}$ and consequently can only be a function of the three expressions

$$\beta^2, \quad \underline{\beta}\cdot\underline{e}, \quad e^2.$$

In order to determine this function, we take $\mu = 0$, $\nu = 0$. For $\lambda > 0$ the above integral (III.27) then becomes

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{\lambda}^{+\infty}(\lambda\lambda_1)^{-9/2}\exp\left\{-(\lambda+\xi)^2 - \left(\frac{\lambda\mu_1}{\lambda_1}+\eta\right)^2 - \left(\frac{\lambda\nu_1}{\lambda_1}+\zeta\right)^2\right\}d\lambda_1 d\mu_1 d\nu_1$$

$$= \pi\lambda^{-13/2}\exp(-(\lambda+\xi)^2\int_{\lambda}^{+\infty}\lambda_1^{-5/2}d\lambda_1$$

$$= \frac{2}{3}\pi\lambda^{-8}\exp(-(\lambda+\xi)^2)$$

and the integral (III.27) will therefore, become equal to

$$\frac{2\pi}{3\beta^8}\exp\left\{-(\underline{\beta}\cdot(\underline{\beta}+\underline{e})^2/\beta^2\right\}.$$

Accordingly, in $\mathscr{F}^*$ we introduce, in place of $\underline{\beta}$, the arguments of ϕ, namely

$$\underline{u}_1 = \underline{u} + \underline{\beta}$$

as integration variables we obtain

$$\mathscr{J}^{*} = \int K^{*}(\underline{u},\underline{u}_1)\ \phi_1 d\underline{u}_1 \tag{III.28}$$

where

$$K^{*} = \frac{2\pi}{\|\underline{u}_1-\underline{u}\|} \exp\left\{-(\underline{u}_1\cdot(\underline{u}_1-\underline{u}))^2/\|\underline{u}_1-\underline{u}\|^2\right\}. \tag{III.29}$$

We now consider the integral

$$\mathscr{J}^{**} = \iint |W| e^{-u_1^2} \phi_1' d\underline{u}_1 d\omega$$

in the same way as we just treated the integral $\mathscr{J}^{*}$. As before, we obtain

$$\mathscr{J}^{**} = 3\iint_{0\leq e^2\leq 1} |\underline{\beta}_1\cdot\underline{e}|\,|e|^7 \exp\left\{-\|\underline{\beta}_1 e^2+\underline{u}\|^2\right\}\phi_1^1 d\underline{\beta}_1 d\underline{e},$$

where now

$$\phi_1' = \phi(\underline{\beta}_1 e^2-\underline{e}(\underline{e}\cdot\underline{\beta}_1)+\underline{u}).$$

Instead of $\underline{e}$ we now choose new integration variables

$$\underline{\beta} = (\lambda,\mu,\nu) = \underline{\beta}_1 e^2-\underline{e}(\underline{e}\cdot\underline{\beta}_1).$$

In view of the fact that

$$\underline{e}\cdot\underline{\beta} = 0$$

$$\beta^2 = e^2(\underline{\beta}\cdot\underline{\beta}_1)$$

and the functional determinant, disregarding sign, becomes

$$\begin{vmatrix} \eta\mu_1+\zeta\nu_1 & \xi\mu_1-2\mu\lambda_1 & \xi\nu_1-2\zeta\lambda_1 \\ \eta\lambda_1-2\xi\mu_1 & \xi\lambda_1+\zeta\nu_1 & \eta\nu_1-2\zeta\mu_1 \\ \zeta\lambda_1-2\xi\nu_1 & \zeta\eta_1-2\eta\nu_1 & \xi\lambda_1+\eta\mu_1 \end{vmatrix} = 2(\underline{\beta}\cdot\underline{\beta}_1)(\underline{e}\cdot\underline{\beta}_1)$$

we obtain by comparison with (III.26) the result

$$\mathscr{J}^{**} = \mathscr{J}^{*}. \qquad \text{(III.30)}$$

We consider now the last term in (III.18),

$$\int |W| \exp(-u^2-u_1^2)\phi_1(u_1)d\underline{u}_1 d\omega$$
$$= 2\pi e^{-u^2} \int \| \underline{u}_1-\underline{u} \| e^{-u_1^2} \phi_1(\underline{u}_1)d\underline{u}_1. \qquad \text{(III.31)}$$

In view of (III.22), (III.28), (III.30), and (III.31) the integral expression (III.18) takes the form of (III.19), where the kernel K is defined by

$$K(\underline{u}_1\underline{u}_1) = 2\pi e^{-u^2}\left\{ V e^{-u_1^2} - \frac{2}{V} \exp\left\{ -(\underline{u}_1\cdot\underline{V})^2/V^2 \right\} \right\} \qquad \text{(III.32)}$$

where $\underline{V} = \underline{u}_1-\underline{u}$. Expression (III.32) shows that the kernel K for $\underline{u} = \underline{u}_1$ only becomes infinite from the first order and the theory of integral equations therefore becomes applicable to it.

Consider $Q_n (n\geq 1)$ and observe that the first and last terms in the sum contain f_0 (the Maxwell distribution function) and f_n, which is the n-th order coefficient in the Hilbert expression of f; the remaining terms $(1\leq k\leq n-1)$ contain *only* f_k of order less than n. If the perturbation expression is applied to Boltzmann's equation (I.19), then we solve a sequence of equations. If this sequence of equations is solved recursively, it is obvious that then n-th step f_k is known for $k\leq n-1$. Therefore,

Q_n splits into the sum

$$Q_n = 2Q(f_0,f_n) + \sum_{k=1}^{n-1} Q(f_k,f_{n-k}) \quad (n\geq 1) \tag{III.33}$$

when the second term is known at the nth step of the approximation and can be written as a source term S_n; as a consequence, the operator to be considered at each step is the linear operator $2Q(f_0,f_n)$ acting on the unknown function f_n. Write $f_n = f_0h_n$ and consider h_n as the new unknown, then we can write

$$Q_n = f_0Lh_n + S_n \quad (n\geq 1) \tag{III.34}$$

where, by definition, the linearized Boltzmann collision operator L is given by

$$Lh = 2f_0^{-1}Q(f_0,f_0h). \tag{III.35}$$

Upon substituting (III.34) into equation (III.11) we obtain

$$\mathscr{D}(f_0h_{n-1}) = f_0Lh_n + S_n \qquad (n\geq 1), \tag{III.36}$$

or

$$f_0Lh_n = \mathscr{D}(f_0h_{n-1}) - S_n \qquad (n\geq 1), \tag{III.37}$$

where $h_0 = 1$.

Accordingly, we have a sequence of equations for the unknowns. We can solve these equations step by step by noting that they have the form

$$Lh = g \tag{III.38}$$

where g is a given source term. Solving this equation amounts to inverting the operator L; this cannot be done in general because zero belongs to the spectrum of $L(\lambda = 0$ is a give fold degenerate eigenvalue and the collision invariants $\psi_\alpha(\alpha = 0,1,2,3,4)$, corresponding to the eigenfunctions $1,\underline{u},u^2$).

Introduce a Hilbert space $\mathscr{H}$ where the inner product is given by

$$(r,s) = \int f_0(\underline{\xi})r(\underline{\xi})s(\underline{\xi})d\underline{\xi}. \tag{III.39}$$

If g is an element of $\mathscr{H}$ and is orthogonal to the ψ_α, e.g.

$$(\psi_\alpha,g) = 0 , \tag{III.40}$$

then a solution h of (III.38) does exist and belongs to $\mathscr{H}$ (see the Fredholm alternative[77]). To show this consider a function g satisfying the condition in (III.40) in the subspace $\tilde{\mathscr{H}}\subset\mathscr{H}$ orthorgonal to the subspace, of $\mathscr{H}$, spanned by the five collision invariants ($\tilde{\mathscr{H}}$ is an invariant subspace for L). In $\tilde{\mathscr{H}}$, L is a self adjoint operator (see[77]); and zero is *not* in its spectrum, since there exists a constant $\delta > 0$ such that

$$-(h,Lh) \geq \delta(h,h) \tag{III.41}$$

for all h which are orthogonal to the collision invariants $\psi_\alpha, \alpha = 0,1,2,3,4$. It follows from the definition of spectrum (see [77]) that L^{-1} exists in $\mathscr{H}$ and a solution $h \in \mathscr{H}$ can be found. While $\bar{h}$ is unique in $\tilde{\mathscr{H}}$, in $\mathscr{H}$ we can add to $\bar{h}$ any linear combination of the five collision invariants (the coefficients being arbitrary) and satisfy equation (III.38).

At each step, h_n can be determined provided the five conditions in (III.40) are satisfied by the source term, however, the solution h_n is determined up to five parameters a_n^α (which depend upon time and space variables). Since the source term is constructed by means of the previous approximations, it can readily be seen that we can combine the restriction on the source term and the five unspecified coefficients cyclically in such a way that the five orthogonality conditions on the n-th source term determine the five parameters left unspecified by the (n-1)th step. The start of the cycle is possible since the zeroth-order approximation already contains the five parameters (the density, temperature, and mass velocity) of the Maxwellian distribution function f_0.

3. The Model Equation

Set $a = n(2\pi\mathscr{R}T)^{-3/2}$, $b = (2\mathscr{R}T)^{-1}$, and $\underline{\alpha} = \underline{u}_0$ ($\underline{u}_0$ some reference velocity), where $\mathscr{R}$ is the universal gas constant. Upon substitution of these quantities into (III.12) we obtain

$$f_0 = \frac{n}{(2\pi RT)^{3/2}} \exp\left(-\frac{C^2}{2\mathscr{R}T}\right) \tag{III.42}$$

where

$$\underline{C} = \underline{u}-\underline{u}_0.$$

With these definitions equation (III.14) becomes

$$\mathscr{D}f_0 = -\frac{\sigma^2 n^2}{2\pi\mathscr{R}T}\left\{m(p)e^{-2p^2}\phi(\underline{p}) + \frac{e^{-p^2}}{\pi}\int \phi(\underline{p}_1)e^{-p_1^2}\left(R-\frac{2}{R}\omega^2\right)d\underline{p}_1\right\} \tag{III.44}$$

or

$$\mathscr{D}f_0 = -\frac{\sigma^2 n^2}{2\pi\mathscr{R}T}\left\{m(p)e^{-2p^2}\phi(\underline{p}) + e^{-p^2}\mathscr{K}\phi\right\} \tag{III.44'}$$

where $\mathscr{K}$ is called the Hilbert operator, n denoted the number density, m the molecular mass, T the temperature, and

$$f = f_0(1+\phi) \text{ (for } \phi \ll 1), \quad \underline{p} = \underline{C}(2RT)^{-\frac{1}{2}} \tag{III.45}$$

$$m(p)=1+\left(2p+\frac{1}{p}\right)P(p), \quad P(p)=e^{p^2}\int_0^p e^{-x^2}dx \tag{III.46}$$

$$m(0)=2, \; \dot{m}(p)\geq 0, \; e^{-p^2}m(p)\rightarrow p/\sqrt{\pi} \text{ as } p\rightarrow\infty,$$

$$R=|\underline{p}-\underline{p}_1|, \quad \omega = \frac{pp_1\sin\theta'}{R}, \tag{III.47}$$

θ' denoting the angle between $\underline{p}$ and $\underline{p}_1$, $\phi = \phi(\underline{x},\underline{p},t)$. This equation (III.44) or (III.44) is called the Boltzmann-Hilbert integral equation, which is a Fredholm integral equation of the second kind.

A function $K(\underline{p},\underline{p}_1)$ is in $\mathscr{L}^2$ provided

$$\| K \|^2 = \iint K^2(\underline{p},\underline{p}_1)d\underline{p}\,d\underline{p}_1 = \int A^2(\underline{p})d\underline{p} = \int B^2(\underline{p}_1)d\underline{p}_1 < +\infty \qquad \text{(III.48)}$$

where

$$A(\underline{p}) = \left[\int K^2(\underline{p},\underline{p}_1)d\underline{p}_1\right]^{\frac{1}{2}}, \; B(\underline{p}_1) = \left[\int K^2(\underline{p},\underline{p}_1)d\underline{p}_1\right]^{\frac{1}{2}} . \qquad \text{(III.49)}$$

See [8].

There is a difficulty in the solution of (III.44). The kernel

$$K(\underline{p},\underline{p}_1) = R - \frac{2}{R}e^{\omega^2} \qquad \text{(III.50)}$$

has a singularity and it has been known by Pekeris [72] that $K(\underline{p},\underline{p}_1)$ is <u>not</u> in $\mathscr{L}^2$ (it can also be seen that $K(\underline{p},\underline{p}_1)$ is in $\mathscr{L}^2$ in each variable separately. See [72]. Thus the theory of Fredholm integral operator of the second kind cannot be used without change. This difficulty can be resolved as follows (see [73]): equation (III.44) may be rewritten as

$$-\frac{2\pi\mathscr{R}T}{\sigma^2\rho^2}e^{p^2}m(p)^{-\frac{1}{2}}\mathscr{D}f_0 = m(p)^{\frac{1}{2}}e^{-p^2}\phi(\underline{p}) + \frac{1}{\pi}\int\phi(\underline{p}_1)e^{-p_1^2}m(p_1)^{\frac{1}{2}}\tilde{K}(\underline{p},\underline{p}_1)d\underline{p}_1 \qquad \text{(III.51)}$$

where

$$\tilde{K}(\underline{p},\underline{p}_1) = K(\underline{p},\underline{p}_1)\Big[m(p)m(p_1)\Big]^{-\frac{1}{2}}. \qquad \text{(III.52)}$$

Write

$$\psi(\underline{p}) = m(\underline{p})^{\frac{1}{2}}e^{-p^2}\phi(\underline{p})$$

$$g(\underline{p}) = -\frac{2\pi\mathscr{R}T}{\sigma^2\rho^2}\; e^{p^2}\, m(p)^{-\frac{1}{2}}\; \mathscr{D}f_0; \tag{III.54}$$

equation (III.51) may be written in the form

$$g(\underline{p}) = \psi(\underline{p}) + \frac{1}{\pi}\int \tilde{K}(\underline{p},\underline{p}_1)\psi(\underline{p}_1)d\underline{p}_1. \tag{III.55}$$

Define the n-th iterate of the kernel $\hat{K}(\underline{p},\underline{p}_1)$ of a Fredholm integral operator, see [81], by

$$\hat{K}^{(n)}(\underline{p},\underline{p}_1) = \int \hat{K}^{(h)}(\underline{p},\underline{p}_2)\; \hat{K}^{(n-h)}(\underline{p}_2,\underline{p}_1)d\underline{p}_2 \tag{III.56}$$

$(n = 2,3,\dots\,;\ h = 1,2,\dots, n-1;\ \hat{K}^{(1)} \equiv \hat{K})$.

It has been shown by Carleman [15] that the second iterate $\tilde{K}^{(2)}$ of $\tilde{K}$ and by Dorfman [31] that the third iterate $K^{(3)}$ of K are square integrable. Hence the operator K (see equation (III.44) is of Hilbert-Schmidt type [72]. This implies in turn that the Hilbert operator is a completely continuous operator [72]. Such an operator has many nice properties: it is bounded; it has a discrete spectrum, each non-zero eigenvalue having finite multiplicity, and zero is the only limit point of the spectrum. Along with the discrete spectrum it has a complete set of square-integrable orthonormal eigenfunctions. Hecke [52] has also shown that the eigenvalues of $\mathscr{K}$ are negative.

Multiply (III.55) by $K^{(2)}(\underline{p},\underline{p}_2)$ and integrate over $\underline{p}_2$; this yields

$$\begin{aligned}\int g(\underline{p}_2)\tilde{K}^{(2)}(\underline{p},\underline{p}_2)d\underline{p}_2 &= \int \psi(\underline{p}_2)\tilde{K}^{(2)}(\underline{p},\underline{p}_2)d\underline{p}_2\\ &\quad + \frac{1}{\pi}\int \psi(\underline{p}_1)\tilde{K}(\underline{p}_2,\underline{p}_1)\tilde{K}^{(2)}(\underline{p}_1\underline{p}_2)d\underline{p}_1 d\underline{p}_2\\ &= \int \psi(\underline{p}_2)\tilde{K}^{(2)}(\underline{p},\underline{p}_2)d\underline{p}_2\\ &\quad + \frac{1}{\pi}\int \psi(\underline{p}_1)\tilde{K}^{(3)}(\underline{p},\underline{p}_1)d\underline{p}_1.\end{aligned} \tag{III.57}$$

This may be written in the form

$$\int \psi(\underline{p}_1)\left[\frac{1}{\pi}\tilde{K}^{(3)}(\underline{p},\underline{p}_1)+\tilde{K}^{(2)}(\underline{p},\underline{p}_1)\right]d\underline{p}_1 = \tilde{g}(\underline{p}) \qquad \text{(III.58)}$$

where

$$\tilde{g}(\underline{p}) = \int g(\underline{p}_2)\tilde{K}^{(2)}(\underline{p},\underline{p}_2)d\underline{p}_2. \qquad \text{(III.59)}$$

Thus we have reduced equation (III.44) to (III.58), a Fredholm integral equation of the first kind. In this transformation from (III.44) to (III.58) we have introduced one additional difficulty; the null space of the operator in (III.58) has infinite dimension, whereas the null space of the operator in (III.44) has dimension five. A detailed discussion of this increase in the null space dimension will be given in Chapter IV.

Let λ_n and ϕ_n be the eigenvalues and corresponding eigenfunctions respectively satisfying

$$\phi_n(\underline{p}) = \frac{\lambda_n}{\pi}\int \tilde{K}(\underline{p},\underline{p}_1)\ \phi_n(\underline{p}_1)d\underline{p}_1. \qquad \text{(III.60)}$$

Then since $\tilde{K}^{(2)}$ and $\tilde{K}^{(3)}$ are square integrable they may be represented by a bilinear expansion, e.g.

$$\tilde{K}^{(j)}(p,p_1) = \pi^j\sum_{n=0}^{\infty}\frac{\phi_n(p)\phi_n(p_1)}{\lambda_n{}^j} \quad (j=2,3) \qquad \text{(III.61)}$$

which converges uniformly and absolutely in $\underline{p}$ and $\underline{p}_1$ individually; and uniformly in $\underline{p}$ and $\underline{p}_1$ together. see [29] . Upon substitution of (III.61) into (III.58), one obtains

$$\tilde{g}(\underline{p}) = \int \psi(\underline{p}_1) \left\{ \sum_{n=0}^{\infty} \frac{\phi_n(\underline{p})\phi_n(\underline{p}_1)}{\lambda_n^2} \left[\frac{1}{\lambda_n} + 1 \right] \right\} d\underline{p}_1 . \qquad \text{(III.62)}$$

Higher order terms in the Hilbert expansion of f are treated in a completely analogous manner.

Equation (III.62) is the model equation that will be solved in Chapter IV.

IV. METHOD OF SOLUTION

1. Construction of Finite Linear Algebraic Equations

Consider the Hilbert expansion of f

$$f = f_0 + f_1 + f_2 + \cdots, \tag{IV.1}$$

where f_0 denotes the Maxwellian distribution; the solution f and $f_i (i = 1,2,\cdots)$ will be expressed as an expansion in Hermite polynomials $H_n(x)$ given by

$$H_n(x) = (-1)^n C_n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}, \quad C_n = (2^n n!)^{-\frac{1}{2}}$$

which are orthonormal with respect to the weight

$$W(x) = \pi^{-\frac{1}{2}} e^{-x^2}, \text{ i.e.}$$

$$\pi^{-\frac{1}{2}} \int H_n(x) H_m(x) e^{-x^2} dx = \delta_{n,m};$$

$\delta_{n,m}$ the Kronecker delta. The set $\left\{ H_n(x) \exp(-\frac{1}{2}x^2) \right\}$ is complete in $\mathscr{L}^2(\mathscr{R})$.

We choose the Hermite polynomials expansion for f because of its weight function e^{-x^2} and it simplifies the numerical computation of the moments of f. Cubic splines could also be used to approximate f with a reduction in the number of points in $\underline{u}$-space, but would make the moment computation more difficult.

The step-by-step procedure for solving the integral equation (III.62) is: divide the time into intervals each of length Δt; and assume that at time $t = n\Delta t$ f_1 (and analogously f) is given by a series

$$f_i(\underline{x},\underline{p},n\Delta t) = \pi^{-\frac{3}{2}}(S_1^n S_2^n S_3^n)^{-\frac{1}{2}} \sum_{i=0}^{M_1}\sum_{j=0}^{M_2}\sum_{h=0}^{M_3} a_{ijk}(\underline{x},t)$$

$$\cdot\, H_i(\zeta_1^n)H_j(\zeta_2^n)H_k(\zeta_3^n)\exp(-\zeta^{n}{}_1^2-\zeta^{n}{}_2^2-\zeta^{n}{}_3^2), \qquad \text{(IV.2)}$$

where $\zeta_\ell^n = (p_\ell - C_\ell^n)/S_\ell^n$, for ℓ = 1,2,3,$\underline{P}$ has components (p_1,p_2,p_3), C_ℓ^n is the center of the expansion and S_ℓ^n is the scale factor of the expansion. C_ℓ^n and S_ℓ^n will be allowed to vary with $\underline{x}$ and time. Appropriate C_ℓ^n, S_ℓ^n, M_1, M_2, and M_3 will be determined below. It will suffice to evaluate $a_{ijk}(\underline{x},t)$ at the points $x_\ell = m_\ell \Delta x_\ell$ for $\ell = 1,2,3$ where m_ℓ is an integer, Δx_ℓ a spatial increment. Our goal is to obtain $f_i(\underline{x},\underline{p},(n+1)\Delta t)$ as a series of the form (IV.2). To achieve this goal we compute the values $f_{ijk}^{n+1}(\underline{x}_m)$ of $f_i(\underline{x},\underline{p},(n+1)\Delta t)$ at the points $\underline{x}_m = (m_1\Delta x_1, m_2\Delta x_2, m_3\Delta x_3)$,

$$P_{1i} = C_1^{n+1}+S_1^{n+1}\xi_{1j}, P_{2j} = C_2^{n+1}+S^{n+1}\xi_{ij},\ P_{3k} = C_3^{n+1}+S_3^{n+1}\xi_{3k},$$

where ξ_{1i}, ξ_{2j}, ξ_{3k} are roots of $H_{N_1}(x)=0$, $H_{N_2}(x)=0$, and $H_{N_3}(x)=0$ respectively. The algorithm for evaluating $f_{ijk}^{n+1}(\underline{x}_m)$ will be described below.

Given $f_i(\underline{x},p,(n+1)\Delta t)$, the coefficients a_{ijk}^{n+1} are defined by

$$a_{ijk}^{n+1}(\underline{x}) = \pi^{-\frac{3}{2}}(S_1^{n+1}S_2^{n+1}S_3^{n+1})^{-\frac{1}{2}}\int f_1(\underline{x},\underline{p},(n+1)\Delta t)H_i(\zeta_1^{n+1})H_i(\zeta_2^{n+1})H_k(\zeta_3^{n+1})d\underline{p}$$

$$= \pi^{-\frac{3}{2}}(S_1^{n+1}S_2^{n+1}S_3^{n+1})^{-\frac{1}{2}}\int f_1(\underline{x},\underline{P},(n+1)\Delta t)H_i(\zeta_1^{n+1})H_i(\zeta_2^{n+1})H_k(\zeta_3^{n+1}) \qquad \text{(IV.3)}$$

$$\exp(\zeta_1^{n+1^2}+\zeta_2^{n+1^2}+\zeta_3^{n+1^2})\exp(-\zeta_1^{n+1^2}-\zeta_2^{n+1^2}-\zeta_3^{n+1^2})d\underline{p}. \qquad \text{(IV.4)}$$

This can be written by a change of variables as

$$\int \tilde{f}_1(\underline{x},\underline{p},(n+1)\Delta t)\exp(-\zeta_1^{n+1^2}-\zeta_2^{n+1^2}-\zeta_3^{n+1^2})d\underline{p},$$

which can be evaluated by Gauss-Hermite quadration (see [80]), using the formula

$$\int \tilde{f}_1(\underline{x},\underline{p},(n+1)\Delta t)\exp(-\zeta_1^{n+1^2}-\zeta_2^{n+1^2}-\zeta_3^{n+1^2})d\underline{p}$$

$$\approx \sum_{i=0}^{NN_1}\sum_{j=0}^{NN_2}\sum_{k=0}^{NN_3} f_1(\underline{x},\underline{\xi}_{ijk},(n+1)\Delta t)w_i w_j w_k, \qquad \text{(IV.5)}$$

where $\underline{\xi}_{ijk} = (\xi_{1i},\xi_{2j},\xi_{3k})$ are roots of $H_{NN_1}(x) = 0$, $H_{NN_2}(x) = 0$, $H_{NN_3}(x) = 0$ respectively and w_i, w_j, w_k are appropriate weights.

The kernel, defined by

$$\hat{K}(\underline{p},\underline{p}_1) = \frac{1}{\pi}\tilde{K}^{(3)}(\underline{p},\underline{p}_1) + \tilde{K}^{(2)}(\underline{p},\underline{p}_1) \qquad \text{(IV.6)}$$

of (III.62) may be evaluated by a bilinear series given by

$$\hat{K}(\underline{p},\underline{p}_1) = \sum_{n=0}^{\infty}\frac{\phi_n(\underline{p})\phi_n(\underline{p}_1)}{\lambda_n^3} + \sum_{n=0}^{\infty}\frac{\phi_n(\underline{p})\phi_n(\underline{p}_1)}{\lambda_n^2}. \qquad \text{(IV.7)}$$

We approximate $\hat{K}$ by a degenerate kernel, which we also denote by $\hat{K}$,

$$\hat{K}(\underline{p},\underline{p}_1) = \sum_{n=0}^{N^{(3)}}\frac{\phi_n(\underline{p})\phi_n(\underline{p}_1)}{\lambda_n^3} + \sum_{n=0}^{N^{(2)}}\frac{\phi_n(\underline{p})\phi_n(\underline{p}_1)}{\lambda_n^2}, \qquad \text{(IV.8)}$$

where $N^{(2)}$ and $N^{(3)}$ will be determined below. The method of computing the eigenvalues λ_n and eigenfunctions ϕ_n is described in Appendix A.

Upon substitution of (IV.8) into (III.62) we obtain

$$\tilde{g}(\underline{p}) = \int \psi(\underline{p}_1) \left\{ \sum_{n=0}^{N^{(3)}} \frac{\phi_n(\underline{p})\phi_n(\underline{p}_1)}{\lambda_n^3} + \sum_{n=0}^{N^{(2)}} \frac{\phi_n(\underline{p})\phi_n(\underline{p}_1)}{\lambda_n^2} \right\} d\underline{p}_1 . \qquad \text{(IV.9)}$$

To see that the null space of (IV.9) is infinite dimensional; let $\tilde{\psi}$ be a particular solution of the homogeneous equation

$$\int \tilde{\psi}(\underline{p}_1)\hat{K}(\underline{p},\underline{p}_1)dp_1 = 0 \ . \qquad \text{(IV.10)}$$

There exists an infinite number of nontrivial functions $\omega \epsilon \mathscr{L}^2$ satisfying $(\omega,\phi_n) = 0$, for $n = 0,1,\cdots, \max\ (N^{(2)},N^{(3)})$; i.e. ω is an element of the orthogonal complement of the subspace spanned by ϕ_i, $i = 0,1, \cdots , \max\ (N^{(2)},N^{(3)})$. Then $\tilde{\tilde{\psi}} = \tilde{\psi} + \omega$ is also a solution of (IV.10). For

$$\int \hat{K}(\underline{p},\underline{p}_1)\ (\tilde{\psi}(\underline{p}_1) + \omega(\underline{p}_1)d\underline{p}_1 = \int \hat{K}(\underline{p},\underline{p}_1)\omega(\underline{p}_1)d\underline{p}_1 \qquad \text{(IV.11)}$$

$$= \int \left\{ \sum_{n=0}^{N^{(3)}} \frac{\phi_n(\underline{p})\phi_n(\underline{p}_1)}{\lambda_n^3} + \sum_{n=0}^{N^{(2)}} \frac{\phi_n(\underline{p})\phi_n(\underline{p}_1)}{\lambda_n^2} \right\} \omega(\underline{p}_1)d\underline{p}_1 \qquad \text{(IV.12)}$$

$$= \sum_{n=0}^{N^{(3)}} \frac{\phi_n(\underline{p})}{{}^{3}_{n}} \int \phi_n(p_1)\omega(p_1)dp_1 + \sum_{n=0}^{N^{(2)}} \frac{\phi_n(\underline{p})}{\lambda_n^2} \int \phi_n(p_1)\omega(p_1)dp_1 \qquad \text{(IV.13)}$$

$$= 0.$$

The transition occurs when the function $\tilde{K}^{(2)}(\underline{p},\underline{p}_1)\psi(\underline{p}_1)$ (the first term on the *right-hand side) in (III.57) is integrated.*

Using any approximate formula for integration, we can approximately replace the integral in (III.9) by some simple form of expression not involving the integral sign.

$$\int \psi(\underline{p}_1)\ \hat{K}(\underline{p},\underline{p}_1)d\underline{p}_1 = \int \psi(\underline{p}_1)\hat{K}(\underline{p},\underline{p}_1)e^{p_1^2}e^{-p_1^2}\ d\underline{p}_1, \tag{IV.14}$$

where $\hat{K}$ is given by (IV.8), which can be evaluated by Gauss-Hermite quadrature (see [80]), i.e. using the formula

$$\int \psi(\underline{p}_1)\hat{K}(\underline{p},\underline{p}_1)e^{p_1^2}e^{-p_1^2}\ d\underline{p}_1 = \sum_{i=0}^{N_1}\sum_{j=0}^{N_2}\sum_{k=0}^{N_3} \psi(\underline{\xi}_{ijk})\ \hat{K}(\underline{p},\underline{\xi}_{ijk})e^{\xi_{ijk}^2} w_{1i}w_{2j}w_{3k} \tag{IV.15}$$

where $\underline{\xi}_{ijk} = (\xi_{ij},\xi_{2j},\xi_{3k})$ are roots of $H_{N_1}(x) = 0$, $H_{N_2}(x) = 0$, $H_{N_3}(x) = 0$ respectively, w_{ij},w_{2j},w_{3k} are weights, and $\xi_{ijk}^2 = \xi_{1i}^2 + \xi_{ij}^2 + \xi_{3k}^2$. N_1,N_2,N_3 will be determined below.

To evaluate $\mathscr{D}f_0$, where

$$\mathscr{D} = \frac{\partial}{\partial t} + (\underline{p}\cdot\underline{\nabla}_x) + \frac{1}{m}(\underline{F}\cdot\underline{\nabla}_p) \tag{IV.16}$$

we use a linear difference operator A such that Af_0^n approximates $\mathscr{D}f_0$ and A is stable. Notice that A acts on f_0 at the previous time step. See Chapter V for a particular choice.

We must exercise considerable care when imposing the boundary conditions. $f(\underline{x},\underline{p},t)$ at a boundary may be imposed only for values of $\underline{p}$ such that the vector $\underline{p}$ points form the boundary into the gas. The distribution of the velocities of the molecules coming from the fluid and striking the boundary depend on the molecular flow and cannot be imposed arbitrarily. See [24] and [44] .

To evaluate $\tilde{g}(p)$ replace $\tilde{K}^{(2)}$ in (III.59) by

$$\tilde{K}^{(2)}(\underline{p},\underline{p}_1) = \sum_{n=0}^{N^{(2)}} \frac{\phi_n(\underline{p})\phi_n(\underline{p}_1)}{\lambda_n^2} \tag{IV.17}$$

then

$$\begin{aligned}\tilde{g}(\underline{p}) &= \int g(\underline{p})\ \tilde{K}^{(2)}(\underline{p},\underline{p}_1)d\underline{p}_1 \\ &= \int g(\underline{p})\ \tilde{K}^{(2)}(\underline{p},\underline{p}_1)e^{p_1^2}e^{-p_1^2}\ d\underline{p}_1\end{aligned} \tag{IV.18}$$

which may be evaluated by Gauss-Hermite quadrature, i.e. by the formula

$$\tilde{g}(\underline{p}) = \sum_{i=0}^{N_4}\sum_{j=0}^{N_5}\sum_{k=0}^{N_6} g(\underline{\xi}'_{ijk})\ \tilde{K}^{(2)}(\underline{p},\xi_{ijk})e^{\xi_{ijk}^2}\ w'_{1i}w'_{2j}w'_{3k} \tag{IV.19}$$

where $\underline{\xi}'_{ijk} = (\xi'_{1i},\xi'_{2j},\xi'_{3k})$ are roots of $H_{N_4}(x) = 0$, $H_{N_5}(x) = 0$, $H_{N_6}(x) = 0$ respectively, $\omega'_{1i},\omega'_{2j},\omega'_{3k}$ are the weights, and $\xi'^2_{ijk} = \xi'^2_{1i} + \xi'^2_{3k}$, N_4, N_5, and N_6 will be determined below.

Combining (IV.15) and (IV.19) we obtain

$$\sum_{i=0}^{N_1}\sum_{j=0}^{N_2}\sum_{k=0}^{N_3}\psi(\underline{\xi}_{ijk})\ \hat{K}(\underline{p}_r,\underline{\xi}_{ijk})e^{\xi_{ijk}^2}\ w_{1i}w_{2j}w_{3k} = \tilde{g}(\underline{p}_r) \tag{IV.20}$$

$$r = 0,1,\cdots,N^*,$$

where $\tilde{g}(\underline{p}_r)$ is given by the right-hand side of (IV.19). This represents a system of linear algebraic equation. We can choose $N^* \geq N_1\cdot N_2\cdot N_3$. so that the matrix represented on the left-hand side of (IV.20) is rectangular (or square as a special case), of order $N^* x(N_1\cdot N_2\cdot N_3)$. This may be written in matrix notation as

$$Q\underline{\psi}^{n+1} = \underline{\tilde{g}}^n. \tag{IV.21}$$

Clearly we seek a solution of the form

$$\underline{\psi}^{n+1} = Q^{-1}\tilde{\underline{g}}^{n} \tag{IV.22}$$

However, certain practical difficulties arise. Since the null space is infinite dimensional, the columns of (IV.20) or of Q is (IV.21) are approximately linearly dependent. Q is very ill-conditioned (or overdetermined if $N^* > N_1 \cdot N_2 \cdot N_3$). For a detailed discussion of the difficulties involved see Philips [74].

If $N^* = N_1 \cdot N_2 \cdot N_3$ one possible way of dealing with this difficulty is to try to invert Q using double precision arithmetic. This method will work provided the eigenvalues of Q are less (in absolute value) than twice the machine precision.

2. Solution of the System of Equations (see [37], [41], [83], and [89]).

It is known (see [41]), that

$$Q = U\Sigma V^T \tag{IV.23}$$

where $U^TU = UU^T = VV^T = V^TV = I_n$ and $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \cdots, \sigma_n)$. The matrix U consists of the n orthonormalized eigenvectors associated with the eigenvalues of QQ^T, and the matrix V consists of the n orthonormalized eigenvectors of Q^TQ. The diagonal elements of Σ are the nonnegative square roots of the eigenvalues of Q^TQ; called the *singular values* of Q.

The use of the decomposition will be to compute the *pseudo-inverse* Q^I of Q which will be represented in the form

$$Q^I = V\Sigma^I U^T \tag{IV.24}$$

where $\Sigma^I = \mathrm{diag}(\sigma_i^I)$ and

$$\sigma_i^I = \begin{cases} 1/\sigma_i, & \text{for } \sigma_i > 0 \\ 0, & \text{for } \sigma_i = 0. \end{cases}$$

The pseudo-inverse's main value, conceptually and practically, is that it provides a solution of the least-squares problem:

> *Of all vectors $\underline{\psi}$ which minimize the sum of the squares $\|\underline{\tilde{g}} - Q\underline{\psi}\|^2$, which has the smallest $\|\underline{\psi}\|^2 = \underline{\psi}^t\underline{\psi}$?*

Let $(V,<\cdot,\cdot>)$ be an inner product space. If $E \epsilon V$, then the *orthogonal complement* $E^{\perp}$ of E is defined by $E^{\perp} = \{x \epsilon V \mid <x,y> = 0 \text{ for all } y \epsilon E\}$.

Let $\hat{\mathscr{K}}$ denote the integral operator in (III.58) and $N(\hat{\mathscr{K}})$ the null space of $\hat{\mathscr{K}}$.

In solving equation (IV.21) we want $\underline{\psi}^{n+1} \epsilon N(\hat{\mathscr{K}})^{\perp}$. The solution $\underline{\psi}^{n+1}$ constructed using the pseudo-inverse, in which the zero (or near zero) singular values have been discarded, lies in a finite dimensional subspace of $N(\hat{\mathscr{K}})^{\perp}$. The singular value decomposition method applied to the algebraic system (IV.21) yields an approximation to the integral equation (III.55). The reason is that when $\|\tilde{\underline{g}} - Q\underline{\psi}\|^2$ is minimized, the component of the solution which lies in the null space is of course zero. To see that we may write $\psi = \Psi + \omega$, where $\Psi \epsilon N(\hat{\mathscr{K}})^{\perp}$ and $\omega \epsilon N(\hat{\mathscr{K}})$, follows from the orthogonal decomposition theorem, provided $N(\hat{\mathscr{K}})$ is closed. See [77]. Since $\hat{K}$ is in $\mathscr{L}^2$, the operator $\hat{\mathscr{K}}$ is continuous (see also page 23) from which it follows that $N(\hat{\mathscr{K}})$ is closed. The null space has arisen because of the multiplication of equation (III.55) by a function (IV.17) defined on a finite dimensional subspace.

Thus, the Hilbert expansion reduces the dimensionality of the integral, and thus the amount of computational labor required, but leads to an ill-posed problem. The singular value decomposition method picks out the appropriate solution of the ill-posed problem, and thus makes the Hilbert expansion useable, allowing us to keep the dowry without the bride.

The solution is $\underline{\psi} = Q^I\tilde{\underline{g}}$. If there were only one vector $\underline{\psi}$ which minimized $\|\tilde{\underline{g}} - Q\psi\|^2$ we could save much work by using $Q^I = (Q^TQ)^{-1}Q^T$ in place of (IV.24). But if Q^TQ is (nearly) singular there will be infinitely many vectors $\underline{\psi}$ which (nearly) minimize $\|\tilde{\underline{g}} - Q\psi\|^2$ and the last formula will have to be modified in a way which takes Q's rank into account.

It should be noted that in computing σ_i^I we actually use the following definition (numerically)

$$\sigma_i^I = \begin{cases} 1/\sigma_i, & \sigma_i > \kappa \\ 0 & , \sigma_i \le \kappa \end{cases}$$

where κ is some small positive number (on the order of the machine precision). The use of the smallest singular values increases the oscillations in ψ; this increase in oscillation of ψ takes place without a meaningful decrease in $\|\tilde{\underline{g}} - Q\underline{\psi}\|$.

The process of *singular value decomposition* first uses Householder's transformation to reduce Q to bidiagonal form and then the QR algorithm to find the singular-values of the bidiagonal matrix. Both phases properly combined produce the singular-value decomposition of Q see [41] and [88].

However, the method of computing the singular-value decomposition of Q and then the pseudo-inverse Q^I is quite slow.

If $N^* = N_1 \cdot N_2 \cdot N_3$, then we can compare the method of singular-value decomposition (time wise) with the standard linear system solvers. See table I.

$\hat{K}$ is symmetric, hence the matrix Q is symmetric; another more direct and faster method of computing the pseudo-inverse Q^I exists. First Q is reduced to a tridiagonal matrix using and accumulating orthogonal similarity transformations, called Householder's algorithm for the tridiagonalization of a real symmetric matrix. Next the eigenvalues and eigenvectors of this symmetric tridiagonal matrix are computed using the QL method to compute the eigenvalues and accumulating the QL transformations to compute the eigenvectors. See [87] and [89] . The method of computing the pseudo-inverse remains unchanged.

This method is much faster than the singular-value decomposition technique discussed above, for the case in which $N^* = N_1 \cdot N_2 \cdot N_3$. See table I under the heading SYMMETRIC.

Higher order terms, $f_n (n \geq 2)$, in the Hilbert expansion are obtained in a completely analogue manner. However, in higher order terms the collision term in Boltzmann's equation must be evaluated (operating on a known function) to obtain the source term $g(\underline{p})$ for equation (III.55).

In the evaluation of the collision integral, since f_n is given in a form analogous to (IV.2), f_n is defined for all arguments $\underline{p}$ (and hence no further interpolation is required); hence we may proceed to use Gaussian quadrature. See [80] . Using this representation (IV.2) and a change of variables, the collision term can be reduced to

$$B(\underline{x},\underline{p}) \int_{-1}^{1} d\phi \int_{-1}^{1} d\chi \int d\underline{p}_1 \; \kappa(\phi_1 \chi, \underline{x}_1 \underline{p}_1) e^{-p_1^2}$$

which can be approximated by

$$Q(f_n, f_n) \simeq B(\underline{x},\underline{p}) \sum_{i=0}^{L_1} \sum_{j=0}^{L_2} \sum_{k=0}^{L_3} \sum_{\ell=0}^{L_4} \sum_{m=0}^{L_5} \kappa(\phi_\ell \, \chi_u, \underline{\xi}_{ijk})$$

$$\cdot \; w_i w_j w_h w_\ell w_m \qquad \text{(IV.25)}$$

where the ϕ_ℓ, χ_m are roots of the Legendre polynomials $P_{L_4}(x) = 0$, $P_{L_5}(x) = 0$ respectively, $\underline{\xi}_{ijk} = (\xi_{1i}, \xi_{2j}, \xi_{3k})$, $\xi_{1i}, \xi_{2j}, \xi_{3k}$ are roots of $H_{L_1}(x) = 0$, $H_{L_2}(x) = 0$, $H_{L_3}(x) = 0$ respectively, and the $w_i, w_j, w_k, w_\ell, w_m$ are the corresponding quadrature weights. See [24].

In order to apply the algorithm just described we need an initial function f^o (and its movements). We will also need a (-1)st function (and its moments) to start the calculation of Af_0^n. The choice of these initial functions will be discussed in Chapter V.

Table I. Times for Computing Q^I (in seconds)

N*	SVD	LS**	SYMMETRIC
4	0.003	0.001	0.001
5	0.005	0.002	0.001
10	0.027	0.012	0.012
15	0.083	0.028	0.033
16	0.100	0.033	0.040
20	0.184	0.058	0.069
25	0.348	0.100	0.134
30	0.587	0.160	0.225
35	0.942	0.243	0.335
36	1.052	0.258	0.352
40	1.357	0.335	0.513
45	1.960	0.460	0.668
49	2.560	0.589	0.843
50	2.757	0.618	0.886

** Wilkinson's method, consisting of Crout's method with row equilibration, column pivoting, and iterative improvement. Double precision arithmatic is used for the fundamental scalar products. The scalar product portion is in machine code. See Algorithm 135, Comm. A.C.M.-November, 1962.

V. APPLICATION TO THE STUDY OF SHOCK STRUCTURE

1. Flow in a Single Space Dimension

We consider the case of a flow in a single space dimension. Assume that f depends on a single space variable $x = x_1$ and that f is invariant under rotation in the u_2,u_3 - plane (i.e. cylindrical symmetry) where $\underline{u} = (u,u_r)$, with $u = u_1$ and $u_r = \sqrt{u_2^2 + u_3^2}$. Then we replace f in page 1 of Chapter I by

$$f(\underline{x},\underline{u},t) = f(x,u,u_r,t).$$

Under the assumption of cylindrical symmetry we obtain

$$f(x,u,u_r,t) = f(x,u,-u_r,t),$$

i.e. f is an even function of u_r. Furtherfore, we assume that there are no external forces ($\underline{F} \equiv 0$). Equations (III.54), (III.58), (III.59), and (III.62) are unchanged except for the corresponding change to the velocity vectors $\underline{p},\underline{p}_1$; i.e.

$$\underline{p} = (2RT)^{-\frac{1}{2}}\underline{u} = (p,p_r),$$

and similarly for $\underline{p}_1$. The expansion (IV.2) now becomes

$$f_1(x,p,p_r,n\Delta t) = \pi^{-3/2}\left(S_1^{n^{-\frac{1}{2}}} S_2^{n-1}\right)\sum_{i=0}^{M_1}\sum_{j=0}^{M_2} a_{ij}(x,t)H_i(\zeta^n)H_i(\zeta_r^n) \cdot \exp\left(-\zeta^{n^2}-\zeta_r^{n^2}\right) \tag{V.1}$$

where $\zeta^n = \dfrac{u-C_1^n}{S_1^n}$ and $\zeta_r^n = u/S_2^n$. A reasonable choice for C_1^n,S_1^n, and S_2^n are

$$S_1^n = S_2^n = \sqrt{2\mathcal{R}\, T^{n-1}} = S^n, \tag{V.2}$$

$$C_1 = \bar{u}^{n-1} = C^n, \tag{V.3}$$

i.e. expand at each time step around the mean velocity at the preceeding time step and use a scale determined by the temperature at the preceeding time step. This is not the only possible choice. See [25] .

Given $f_1(x,p,p_r,n\Delta t)$ we evaluate $f_1(x,p,p_r,(n+1)\Delta t)$ at the points (x_k,p_i,p_{r_j}) where $p_i = C^n + S^n\xi_{1i}$, $p_{r_j} = S^n\xi_{2j}$, where ξ_{1i} and ξ_{2j} are roots of $H_{N_1}(x) = 0$ and $H_{N_2}(x) = 0$ respectively. The coefficients $a_{ij}(x,(n+1)\Delta t)$ are given by

$$a_{ij}(x,(n+1)\Delta t) = a_{ij}^{n+1}(x) = \pi(S^{n+1})^{-1}\iint f_1(x,p,p_r,(n+1)\Delta t) \cdot H_i(\zeta^{n+1})H_j(\zeta_r^{n+1})\,dp\,dp_r. \tag{V.4}$$

Notice the $a_{ij} = 0$ for j odd (because f_1 is an even function of p_r and H_j is an odd function for j odd).

Let $x_k = k\Delta x$, k being an integer and Δx a spatial increment. Our choice of the difference operator A is given by

$$AF_{ijk}^{\,n} = \frac{F_{ijk}^{\,n} - F_{ijk}^{\,n-1}}{\Delta t} + p^n\,\frac{F_{ijk}^{\,n-1} - F_{ijk+S(p)}^{\,n-1}}{\Delta x}, \tag{V.5}$$

where

$$S(p) = \begin{cases} 1, & \text{for } p < 0, \\ -1, & \text{for } p > 0. \end{cases}$$

Despite A having only first order accuracy, at the boundaries .c ensures automatically that only relevant boundary conditions are used. For stability, we require that

$$\max_k \left| p_k \right| \frac{\Delta t}{\Delta x} < 1 \ . \qquad \text{(V.6)}$$

In computing the appropriate $g(\underline{p})$ for higher order terms of the Hilbert expansions the evaluation of (IV.24) carries over to the one spatial dimension directly.

We must consider the question of numerical stability. For the second term (f_1) in the Hilbert expansion, stability of the scheme (IV.20) is implied by the stability of A. To see this it suffices to show that $\|Q^I\|$ is uniformly bounded independent of the mesh size. We see that

$$\| Q^I \| = \| V \Sigma^I U^T \| \leq \| \Sigma^I \| \leq \max_{\substack{i \\ \sigma_i > 0}} \left| \frac{1}{\sigma_i} \right| \ .$$

We have put a bound κ on how small σ_i can become, i.e. $0 < \kappa \leq \sigma_i$. This implies that $\|Q^I\| < \kappa^{-1}$ (uniformly). However, for the higher order terms in the Hilbert expansion in which the collision integral appears in the source term, stability analysis is slightly more complicated. Stability of A would imply stability of the entire scheme if the integral of the collision term had compact support. This condition cannot be satisfied; however, $f_j (j \geq 1)$ does decay rapidly with increasing $|p|$ and $|p_r|$ and this might be considered sufficient for stability. It has been considered by Chorin [25], with the conclusion that for $M_1 \leq 3$, $M_2 \leq 3$ this is the case; where as when M_1 or M_2 is larger, the range of P and p_r over which f_j is not negligable increases, and it is necessary to truncate the support of f_j. One way of achieving this is to set $f_j = 0$ whenever $|p| \geq C_1^n + \xi\lambda S^n$, $|p_r| \geq \xi\lambda S^n$, where ξ is the largest root of $H_m(x) = 0$, $M = \max(M_1, M_2)$, and λ is a constant greater than 1. See [24].

Once the expansion (V.1) for f is known the various moments of f can be computed using the following identities

$$\pi^{-\frac{1}{2}} \int_{-\infty}^{+\infty} p^n \exp(-p^2)dp = \begin{cases} (n-1)(n-3)\cdots(1)2^{-n/2}, & n \text{ even} \\ 0 & , n \text{ odd}, \end{cases}$$

and

$$2\int_0^{\infty} p_r^{n+1} \exp(-p_r^2)dp_r = n(n-2)\cdots(2)2^{-n/2}, \ n \text{ even}.$$

Using these identities we obtain the density at time $t = n\Delta t$; it is

$$\rho^n(x) = a_{00}^n(x), \tag{V.7}$$

the mean velocity is

$$\bar{u}^n(x) = S^n(x) + 2^{-\frac{1}{2}}C^n(x)a_{10}^n(x)/\rho^n(x), \tag{V.8}$$

and the temperature is

$$T^n(x) = C^n(x)^2 \left\{\frac{3}{2}a_{00}^n(x) + 2^{-\frac{1}{2}}a_{20}^n(x) + 2^{\frac{1}{2}}a_{02}(x)\right\}/3\mathscr{R}\rho^n(x), \tag{V.9}$$

where $\mathscr{R}$ is the universal gas constant.

2. The Shock Problem

If the velocity in a particular flow field exceeds that of the local sound speed, then it is possible that a shock wave may exist in the region in which this occurs. Macroscopically a shock wave appears as a discontinuity across which there occurs measurable changes in the thermal-fluid properties. For a detailed discussion see [28], [42], and [86].

We assume that f is constant in the x_2 and x_3 directions; that we have cylindrical symmetry in the u_2,u_3 velocity plane; and there are no external forces, $\underline{F} \equiv 0$. Also we treat the shock wave in terms of a coordinate system attached to the shock, i.e. the frame of reference is moving with the velocity of the shock.

Consider a gas of rigid spheres flowing in $-\infty \leq x \leq \infty$ with

$$f(-\infty,u,u_{r,t}) = \rho_1 \pi^{-3/2} C_1^{-3} \exp\left\{-\frac{(u-v_1)^2+u_r^2}{C_1^2}\right\}, \tag{V.10}$$

$$f(+\infty,u,u_r,t) = \rho_2 \pi^{-3/2} C_2^{-3} \exp\left\{-\frac{(u-v_2)^2+u_r^2}{C_2^2}\right\}, \tag{V.11}$$

where v_1 is the upstream mass velocity, C_1 is the upstream thermal velocity, defined by

$$C_1 = \sqrt{2\mathcal{R}T_1}, \tag{V.12}$$

where T_1 is the upstream temperature, and ρ_1 is the upstream density. Analogously, v_2,ρ_2,C_2, and T_2 are the downstream terms.

The net flow of mass, momentum, and energy into the shock must be equal to the net flow of these quantities out of the shock, so we can relate the upstream and downstream values of the macroscopic variables through the Rankine-Hugoniot equations:

$$\rho_1 v_1 = \rho_2 v_2, \tag{V.13}$$

$$\rho_1(v_1^2+\tfrac{1}{2}C_1^2) = \rho_2(v_2^2+\tfrac{1}{2}C_2^2), \tag{V.14}$$

$$\rho_1 v_1(v_1^2+\tfrac{5}{2}C_1^2) = \rho_2 v_2(v_2^2+\tfrac{5}{2}C_2^2), \tag{V.15}$$

where the ratio of specific heats is $\gamma = 5/3$.

If we define the sound speed, $\hat{C}$, is the value of v_1 when $v_1 = v_2$ then the Mach number M, of the shock wave, is

$$M = \left(\frac{6}{5}\right)^{\frac{1}{2}} v_1/C_1, \tag{V.16}$$

where we used the fact that (using (V.13), (V.14), and (V.15)

$$\left(\frac{C_1}{v_1}\right)^2 = \frac{2}{5}\left(4\,\frac{v_2}{v_1} - 1\right), \tag{V.17}$$

and

$$M = \frac{v_1}{\hat{C}}, \tag{V.18}$$

by definition. It can be seen that the condition for the existence of a shock wave is $M > 1$. See [43]. Equations (V.13), (V.14), (V.15), and (V.16) may be rearranged to yield

$$\left(\frac{C_2}{C_1}\right)^2 = \frac{(M^2+3)(5M^2-1)}{16M^2} \tag{V.19}$$

and

$$\frac{v_2}{v_1} = \frac{M^2+3}{4M^2} \quad .$$

The shock thickness based on maximum variations of mean velocity is defined to be

$$X = \frac{v_2 - v_1}{\max\limits_{x}\left|\frac{d\bar{u}}{dx}\right|}, \tag{V.21}$$

See Fig. 1.

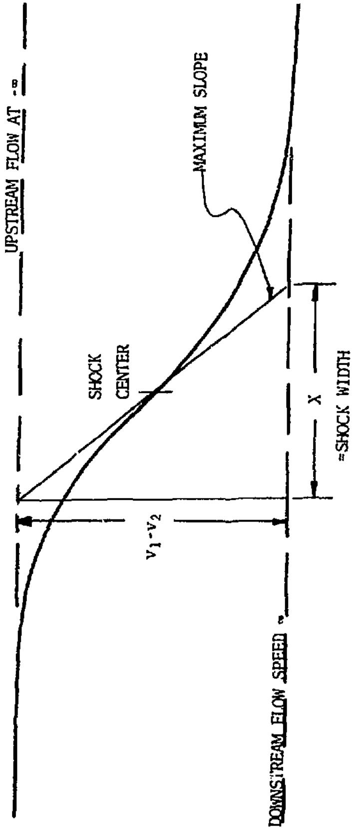

Fig. 1. Definition of shock width.

Choose $\rho_1 = 1, v_1 = 1$ then given M, equations (V.16), (V.19), and (V.20) yields C_1, ρ_2, v_2, C_2 (M completely determines the structure of the shock). Choose units so that the upstream means free path $(\sqrt{2}\pi\rho\sigma^2)^{-1}$ is one, i.e. pick $\sigma^2 = 1/\sqrt{2}\pi$.

For practical reasons we replace the region R: $-\infty \leq x \leq +\infty$ with a compact region $-\alpha \leq x \leq \alpha$, where we choose α sufficiently large that any further increase in α will have no measureable effect on the shock wave. Under this assumption the boundary conditions (V.10) and (V.11) become

$$f(-\alpha,u,u_r,t) = \rho_1\pi^{-3/2}C_1^{-3}C_1^{-3} \exp\left\{\frac{-(u-v_1)^2-u_r^2}{C_1^2}\right\}, \text{ for } u < 0 \qquad (V.22)$$

and

$$f(\alpha,u,u_r,t) = \rho_2\pi^{-3/2}C_2^{-3}\exp\left\{\frac{-(u-v_2)^2-u_r^2}{C_2^2}\right\}, \text{ for } u > 0. \qquad (V.23)$$

Divide $[-\alpha_1\alpha]$ into intervals of length Δx, where $\Delta x = 2\alpha/Nx$ where Nx is a positive integer indicating the number of intervals in which $[-\alpha_1\alpha]$ is divided.

Our goal is to obtain the steady solution as a limit, for large time, of a flow which evolves from an initial distribution $f_0 = f_0(x,u,u_r,o)$. This initial distribution function should be chosen so that the steady unit is achieved as fast as possible. It is clear that the convergence to the steady limit is inherently slow. If we use $\bar{N}$ points across the shock, and if the stability condition (V.6) is respected, it will take a minimum of $\bar{N}$ steps for the fastest particles to cross the shock. The choice of the initial distribution as well as the other numerical parameters will be discussed in the next section of this chapter.

3. Numerical Results

There remains a great many numerical parameters to be chosen: the number NTERMS of terms in the Hilbert expansion of f; the number $(M_1+1)(M_2+1)$ of terms in the Hermite expansion of f (and f_j); the size $2a$ of the region, the spatial increment Δx, the time step Δt.

The number of terms in the Hilbert expansion for this study are 2 and 3 for Mach numbers 1.1 and 1.6 respectively.

The width $2a$ of the region is chosen to be about 16 mean free paths. The spatial increment Δx is chosen small enough so that any further decrease in Δx will not affect the outcome of the calculation. The way in which this is accomplished (due to Chorin [24]) is as follows: evaluate $\frac{d\bar{u}}{dx}$ (which enters the definition of the shock thickness X) using the two formulas

$$\frac{d\bar{u}}{dx} \approx \frac{\bar{u}_{k+1}-\bar{u}_{k-1}}{2\Delta x}, \qquad (V.24)$$

and

$$\frac{d\bar{u}}{dx} \approx \frac{\bar{u}_{k+1}-\bar{u}_{k}}{\Delta x}. \qquad (V.25)$$

When they are in substantial agreement Δx can be considered small enough. We took Δx on the order of 1 mean free path. The stability condition (V.6) will give a good estimate of the appropriate value of Δt. However, we took Δt to be 0.8 times the maximum value allowed by (V.6), because higher values of Δt could give rise to an instability due to temperature overshoots. See [91] .

In the evaluation of the shock thickness X, using (V.21), the use of (V.25) will yield a more reliable estimate of the value of X, since X is a local property of the shock center and an estimate using (V.25) uses values of f in a smaller neighborhood.

In the matter of choosing these parameters, we took $M_1=M_2=M$, $NN_1=NN_2=NN$, and $N_1=N_2=N_4=N_5=N$. Clearly, we must have $M < NN$; we generally choose NN=M+1 (choosing NN much larger than M would result in information being generated and immediately discarded). The choice of $N^{(3)}$ and $N^{(2)}$ used in the bilinear expansion of the various iterates of the kernel will be discussed in Appendix A.

As our initial distribution function f^0, we choose

$$f^0 = f(x,p,p_r,0) = \begin{cases} f(-\infty,p,p_r), & x \leq 0, \\ f(+\infty,p,p_r), & x > 0, \end{cases}$$

which corresponds to a shock of zero width. However, on the finite grid that we are using, this initial distribution function corresponds to a shock of width Δx. As our (-1)-st distribution function we took f^0 also. This was not the only possibility.

No conservation is built into our scheme, so the use of the conservation laws (mass, momentum, and energy) provides a check on the accuracy of the scheme. For example, the total mass is evaluated by

$$Q_{mass} = \sum_k \rho(k\Delta x)\Delta x. \qquad (V.26)$$

Details of runs will be presented for the case where the Mach number is 1.1 and 1.6, M=5, and N=5. Other runs were made where M=N=3 and M=N=4; but these runs were poor because with our choice of center and scale given by (V.2) and (V.3) on the upstream side of the shock the $\mathscr{D}f_0$ term shows no change. The reason for this is that $p = C^n + S^n\xi$, where ξ is any root of $H_3(x) = 0$ or $H_4(x) = 0$, is such that $p \geq 0$, so then in our approximation A does not take values across the shock.

In table II we display the singular-values for the cases in which $N=5$. *In tables III and IV the relaxation from the initial data are displayed.* In table IIIa and IIIb the mean velocities are tabulated as a function of x for low values of $t/\Delta t$ and at Mach numbers of 1.6 and 1.1 respectively; this gives a qualitative picture of the behavior of our numerical scheme. In table IV the instantaneous value X^{-1} of the reciprocal of the shock thickness and the computed total mass Q_{mass} in the region of the shock are tabulated for $t/\Delta t = 1, \cdots, 10$ and Mach number 1.6. One of the most important characteristics of the relaxation to equilibrium is the lack of monotonicity and extreme slowness. The reason for this (see Chorin [24]) can be seen if we consider the equation of mass conservation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) = 0.$$

Momentum must be transfered to the boundary to allow a change in ρ, and then transported back to allow steady state convergence. It can also be observed that Q_{mass} varies a little.

In tables V the structure of a shock is displayed. The mean velocity $\bar{u}$, density ρ, temperature T, and the Boltzmann H-function divided by ρ, are given as a function of x for M=1.6 and M=1.1, t=8.278. We observe the monotonic variation of $\bar{u}$ and ρ, T exhibits a slight overshoot (see [91]), H/ρ (determined up to an additive constant) displays a dip. It should be noted that during the first four time steps $\bar{u}$ and ρ did not vary monotonically; however, after the fourth time step monotonic variation was observed. This can be explained by the fact that during the first four time steps the wave had not reached the boundary yet. Once it reached the boundary the returning wave began to enter.

In table VI we present the coefficients a_{ij} of the Hermite expansion of f for x = - 2, M = 1.6, and t = 4.967. We see that the coefficient a_{40} is not small, which contradicts Grad's assumption that all coefficients of Hermite polynomials of degree greater than 3 are zero (or negligible). The range of oscillations of X^{-1} (for 50 time steps) for a Mach number of 1.6 is 0.226 to 0.230, compared with: 0.22 to 0.24 of Chorin [24]; 0.164 of the Monte-Carlo determination by Bird [6] ; 0.222 of Gilbarg and Paolucci [40] ; and 0.238 of Ziering et al. [95] .

Finally, in table VII the timing results of our program are given for M=3,4, and 5, and compared with the time of Chorin's program COLLIDE for M=4. Both programs were run on a CDC 7600, using the same compiler.

4. Conclusions and Remarks

Clearly, as with Chorin's method, our procedure will break down for a fixed number of terms in the Hermite and Hilbert expansions, whenever the Mach number is sufficiently large; certainly by the time all the velocities $p = C^n+S^n\xi_i$, $i = 0,1,\cdots, NN$, ξ_i roots of $H_{NN}(x) = 0$, are all of the same sign. This was exhibited above for M = 3 and M = 4.

Our method has one other advantage over Chorin's and others, that is, it can deal with weak shocks. Chorin's procedure breaks down just below a Mach number of 1.2: This breakdown is due to the large number of operators that required in the computation of the collision term. For our weak shocks the changes across the shock are very small and hence is computing $f'f_1'-ff_1$ in (1.19) this difference is very small; and round off error begins to effect this difference greatly. Thus the collision time produces a great deal of noise for low Mach number. However, our procedure for weak shocks need only two terms in the Hilbert expansion and then the number of operations is quite small. Hence, round off error plays a much smaller role. Also, the Monte-Carlo techniques are not suited to low Mach numbers because the solution is near equilibrium, and the small deviations from equilibrium would be lost in the statistical fluctuations.

From the times given in table VII as well as the small storage requirements (· 90 K_8) it can readily be seen that this method is well suited to the smaller computers, provided one has the required data. See Appendix A.

One possible modification to this method (that is currently being studied) is to assume that $Q(f_i,f_j) = 0$ for terms higher than 3 ($n = 2$) in Hilbert's expansion. If this is assumed, then the program is greatly simplified as well as being tremendously speeded up. If the terms f_i,f_j are sufficiently small, then it seems reasonable to take $Q(f_i,f_j)$. However, this remains to be proved.

A more direct approach to solve (IV.21) would be to expand the distribution function directly in a series of the eigenfunctions of the integral operator. This method was considered but convergence of this series as well as the computation of the coefficients would be extremely slow. This expansion would have to be carried out for each spatial point, velocity point, and time step. Our method requires the summation of the bilinear expansion of the kernel for each velocity point once and only once. This results in a great savings of computing time.

Our method reduces Boltzmann's equation, which is an extremely complex integro-differential equation, to a Fredholm integral equation of the first kind. The resulting integral equation is much less complex and requires substantially less work to solve. The price for this savings is that the system of algebraic equations obtained from the integral equation is ill-conditioned. This system of equations is solved using the singular value decomposition technique to compute the pseudo-inverse; this technique yields the appropriate solution.

Table II. Singular Values of Q (order 25×25).

1.87745×10^{0}
7.99143×10^{-1}
8.31776×10^{-2}
5.96706×10^{-2}
5.67885×10^{-2}
2.50292×10^{-3}
1.87648×10^{-3}
9.01666×10^{-5}
1.80434×10^{-6}
3.15672×10^{-7}
6.92570×10^{-9}
1.96833×10^{-10}
4.24124×10^{-11}
3.74937×10^{-11}
9.07109×10^{-12}

Table IIIa. $\bar{u}$ as a function of x and t ($\Delta x = 2.00$, $\Delta t = 0.5518$, Mach = 1.6)

x	$t/\Delta t=1$	$t/\Delta t=3$	$t/\Delta t=6$
-8	1.000	1.000	1.000
-6	1.000	1.000	1.000
-4	1.000	1.000	0.993
-2	0.986	0.958	0.931
0	0.568	0.622	0.701
2	0.542	0.543	0.552
4	0.542	0.542	0.543
6	0.542	0.542	0.542
8	0.542	0.542	0.542

Table IIIb, $\bar{u}$ as a function of x and t ($\Delta x = 2.00$, $\Delta t = 0.5518$, Mach = 1.1)

x	t/Δt=1	t/Δt=3	t/Δt=6
-8	1.000	1.000	1.000
-6	1.000	1.000	1.000
-4	1.000	1.000	0.998
-2	0.995	0.991	0.990
0	0.873	0.875	0.878
2	0.869	0.870	0.872
4	0.869	0.869	0.870
6	0.869	0.869	0.869
8	0.869	0.869	0.869

Table IV. Relaxation to a Steady Shock ($\Delta x = 2.00$, $\Delta t = 0.5518$, Mach = 1.6)

$t/\Delta t$	X^{-1}	MASS
1	0.456	26.43
2	0.414	26.43
3	0.368	26.42
4	0.325	26.42
5	0.286	26.42
6	0.252	26.40
7	0.224	26.40
8	0.224	26.38
9	0.223	26.37
10	0.242	26.37

Table Va. Structure of a Shock (Mach = 1.6, t = 8.278)

x	$\bar{u}$	ρ	T
-8	1.00	1.00	0.47
-6	0.99	1.00	0.47
4	0.94	1.01	0.48
-2	0.82	1.12	0.51
0	0.58	1.59	0.68
2	0.56	1.78	0.74
4	0.56	1.78	0.74
6	0.54	1.84	0.72
8	0.54	1.84	0.75

Table Vb. Structure of a Shock (Mach = 1.1, $t = 8.278$)

x	$\bar{u}$	ρ	T
-8	1.00	1.00	0.99
-6	1.00	1.00	0.99
-4	0.99	1.00	0.99
-2	0.97	1.04	1.00
0	0.89	1.12	1.06
2	0.88	1.14	1.08
4	0.87	1.14	1.08
6	0.87	1.15	1.09
8	0.87	1.15	1.09

Table VI. Coefficients a_{ij} (Mach = 1.6, $\Delta x = -2$, $t = 4.967$)

j \ i	0	1	2	3	4
0	1.06	0.20	0.09	-0.09	-0.19
1	0.	0.	0.	0.	0.
2	0.08	-0.02	-0.05	0.07	0.05
3	0.	0.	0.	0.	0.
4	-0.11	-0.12	0.03	0.03	-0.03

Table VII. Time per Time Step(seconds)

M	Our Method	Chorin's Method
3	0.28	—
4	0.85	~ 240.00
5	3.00	—

APPENDIX A

Computation of Eigenvalues and Eigenvectors

The eigenvalues and eigenfunctions of the linearized Boltzmann collision operator for a Maxwellian gas have been extensively studied by Burnett [13] and [14], Mott-Smith [68], and Wang-Chang and Uhlenbeck [85]. It has been shown that the eigenfunctions are

$$\Phi_{r\ell}(\underline{p}) = N_{r\ell} P_\ell(\cos\theta) p^\ell L_r^{\ell+\frac{1}{2}}(p^2) \tag{A.1}$$

where

$$N_{r\ell} = \left[\frac{r!(\ell+\frac{1}{2})}{\pi\Gamma(\ell+r+\frac{1}{2})}\right]^{\frac{1}{2}}$$

is a normalization factor with respect to the weight e^{-p^2}, P denotes the Legendre polynomials, and L denotes the Laguerre polynomials. See [64]. Dependence on the azimuthal angle ϕ can be included by replacing $P_\ell(\cos\theta)$ by $e^{im\phi}P^m(\cos\theta)$, and the eigenvalues are independent of m.

Our goal is to obtain the eigenvalues λ_i and the eigenfunction ϕ_i satisfying the integral equation

$$\phi_i(\underline{p})e^{-p^2}m(p) = \frac{\lambda_i}{\pi}\int K(\underline{p},\underline{p}_1)e^{-p_1^2}\phi_i(\underline{p}_1)d\underline{p}_1. \tag{A.2}$$

Define

$$\psi_i(\underline{p}) = \phi_i(\underline{p})e^{-p^2}m(p)^{\frac{1}{2}}, \tag{A.3}$$

then by substitution of (A.3) into (A.2) we obtain the integral equation

$$\psi_i(\underline{p}) = \frac{\lambda_i}{\pi}\int \tilde{K}(\underline{p},\underline{p}_1)\psi_i(\underline{p}_1)d\underline{p}_1 \tag{A.4}$$

where

$$\tilde{K}(\underline{p},\underline{p}_1) = K(\underline{p},\underline{p}_1)\left[m(p)m(p_1)\right]^{-\frac{1}{2}} . \tag{A.5}$$

The integral equation (A.4) will be solved using a method introduced by Wang-Chang and Uhlenbeck [85] also by Pekeris et al. [2]; expand ψ (dropping the subscript i) in a complete set of functions $\{h_i(\underline{p})\}$, i.e.

$$\psi(\underline{p}) = \sum_{i=0}^{\infty} a_i h_i(\underline{p}) \tag{A.6}$$

following Galerkins method, in which we require that the error term be orthogonal to these functions h_i. See [27] . Upon substitution of (A.6) into (A.4) we obtain

$$\sum_{i=0}^{\infty} a_i \left[\frac{\lambda}{\pi}\int \tilde{K}(\underline{p},\underline{p}_1) h_i(\underline{p}) d\underline{p}_1 - h_i(\underline{p})\right] = 0. \tag{A.7}$$

The sum is (A.7) has to be orthogonal to each base function $h_k(\underline{p})$, thus

$$\sum_{i=0}^{\infty} a_i \left[\frac{\lambda}{\pi}\iint K(\underline{p},\underline{p}_1) h_i(\underline{p}_1) h_k(\underline{p}) d\underline{p}_1 d\underline{p} - \int h_i(\underline{p}) h_k(\underline{p}) d\underline{p}\right] = 0. \tag{A.8}$$

Equation (A.8) represents a system of linear equations, the vanishing of whose determinant yields the eigenvalues $\lambda_{r\ell}$ and the eigenvectors $\underline{a}_{r\ell}$ for the expansion in (A.8).

For this orthogonal family we choose

$$\left\{ \exp(-p^2) m(p)^{\frac{1}{2}} \, \phi_{r\ell m}(\underline{p}) \right\}$$

i.e.
$$h_{r\ell m}(\underline{p}) = \exp(-p^2) m(p)^{\frac{1}{2}} \phi_{r\ell m}(\underline{p}) \tag{A.9}$$

where $\phi_{r\ell m}$ is given by (A.1). Thus

$$\psi_{r\ell m}(\underline{p}) = \exp(im\phi) P_\ell^m(\cos\theta) \exp(-p^2) m(p)^{\frac{1}{2}} p^\ell \sum_{k=0}^{\infty} a_{r\ell k} L_k^{\ell+\frac{1}{2}}(p^2). \tag{A.10}$$

Upon the explicit substitution of (A.10) into (A.8) we obtain

$$\sum_{r',\ell'=0}^{\infty} a_{r'\ell'} \left\{ \frac{\lambda}{\pi} \iint \left(R - \frac{2}{R} e^{\omega^2} \right) \exp(-p^2 - p_1^2) \, \phi_{r'\ell'}(\underline{p}_1) \phi_{r\ell}(\underline{p}) d\underline{p}_1 d\underline{p} \right.$$

$$\left. - \int \exp(-2p^2) m(p) \phi_{r'\ell'}(\underline{p}) \phi_{r\ell}(\underline{p}) d\underline{p} \right\} = 0. \tag{A.11}$$

Here $\phi_{r\ell}$ denotes $\phi_{r\ell 0}$, for it was pointed out by Wang-Chang and Uhlenbeck [85], that when L (the linearized Boltzmann collision operator) is applied (and hence $\mathscr{K}$) to a function of the form $g(p^2) P_\ell^m(\cos\theta) e^{im\phi}$ the result is of the form $g_\ell(p^2) P_\ell^m(\cos\theta) e^{im\phi}$, where $g_\ell(p^2)$ does not depend on m.

Write the linearized collision operator L in the form (in the notation of Mott-Smith)

$$Lf = O_1 R \int_0^{2\pi} d\varepsilon (f + f_1 - f' - f_1') \tag{A.12}$$

where

$$O_1 \text{ = integral operator } \pi^{-3/2}\int e^{-p_1^2}\,dp_1 \tag{A.13}$$

$$R \text{ = integral operator } \frac{\sigma^2}{4}\int_0^{\pi} V\sin\theta d\theta \tag{A.14}$$

(for the case of rigid sphere molecules of diameter σ). Similarly, we define

$$O \text{ = integral operator } \pi^{-3/2}\int e^{-p^2}dp \tag{A.15}$$

and

$$Qf' = f+f_1-f'-f_1'. \tag{A.16}$$

We define the Chapman brackets, denoted $[r\ell m,r'\ell'm']$, by

$$[r\ell m,r'\ell'm'] = O\Phi^*_{r\ell m}L\Phi_{r'\ell'm'}. \tag{A.17}$$

As pointed out above L is independent of m. From this it follows (by orthogonality) that the Chapman brackets vanish unless $\ell = \ell'$ and $m = m'$. Furthermore, the normalized matrix elements are independent of m, i.e.

$$[r\ell m,r'\ell m]/Nr\ell m = [r\ell 0,r'\ell 0]/N_{r\ell 0}. \tag{A.18}$$

Therefore, we need only calculate $[r\ell 0,r'\ell 0]$ denoted by $[r\ell,r'\ell]$.

Using Q the expression for L given in (A.12) can be rewritten as

$$Lf = O_1R\int_0^{2\pi} Qf'd\varepsilon \tag{A.19}$$

and (A.17) becomes for $m = m' = 0$,

$$[r\ell,r'\ell] = O\Phi_{r\ell}O_1R\int_0^{2\pi} d\varepsilon Q\Phi_{r'\ell}, \tag{A.20}$$

where the conjugate sign "*" is dropped since $\Phi_{r\ell}$ is real for $m = m' = 0$. Upon substitution of the explicit form of the operators

Q and Q_L, (A.15) and (A.13) respectively, we obtain

$$[r\ell, r'\ell] = \pi^{-3}\int d\underline{p}\int d\underline{p}_1 \exp(-p^2-p_1^2)\; R\int_0^{2\pi} d\varepsilon \Big(Q\phi_{r'\ell}(\underline{p}_1)\Big)\phi_{r\ell}(\underline{p}). \qquad \text{(A.21)}$$

However, using Hilbert's representation of (A.12), we see

$$Lf = \sigma^2\left\{\pi^2 m(p)e^{-p^2}f(\underline{p}) + \pi\int K(\underline{p},\underline{p}_1)e^{-p_1^2}f(\underline{p}_1)d\underline{p}_1\right\}, \qquad \text{(A.22)}$$

where we have multiplied by 2 the contents of the { - } because we are integrating $\int_0^{\pi/2} \cdot d\theta$, R rather than $\int_0^{2} \cdot d$ in Boltzmann's equation due to Hilbert. Upon substituting (A.22) into (A.21) we obtain

$$[r\ell, r'\ell] = \sigma^2\Big\{\pi^{-2}\iint d\underline{p}d\underline{p}_1 K(\underline{p},\underline{p}_1)\exp(-p^2-p_1^2)\phi_{r'\ell}(\underline{p}_1)\phi_{r\ell}(\underline{p})$$

$$+\; \pi^{-1}\int d\underline{p}\; \exp(-2p^2)m(p)\;\; \phi_{r'\ell}(\underline{p})\phi_{r\ell}(\underline{p})\Big\}. \qquad \text{(A.23)}$$

The Chapman brackets were evaluated by Mott-Smith [68] yielding

$$[r\ell, r'\ell'] = \delta_{\ell\ell'}\;\frac{\sigma^2(2\pi)^{\frac{1}{2}}(2\ell)!}{\Gamma(\ell+\frac{3}{2})2^{r+r'+3\ell}}\sum_{n=0}^{\min(r,r')}\;\sum_{m=0}^{\ell}\frac{4^n\Gamma(\ell-m+r+r'-2n-\frac{1}{2})}{(r-n)!\,(r'-n)!\,(\ell-m)!}\,B_m^n$$

(A.24)

where

$$B_m^n = \begin{cases} 0, & m=n=0 \\ \dfrac{(m+2n+1)!}{(2n+1)!\,m!} - \dfrac{2^{m-1}(m+n+1)!}{n!\,m!}, & \text{otherwise.} \end{cases} \qquad \text{(A.25)}$$

Upon substitution of (A.23) into (A.11) we obtain

$$\sum_{r',\ell'=0}^{\infty} a_{r'\ell'}\left\{\frac{\lambda\pi}{2}\,[r\ell,r'\ell] - (\lambda+1)\int \exp(-2p^2)m(p)\Phi_{r'\ell'}(\underline{p})\Phi_{r\ell}(\underline{p})d\underline{p}\right\} = 0. \qquad (A.26)$$

We consider the integral

$$\int \exp(-2p^2)m(p)\Phi_{r'\ell}(\underline{p})\Phi_{r\ell}(\underline{p})d\underline{p}$$

which can be rewritten by changing to spherical coordinates yielding

$$\int \exp(-2p^2)m(p)\Phi_{r'\ell}(\underline{p})\Phi_{r\ell}(\underline{p})d\underline{p} = \delta_{\ell\ell'}\frac{4\pi}{(2\ell+1)}\int_0^{\infty} \exp(-2p^2)m(p)$$

$$\cdot\, p^{2\ell+2}\, L_r^{\ell+\frac{1}{2}}(p^2)L_{r'}^{\ell+\frac{1}{2}}(p^2)dp \qquad (A.27)$$

$$= -\,\delta_{\ell\ell'}\,b_{rr'}^{\ell}\ . \qquad (A.28)$$

The integral on the right in (A.27) can be evaluated numerically using the FORTRAN subroutine CADRE which uses cautious adaptive Romberg extrapolation. See [30] . Gaussian quadrature is very poor since the integrand is very oscillatory. However, this can become very expansive as r and ℓ increase.

The integral (A.27) (or (A.28)) can be written in a closed form which enables efficient numerical compuation for a large range of values of ℓ, r, and r'. The approach that will be used was suggested by K. Frankowski (private communication).

Expand $p^{\ell+\frac12}L_r^{\ell+\frac12}(p)L_{r'}^{\ell+\frac12}(p)$ a series of Hermite polynomials

$$p^{\ell+\frac12}L_r^{\ell+\frac12}(p)L_{r'}^{\ell+\frac12}(p) = \sum_j d_j H_{2j+1}(p^{\frac12}). \tag{A.29}$$

Apply the Laplace transform to both sides of (A.29),

$$\mathscr{L}\left\{p^{\ell+\frac12}L_r^{\ell+\frac12}(p)L_{r'}^{\ell+\frac12}(p)\right\}=\mathscr{L}\left\{\sum_j d_j H_{2j+1}(p^{\frac12})\right\}.$$

Let $(2n-1)!! = 1\cdot3\cdot5\cdots(2n-1)$, where $(-1)!! = 1$, and $(n)_m = n(n+1)\cdots(n+m-1)$, where $(n)_0 = 1$. Using Bateman [35], page 175 formula (35) and page 172 formula (12), we obtain

$$\mathscr{L}\left\{p^{\alpha}L_r^{\alpha}(p)L_{r'}^{\alpha}(p)L_{r'}(p)\right\} = (r!\,r'!)^{-1}\,\Gamma(r+r'+\alpha+1)\,(p-1)^{r+r'}p^{-r-r'-\alpha-1}$$
$$ {}_2F_1\left(-r,-r'\,|\,-r-r'-\alpha\,|\,\frac{p(p-2)}{(p-1)^2}\right) \tag{A.30}$$

and

$$\mathscr{L}\left\{H_{2j+1}(p^{\frac12})\right\} = \sqrt{\pi}\,2^j(2j+1)!!\,(1-p)^j p^{-j-3/2} \tag{A.31}$$

respectively.

Using the notation $(1-p)/p = q$ the transformed equation (A.29) becomes

$$(-1)^{r+r'}(r!\,r'!)^{-1}\,\Gamma(r+r'+\ell+\tfrac32)q^{r+r'+\ell}(q^{-1}+1)^{\ell}{}_2F_1(-r,-r'\,|\,-r-r'-\ell-\tfrac12\,|\,1-(q^{-1}+1)^2)$$
$$= \sqrt{\pi}\sum_j d_j 2^j(2j+1)!!\,q^j. \tag{A.32}$$

Apply formulas

$$ {}_2F_1(a,b|c|1-x) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\; {}_2F_1(a,b|a+b-c+1|x) $$

$$ + x^{c-a-b}\,\frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}\; {}_2F_1(c-a,c-b|c-a-b+1|x) \qquad (A.34) $$

and

$$ \Gamma(n\pm\tfrac{1}{2}) = \sqrt{\pi}\,(\pm1)^n\,[2^{-n}(2n-1)!!]^{\pm1}. \qquad (A.35) $$

See [61]. Expand ${}_2F_1$ in a Taylor series expansion in $(q^{-1}+1)$ and then expand the different powers of $(q^{-1}+1)$ in a Taylor series expansion in q^{-1}. Comparing coefficients of equal powers of q we obtain

$$ d_j = \frac{(-1)^{\ell}(2r+2\ell+1)!!(2r'+2\ell+1)!!}{2^{r+r'+\ell}(2\ell+1)!!r!r'!}\,\frac{(-1)^j}{2^j(2j+1)!!(r+r'+\ell-j)!} $$

$$ \times \sum_{k\geq\max\{0,(r+r'-j)/2\}}^{r} \frac{(-r)_k\,(-r')_k\,(-\ell-2k)_{r+r'+\ell-j}}{(\ell+3/2)_k k!}, \qquad (A.36) $$

$$ j = |r-r'|, |r-r'|+1, \cdots, r+r'+\ell. $$

Consider the Hermite function of order -1 defined by

$$ H_{-1}(p) \equiv -e^{p^2}\int_0^p e^{-x^2}dx . \qquad (A.37) $$

This satisfies the differential equation for Hermite polynomials

$$H''_n(p) - 2pH'_n(p) + 2nH_n(p) = 0. \tag{A.38}$$

See[61] . Using (A.37) and the recurence relation

$$2nH_{n-1}(p) = H'_n(p), \tag{A.39}$$

we define other Hermite functions $H_{-n}(p)$ for n natural. Define

$$H_{m,n} \equiv \int_0^\infty e^{-2p^2} H_m(p)H_n(p)dp, \tag{A.40}$$

for m+n even and assume that at least one of m,n is non-negative. Integrate (A.40) by parts several times, noting that $H_n(p)$ is an even (odd) function of p corresponding to n even (odd), and using the relations

$$H_n(p) + 2(n-1)H_{n-2}(p) - 2pH_{n-1}(p) = 0, \tag{A.41}$$

and

$$\left(e^{-p^2}H_n(p)\right)' + e^{-p^2}H_{n+1}(p) = 0 \tag{A.42}$$

we obtain

$$H_{m,n} = (-1)^n \int_0^\infty e^{-p^2} H_{m+n}(p)dp = (-1)^n H_{m+n,0}. \tag{A.43}$$

Using (A.41) along with setting m+n=2k we define

$$T_k = \int_0^\infty e^{-2p^2} H_{2k}(p)dp = \int_0^\infty e^{-p^2} d\left(e^{-p^2} H_{2k-1}(p)\right) = \int_0^\infty e^{-p^2} H_{2k-1}(p)\left(-2pe^{-p^2}\right)dp$$

$$= -\int_0^\infty e^{-2p^2}\left(H_{2k}(p) + 2(2k-1)H_{2k-2}(p)\right) dp.$$

This yields the recurence relation $T_k = (1-2k)T_{k-1}$ from which we obtain

$$T_k = \begin{cases} (-1)^k(2k-1)!!\ T_0, & k \geq 0 \\ [(2k-1)!!]^{-1}\ T_0, & k \leq 0 \end{cases} \tag{A.44}$$

where $T_0 = \sqrt{\frac{\pi}{8}}$. Using (A.35) we obtain

$$\int_0^\infty e^{-2p^2} H_{2k}(p)dp = 2^{-\frac{3}{2}}(-2)^k \Gamma(k+\tfrac{1}{2}) \, . \tag{A.45}$$

Using (A.40), (A.43), and Bateman [36] page 289 formula (10) we obtain

$$\int_0^\infty e^{-2p^2} H_m(p)H_n(p)dp = (-1)^{(m+n)/2} 2^{(m+n-3)/2} \Gamma\left(\frac{m+n+1}{2}\right). \tag{A.46}$$

where m+n is even and atleast one of m,n is nonnegative.

Considering the case inwhich $n = -3$ and $m = 2i + 1$ we obtain

$$\int_0^\infty e^{-2p^2} H_{-3}(p) \, H_{2j+1}(p)dp = (-1)^j \, 2^{-\frac{3}{2}} \frac{(2j-1)!!}{2j-1} \sqrt{\pi} \, . \tag{A.47}$$

It can readily be seen, using (III.46), that

$$pm(p) = - 4 \, H_{-3}(p). \tag{A.48}$$

As a result

$$b_{rr'}^{\ell} = \frac{16\pi}{2\ell+1} \sum_j d_j \int_0^\infty e^{-2p^2} H_{-3}(p) H_{2j+1}(p)dp.$$

Upon substitution of (A.36) for d_i we obtain

$$b_{rr'}^{\ell} = \frac{(2\pi)^{\frac{3}{2}}(-1)^{\ell}(2r+2\ell+1)!!(2r'+2\ell+1)!!}{(2\ell+1)2^{r+r'+\ell+1}(2\ell+1)!!r!r'!} \sum_{j=r'-r}^{r+r'+\ell} \left(2^{j-1}(4j^2-1)(r+r'+\ell-j)\right)^{-1}$$
$$\sum_{k\geq\max\{0,(r+r'-j)/2\}}^{r} \frac{(-r)_k(-r')_k(-\ell-2k)_{r+r'+\ell-j}}{(\ell+3/2)_k \, k!} \, . \tag{A.49}$$

Next interchange the order of summation in (A.49) and consider the term

$$\mathscr{T}_k = \sum_j \frac{(-\ell-2k)_{r+r'+\ell-j}}{2^{i-1}(2j+1)(2j+1)(r+r'+\ell-j)!} \qquad \text{(A.50)}$$

Let $r+r'+1-i=\alpha$, from which (A.50) becomes

$$\mathscr{T}_k = \sum_{s=0}^{\ell+2k} \frac{(-\ell-2k)_\alpha \; 2^\alpha}{2^{r+r'+\ell+1}(r+r'+\ell-\alpha-\frac{1}{2})(r+r'+\ell-\alpha+\frac{1}{2})}. \qquad \text{(A.51)}$$

$$= \left[2^{r+r'+\ell+1}(r+r'+\ell-\tfrac{1}{2})_2\right]^{-1} {}_2F_1(-\ell-2k,-r-r'-\ell-\tfrac{1}{2} \;|{-r}-r'-\ell+\tfrac{3}{2}|\,2).$$

(A.52)

Using Bateman [34] page 109 formula (3) for analytic continuation of hypergeometric functions, and explicitly writing the representation (-)!! we obtain

$$b^{\ell}_{rr'} = \frac{(2\pi)^{3/2}\;(\frac{3}{2})_{r'+\ell}}{(2\ell+1)2^{r+r'+\ell+1}} \sum_{k=0}^{r} \frac{(-\ell-r-\frac{1}{2})_k(-1)^k}{k!(r-k)!(r'-r+k)!} \sum_{\alpha=0}^{\ell+2r-2k} \frac{(-\ell-2r+2k)_\alpha(-1)^\alpha(\alpha+1)}{(r'-r+2k-\frac{1}{2})_{\alpha+2}}$$

(A.53)

which can be written in a more convenient form for numerical computation

$$b^{\ell}_{rr'} = A\sum_{k=0}^{r}\tau_k \sum_{\alpha=0}^{\ell+2r-2k} (\alpha+1)\sigma_{\alpha k}, \qquad \text{(A.54)}$$

where

$$A = \frac{2\pi\ \sqrt{2}\ \Gamma(\ell+r'+\frac{3}{2})}{(2\ell+1)2^{r+r'+\ell+1}}\ , \tag{A.55}$$

$$\tau_{k+1} = \frac{(\beta-2k)\ (\gamma-k)}{2(k+1)(\gamma+k)}\ \tau_k, \qquad \tau_0 = \frac{1}{r!(r'-r)!}\ , \tag{A.56}$$

$$\sigma_{\alpha+1,k} = \frac{2(\delta-2k-\alpha)}{(2\gamma+4k+2\alpha+1)}\ \ \sigma_{\alpha k}, \quad \sigma_{0k} = \frac{1}{(2k+\gamma-\frac{3}{2})(2k+\gamma-\frac{1}{2})}\ , \tag{A.57}$$

$$\beta = 2(\ell+r) + 1,\ \gamma = r'-r + 1,\ \delta = \ell+2r, \tag{A.58}$$

for $r \leq r'$. Interchange r and r' in (A.54) - (A.58) for $r' \leq r$. This computation was originally done by Pekeris, et al. [72] ; however, there are several misprints in the paper. Equation (A.26) now takes the form

$$\sum_{r'=0}^{\infty} a_{r'\ell} \left\{ \frac{\lambda\pi}{\sigma^2} [\,r\ell, r'\ell] + (\lambda+1) b^{\ell}_{rr'} \right\} = 0\ . \tag{A.59}$$

$$r,\ell\ = 0,1,\ \cdots\cdots\ .$$

For a given value of ℓ, the vanishing of the determinant of (A.59) determines the eigenvalues $\lambda_{r\ell}$ of (A.4).

Writing, for a given value of ℓ and $r,r' = 0,1, \cdots , N < +\infty$,

$$A^{\ell} = (b^{\ell}_{rr'}), \tag{A.60}$$

$$B^{\ell} = -\left(\frac{\pi}{\sigma^2} [\,r\ell, r'\ell] + b^{\ell}_{rr'} \right), \tag{A.61}$$

$$\underline{a}^{\ell} = (a_{r'\ell})\ , \tag{A.62}$$

equation (A.59) becomes a generalized eigenvalue problem of order N, for each ℓ,

$$A^{\ell}\underline{a}^{\ell} = \lambda B^{\ell}\underline{a}^{\ell} . \qquad (A.63)$$

The matrices A^{ℓ} and B^{ℓ} are negative and positive definite respectively. It is observed that the off diagonal terms of A^{ℓ} and B^{ℓ} decay so rapidly that, for the expansion (A.6), $\underline{a}^{\ell}$ should be of order 30×1. Although N may be larger than 30, only the first 30 components of each eigenvector $\underline{a}^{\ell}$ need be retained for the expansion.

The method used to solve (A.63) consists of four parts: (1) Perform Cholesky decomposition of B^{ℓ} into $L^{\ell}L^{\ell T}$, where L^{ℓ} is lower triangular. The composition $L^{\ell -1}A^{\ell}L^{\ell T-1}$ is performed, resulting in a symmetric matrix. (2) Reduce the symmetric matrix obtained in (1) to a symmetric tridiagonal matrix using accumulating orthogonal similarity transforms. (3) Compute eigenvalues and eigenvectors of the symmetric tridiagonal matrix obtained in (2) by the implicit QL method. (4) Form eigenvectors of (A.63) by back transforming those obtained in (3). See [38].

From (A.4), (A.6), and (A.9) we see that

$$\phi_{r\ell}(\underline{p}) = e^{-p^2} m(p)^{\frac{1}{2}} p^{\ell} P_{\ell}(\cos\theta) \sum_{k=0}^{\infty} a_{r\ell k}\, L_k^{\ell+\frac{1}{2}}(p^2). \qquad (A.64)$$

For our approximation, by the above discussion, we shall truncate the expansion at N = 29 and assume that

$$\phi_{r\ell}(\underline{p}) = e^{-p^2} m(p)^{\frac{1}{2}}\, p^{\ell} P_{\ell}(\cos\theta) \sum_{k=0}^{29} a_{r\ell k}\, L_k^{\ell+\frac{1}{2}}(p^2). \qquad (A.65)$$

In the work discussed in Chapter V, the bilinear expansion ranged over $\ell = 0, \cdots, 10$ and $r = 0, \cdots, 59$. For this case the computation of the eigenvalues and is very costly (about 25 minutes on CDC 7600); also, the computation of the two bilinear expansion to compute the kernel for each velocity point is costly (from about 10 minutes for three points per velocity coordinate to 45 minutes for seven points per velocity coordinate on CDC 7600). Hence, it is advisable to compute the bilinear expansions of the iterates of the kernel and store them as data to be read in by the main program. For a sample of the eigenvalues and coefficients $a_{r\ell k}$ for $\ell = 0,1$, $r = 0,1, \cdots, 29$, and $k = 0,1,\cdots, 29$ see table AI.

A disadvantage of this method of computing the $a_{r\ell k}$'s is the difficulty in ascertaining its accuracy without repeating the complete calculation with a larger determinant. However, due to the structure of the matrix obtained from (A.59) the matrix elements for a given value of rapidly approach zero as $|r-r'|$ becomes large, i.e. the off-diagonal elements rapidly decay, away from the diagonal. See [68] . The matrix, for Maxwellian molecules, corresponding to (A.59) is diagonal, with its eigenvalues along the diagonal. So some advantage can be taken of part of the previous computation. Also, from this, one can see that the Laguerre-Sonine polynomials given by (A.1) are good approximation to the eigenfunction even for rigid-sphere molecules. For a comparison of matrix elements for rigid sphere molecules and matrix elements for Maxwellian molecules for $\ell = 0,1,\cdots,11$ and $r = 0,1,\cdots, 7$, see table AII. From this it can be observed that for r large and ℓ fixed the matrix element for the rigid sphere molecules varies like $r^{\frac{1}{2}}$ (a result predicted by Mott-Smith [68]).

Table A-1

Eigenvalues $\lambda_{r\ell}$ and coefficients of the expansion $a_{r\ell k}$ in equation (A.10) for the eigenfunctions of the linearized Boltzmann collision operator for a rigid sphere gas.

```
L                           0                   0                   0
R                           0                   1                   2

EIGENVALUE          -1.00000000E+00     -1.00000000E+00     -1.57971633E+00

COEFFICIENT
 K
 0                  -1.23105631E-01      2.24622114E-01      1.85468841E-02
 1                  -1.74633757E-01     -5.80200252E-02      5.16782156E-02
 2                   0.                  0.                  1.85265673E-01
 3                   0.                  0.                 -1.90086175E-02
 4                   0.                  0.                 -4.96154072E-03
 5                   0.                  0.                 -1.80348774E-03
 6                   0.                  0.                 -7.77615594E-04
 7                   0.                  0.                 -3.65746476E-04
 8                   0.                  0.                 -1.82671270E-04
 9                   0.                  0.                 -9.55486179E-05
10                   0.                  0.                 -5.19195077E-05
11                   0.                  0.                 -2.91547182E-05
12                   0.                  0.                 -1.68549791E-05
13                   0.                  0.                 -1.00026427E-05
14                   0.                  0.                 -6.07856424E-06
15                   0.                  0.                 -3.77441030E-06
16                   0.                  0.                 -2.39008582E-06
17                   0.                  0.                 -1.54072249E-06
18                   0.                  0.                 -1.00944135E-06
19                   0.                  0.                 -6.71196475E-07
20                   0.                  0.                 -4.52334524E-07
21                   0.                  0.                 -3.08604103E-07
22                   0.                  0.                 -2.12923421E-07
23                   0.                  0.                 -1.48431065E-07
24                   0.                  0.                 -1.04460592E-07
25                   0.                  0.                 -7.41642427E-08
26                   0.                  0.                 -5.30854374E-08
27                   0.                  0.                 -3.82869470E-08
28                   0.                  0.                 -2.78101567E-08
29                   0.                  0.                 -2.03347905E-08
```

```
L                                 0                  0                  0
R                                 3                  4                  5

EIGENVALUE              -2,13148483E+00    -2,67331135E+00    -3,20941971E+00

COEFFICIENT
 K
 0                      -1,05490921E-02     6,78790049E-03     4,68301004E-03
 1                      -2,76991339E-02     1,74903065E-02     1,19775929E-02
 2                      -7,42274434E-02     4,37056257E-02     2,00981354E-02
 3                      -1,79391206E-01     8,74398391E-02     5,56071136E-02
 4                       3,60149896E-02     1,70058071E-01     9,52495316E-02
 5                       8,86770647E-03    -5,17357198E-02     1,58842507E-01
 6                       3,31439714E-03    -1,21040605E-02    -6,62608714E-02
 7                       1,44412287E-03    -4,51770493E-03    -1.45857011E-02
 8                       6,83833948E-04    -1,97581568E-03    -5.40435939E-03
 9                       3,42037854E-04    -9,37215002E-04    -2.36020588E-03
10                       1,78209107E-04    -4,67534068E-04    -1,11624523E-03
11                       9,59937056E-05    -2,41668019E-04    -5.52802991E-04
12                       5,32239471E-05    -1,28426906E-04    -2.81974637E-04
13                       3,02923580E-05    -6,98673397E-05    -1.46801096E-04
14                       1,76646364E-05    -3,88228482E-05    -7.75913499E-05
15                       1,05387214E-05    -2,20094586E-05    -4.15024410E-05
16                       6,42424599E-06    -1,27244156E-05    -2,24231321E-05
17                       3,99634193E-06    -7,50087625E-06    -1,22251224E-05
18                       2,53370287E-06    -4,50829342E-06    -6,72351503E-06
19                       1,63506431E-06    -2,76241769E-06    -3,73074176E-06
20                       1,07257776E-06    -1,72512098E-06    -2,08976532E-06
21                       7.14289559E-07    -1,09744102E-06    -1.18277384E-06
22                       4.82313624E-07    -7,10644598E-07    -6,77222242E-07
23                       3.29826023E-07    -4,67977240E-07    -3.92830700E-07
24                       2.28176310E-07    -3,13058841E-07    -2.31207564E-07
25                       1,59536429E-07    -2,12494779E-07    -1.38295696E-07
26                       1,12634197E-07    -1,46175418E-07    -8.41908100E-08
27                       8,02345572E-08    -1,01788737E-07    -5.22274713E-08
28                       5.76278465E-08    -7,16718790E-08    -3.30424856E-08
29                       4.17078078E-08    -5,09782312E-08    -2.13274001E-08
```

```
L                        0                    0                    0
R                        6                    7                    8

EIGENVALUE       -3.74166824E+00      -4.27108206E+00      -4.79829990E+00

COEFFICIENT
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 1               -8.[illegible]        6.[illegible]        4.[illegible]
 2               -2.[illegible]        1.[illegible]        1.[illegible]
 3               -3.[illegible]        2.[illegible]        2.[illegible]
 4               -6.[illegible]        4.[illegible]        3.[illegible]
 5               -9.[illegible]        7.[illegible]        5.[illegible]
 6               -1.[illegible]        1.[illegible]        7.[illegible]
 7                7.[illegible]        1.[illegible]        1.[illegible]
 8                1.[illegible]       -9.[illegible]        1.[illegible]
 9                5.[illegible]       -1.[illegible]       -1.[illegible]
10                2.[illegible]       -6.[illegible]       -1.[illegible]
11                1.[illegible]       -2.[illegible]       -6.[illegible]
12                5.[illegible]       -1.[illegible]       -2.[illegible]
13                2.[illegible]       -5.[illegible]       -1.[illegible]
14                1.[illegible]       -2.[illegible]       -5.[illegible]
15                7.[illegible]       -1.[illegible]       -2.[illegible]
16                3.[illegible]       -6.[illegible]       -1.[illegible]
17                1.[illegible]       -2.[illegible]       -4.[illegible]
18                8.[illegible]       -1.[illegible]       -1.[illegible]
19                3.[illegible]       -2.[illegible]        6.[illegible]
20                1.[illegible]        6.[illegible]        5.[illegible]
21                4.[illegible]        1.[illegible]        7.[illegible]
22               -2.[illegible]        2.[illegible]        6.[illegible]
23               -2.[illegible]        1.[illegible]        5.[illegible]
24               -2.[illegible]        1.[illegible]        4.[illegible]
25               -2.[illegible]        1.[illegible]        3.[illegible]
26               -2.[illegible]        9.[illegible]        2.[illegible]
27               -1.[illegible]        7.[illegible]        1.[illegible]
28               -1.[illegible]        5.[illegible]        1.[illegible]
29               -9.[illegible]        3.[illegible]        9.[illegible]E-07
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L                                0                  0                  0
R                                9                 10                 11

EIGENVALUE          -5.32375194E+00    -5.84774422E+00    -6.37050354E+00

COEFFICIENT
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 1                   3.[illegible]     -3.[illegible]     -2.[illegible]
 2                   9.[illegible]     -7.[illegible]     -5.[illegible]
 3                   1.[illegible]     -1.[illegible]     -1.[illegible]
 4                   2.[illegible]     -2.[illegible]     -1.[illegible]
 5                   4.[illegible]     -3.[illegible]     -2.[illegible]
 6                   5.[illegible]     -4.[illegible]     -3.[illegible]
 7                   7.[illegible]     -6.[illegible]     -5.[illegible]
 8                   9.[illegible]     -7.[illegible]     -6.[illegible]
 9                   1.[illegible]     -9.[illegible]     -8.[illegible]
10                  -1.[illegible]     -9.[illegible]     -8.[illegible]
11                  -1.[illegible]      1.[illegible]     -8.[illegible]
12                  -6.[illegible]      1.[illegible]      1.[illegible]
13                  -2.[illegible]      5.[illegible]      1.[illegible]
14                  -1.[illegible]      2.[illegible]      6.[illegible]
15                  -4.[illegible]      9.[illegible]      1.[illegible]
16                  -2.[illegible]      3.[illegible]      7.[illegible]
17                  -7.[illegible]      1.[illegible]      2.[illegible]
18                  -1.[illegible]      2.[illegible]      5.[illegible]
19                   7.[illegible]     -1.[illegible]     -2.[illegible]
20                   1.[illegible]     -3.[illegible]     -5.[illegible]
21                   1.[illegible]     -3.[illegible]     -6.[illegible]
22                   1.[illegible]     -2.[illegible]     -5.[illegible]
23                   1[illegible]      -2.[illegible]     -4.[illegible]
24                   8.[illegible]     -1.[illegible]     -3.[illegible]
25                   7.[illegible]     -1.[illegible]     -2.[illegible]
26                   5.[illegible]     -1.[illegible]     -2.[illegible]
27                   4.[illegible]     -8.[illegible]     -1.[illegible]
28                   2.[illegible]     -5.[illegible]     -1.[illegible]
29                   2.[illegible]     -4.[illegible]     -7.[illegible]
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L                          0                    0                    0
R                         12                   13                   14

EIGENVALUE       -6.89220350E+00      -7.41298040E+00      -7.93294360E+00

COEFFICIENT
 K
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 2               -4.[illegible]       -3.[illegible]       -3.[illegible]
 3               -8.[illegible]       -7.[illegible]       -5.[illegible]
 4               -1.[illegible]       -1.[illegible]       -9.[illegible]
 5               -2.[illegible]       -1.[illegible]       -1.[illegible]
 6               -3.[illegible]       -2.[illegible]       -2.[illegible]
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 8               -5.[illegible]       -4.[illegible]       -3.[illegible]
 9               -6.[illegible]       -5.[illegible]       -4.[illegible]
10               -7.[illegible]       -6.[illegible]       -5.[illegible]
11               -8.[illegible]       -7.[illegible]       -6.[illegible]
12               -6.[illegible]       -7.[illegible]       -7.[illegible]
13                1.[illegible]       -5.[illegible]       -7.[illegible]
14                1.[illegible]        1.[illegible]       -4.[illegible]
15                4.[illegible]        1.[illegible]        1.[illegible]
16                1.[illegible]        3.[illegible]        9.[illegible]
17                5.[illegible]        1.[illegible]        2.[illegible]
18                1.[illegible]        2.[illegible]        5.[illegible]
19               -3.[illegible]       -4.[illegible]       -3.[illegible]
20               -9.[illegible]       -1.[illegible]       -2.[illegible]
21               -1.[illegible]       -1.[illegible]       -2.[illegible]
22               -9.[illegible]       -1.[illegible]       -2.[illegible]
23               -7.[illegible]       -1.[illegible]       -2.[illegible]
24               -6.[illegible]       -1.[illegible]       -1.[illegible]
25               -4.[illegible]       -7.[illegible]       -1.[illegible]
26               -3.[illegible]       -5.[illegible]       -9.[illegible]
27               -2.[illegible]       -4.[illegible]       -7.[illegible]
28               -1.[illegible]       -3.[illegible]       -5.[illegible]
29               -1.[illegible]       -2.[illegible]       -3.[illegible]
```

```
L                          0               0               0
R                         15              16              17

EIGENVALUE   -8.45218239E+00 -8.97077082E+00 -9.48877109E+00

COEFFICIENT
 K
 0            4.52910741E-04 -3.81856411E-04 -3.23956541E-04
 1            1.14929851E-03 -9.68861985E-04 -8.21858059E-04
 2            2.67881026E-03 -2.25625862E-03 -1.91244559E-03
 3            4.96894539E-03 -4.18555179E-03 -3.54808085E-03
 4            8.19063465E-03 -6.90551271E-03 -5.85850202E-03
 5            1.25020659E-02 -1.05583135E-02 -8.97102686E-03
 6            1.80275750E-02 -1.52634283E-02 -1.29982158E-02
 7            2.48295656E-02 -2.10963095E-02 -1.80214800E-02
 8            3.28705550E-02 -2.80602995E-02 -2.40697643E-02
 9            4.19591350E-02 -3.60486164E-02 -3.10916266E-02
10            5.16665895E-02 -4.47899486E-02 -3.89174036E-02
11            6.11844597E-02 -5.37642211E-02 -4.72049075E-02
12            6.90491886E-02 -6.20588239E-02 -5.53552692E-02
13            7.25171293E-02 -6.80920173E-02 -6.23696388E-02
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17           -6.55311108E-03  1.59391433E-01 -1.06246359E-02
18           -1.27050870E-03  3.31364824E-03  1.62748680E-01
19           -7.71744332E-06  5.33765280E-05 -2.32322720E-04
20            3.48605907E-04 -5.89910020E-04 -1.23035375E-03
21            4.17022024E-04 -6.81629523E-04 -1.21143758E-03
22            3.86092441E-04 -6.17255191E-04 -1.02502278E-03
23            3.24768581E-04 -5.12793454E-04 -8.22344589E-04
24            2.59978562E-04 -4.07890307E-04 -6.41796454E-04
25            2.01884513E-04 -3.15943735E-04 -4.92053253E-04
26            1.53543338E-04 -2.40266805E-04 -3.72314066E-04
27            1.14995474E-04 -1.80202412E-04 -2.78736960E-04
28            8.50983168E-05 -1.33663061E-04 -2.06798574E-04
29            6.23842935E-05 -9.82292056E-05 -1.52203980E-04
```

```
L                           0                    0                    0
R                          18                   19                   20

EIGENVALUE      -1.00062361E+01      -1.05232111E+01      -1.10397364E+01

COEFFICIENT
 K
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 1              -7.[illegible]        6.[illegible]        5.[illegible]
 2              -1.[illegible]        1.[illegible]        1.[illegible]
 3              -3.[illegible]        2.[illegible]        2.[illegible]
 4              -4.[illegible]        4.[illegible]        3.[illegible]
 5              -7.[illegible]        6.[illegible]        5.[illegible]
 6              -1.[illegible]        9.[illegible]        8.[illegible]
 7              -1.[illegible]        1.[illegible]        1.[illegible]
 8              -2.[illegible]        1.[illegible]        1.[illegible]
 9              -2.[illegible]        2.[illegible]        2.[illegible]
10              -3.[illegible]        2.[illegible]        2.[illegible]
11              -4.[illegible]        3.[illegible]        3.[illegible]
12              -4.[illegible]        4.[illegible]        3.[illegible]
13              -5.[illegible]        5.[illegible]        4.[illegible]
14              -6.[illegible]        5.[illegible]        5.[illegible]
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17              -4.[illegible]        5.[illegible]        5.[illegible]
18              -6.[illegible]        3.[illegible]        5.[illegible]
19               1.[illegible]       -8.[illegible]        3.[illegible]
20              -4.[illegible]       -1.[illegible]       -1.[illegible]
21              -2.[illegible]        8.[illegible]       -1.[illegible]
22              -1.[illegible]        3.[illegible]        1.[illegible]
23              -1.[illegible]        2.[illegible]        5.[illegible]
24              -1.[illegible]        1.[illegible]        3.[illegible]
25              -7.[illegible]        1.[illegible]        2.[illegible]
26              -5.[illegible]        8.[illegible]        1.[illegible]
27              -4.[illegible]        6.[illegible]        1.[illegible]
28              -3.[illegible]        4.[illegible]        7.[illegible]
29              -2.[illegible]        3.[illegible]        5.[illegible]
```

```
L                                0                   0                   0
R                               21                  22                  23

EIGENVALUE         -1,15558433E+01     -1,20715650E+01     -1,25869270E+01

COEFFICIENT
 K
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 1                  4,48047914E-04      3,89182157E-04      3,39295022E-04
 2                  1,04018654E-03      9,03125533E-04      7,87043222E-04
 3                  1,93043847E-03      1,67618707E-03      1,46083354E-03
 4                  3,19542311E-03      2,77589836E-03      2,42031617E-03
 5                  4,91579689E-03      4,27418669E-03      3,72967483E-03
 6                  7,17187352E-03      6,24397860E-03      5,45499059E-03
 7                  1,00375396E-02      8,75441111E-03      7,66046535E-03
 8                  1,35722453E-02      1,18644650E-02      1,04033449E-02
 9                  1,78108245E-02      1,56148326E-02      1,37273891E-02
10                  2,27508010E-02      2,00177944E-02      1,76547256E-02
11                  2,83366156E-02      2,50447671E-02      2,21758770E-02
12                  3,44397849E-02      3,06109661E-02      2,72376340E-02
13                  4,08332285E-02      3,65562087E-02      3,27282296E-02
14                  4,71565852E-02      4,26201590E-02      3,84588782E-02
15                  5,28666148E-02      4,84089810E-02      4,41400587E-02
16                  5,71610928E-02      5,33478244E-02      4,93496898E-02
17                  5,88514582E-02      5,66082510E-02      5,34879828E-02
18                  5,61249019E-02      5,69874714E-02      5,57088493E-02
19                  4,60289703E-02      5,26841900E-02      5,48064476E-02
20                  2,30859458E-02      4,08166277E-02      4,90059958E-02
21                 -2,60433840E-02      1,61392289E-02      3,55173477E-02
22                 -1,69465235E-01     -3,38217857E-02      9,35760267E-03
23                  1,69044090E-02     -1,69626075E-01     -4,10443922E-02
24                  6,71538742E-03      2,15604755E-02     -1,69241802E-01
25                  3,77651941E-03      8,10344340E-03      2,63620626E-02
26                  2,41323623E-03      4,40278083E-03      9,47303575E-03
27                  1,63832675E-03      2,74488887E-03      5,01111364E-03
28                  1,14784392E-03      1,82997639E-03      3,06396391E-03
29                  8,17808922E-04      1,26488[illegible]1E-03     2,01294605E-03
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L                              0                   0                   0
R                             24                  25                  25

EIGENVALUE         -1.31019531E+01     -1.36166645E+01     -1.41310803E+01

COEFFICIENT
  K
  0                -1.[illegible]       1.[illegible]      -9.[illegible]-05
  1                -2.[illegible]       2.[illegible]      -2.[illegible]-04
  2                -6.[illegible]       6.[illegible]      -5.[illegible]-04
  3                -1.[illegible]       1.[illegible]      -9.[illegible]-04
  4                -2.[illegible]       1.[illegible]      -1.[illegible]-03
  5                -3.[illegible]       2.[illegible]      -2.[illegible]-03
  6                -4.[illegible]       4.[illegible]      -3.[illegible]-03
  7                -6.[illegible]       5.[illegible]      -5.[illegible]-03
  8                -9.[illegible]       8.[illegible]      -7.[illegible]-03
  9                -1.[illegible]       1.[illegible]      -9.[illegible]-03
 10                -1.[illegible]       1.[illegible]      -1.[illegible]-02
 11                -1.[illegible]       1.[illegible]      -1.[illegible]-02
 12                -2.[illegible]       2.[illegible]      -1.[illegible]-02
 13                -2.[illegible]       2.[illegible]      -2.[illegible]-02
 14                -3.[illegible]       3.[illegible]      -2.[illegible]-02
 15                -4.[illegible]       3.[illegible]      -3.[illegible]-02
 16                -4.[illegible]       4.[illegible]      -3.[illegible]-02
 17                -4.[illegible]       4.[illegible]      -4.[illegible]-02
 18                -5.[illegible]       5.[illegible]      -4.[illegible]-02
 19                -5.[illegible]       5.[illegible]      -5.[illegible]-02
 20                -5.[illegible]       5.[illegible]      -5.[illegible]-02
 21                -4.[illegible]       4.[illegible]      -5.[illegible]-02
 22                -3.[illegible]       4.[illegible]      -4.[illegible]-02
 23                -2.[illegible]       2.[illegible]      -3.[illegible]-02
 24                 4.[illegible]      -3.[illegible]      -1.[illegible]-02
 25                 1.[illegible]      -5.[illegible]       9.[illegible]-03
 26                -3.[illegible]      -1.[illegible]       5.[illegible]-02
 27                -1.[illegible]       3.[illegible]       1.[illegible]-01
 28                -5.[illegible]       1.[illegible]      -4.[illegible]-02
 29                -3.[illegible]       6.[illegible]      -1.[illegible]-02
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L                              O                 O                  O
R                             27                28                 29

EIGENVALUE       -1,46452176E+01   -1.51590920E+01    -1.66727178E+01

COEFFICIENT
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  0              -7,98285943E-05   -7.06508196E-05    -6,26830283E-05
  1              -2.02377650E-04   -1.79103067E-04    -1,58898145E-04
  2              -4,68836862E-04   -4,14808723E-04    -3,67923537E-04
  3              -8,70401436E-04   -7,70134216E-04    -6,83117961E-04
  4              -1,44414[illegible]22E-03   -1,27815434E-03    -1,13404584E-03
  5              -2,23116133E-03   -1,97575109E-03    -1,75384252E-03
  6              -3.27565244E-03   -2.90288342E-03    -2,57865658E-03
  7              -4,62341500E-03   -4,10142078E-03    -3,64672927E-03
  8              -6,31976571E-03   -5,61346091E-03    -4,99704251E-03
  9              -8,40673838E-03   -7,47905437E-03    -6,66746725E-03
 10              -1,09194989E-02   -9,73326432E-03    -8,69234806E-03
 11              -1,38819022E-02   -1,24024979E-02    -1,10994671E-02
 12              -1,73011232E-02   -1,55000533E-02    -1,39063382E-02
 13              -2.11612869E-02   -1,90208291E-02    -1,71157898E-02
 14              -2,54159968E-02   -2,29351324E-02    -2,07107933E-02
 15              -2,99796059E-02   -2,71815003E-02    -2,46484887E-02
 16              -3,47169750E-02   -3,16583920E-02    -2,88533308E-02
 17              -3,94312993E-02   -3,62145252E-02    -3,32092344E-02
 18              -4,38493090E-02   -4,06374795E-02    -3,75505183E-02
 19              -4,76026923E-02   -4,46399510E-02    -4,16513182E-02
 20              -5.02037704E-02   -4,78426440E-02    -4,52129355E-02
 21              -5,10119056E-02   -4,97520711E-02    -4,78482448E-02
 22              -4,91839263E-02   -4,97301952E-02    -4,90616820E-02
 23              -4,35945813E-02   -4,69500819E-02    -4,82221960E-02
 24              -3,26943445E-02   -4,03254584E-02    -4,45242113E-02
 25              -1,42156281E-02   -2,83860290E-02    -3,69263669E-02
 26               1,55732539E-02   -9,02230966E-03    -2,40443175E-02
 27               6,44999130E-02    2,11558315E-02    -3,93371102E-03
 28               1,62847752E-01    6.90515194E-02     2,64495032E-02
 29              -4,65793796E-02    1,60178160E-[illegible]     7,31016840E-02
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L                            1                  1                  1
R                            0                  1                  2

EIGENVALUE       -1.00000000E+00    -1.62519664E+00    -2.17741228E 00

COEFFICIENT
 K
 0                3.29918525E-01    -7.[illegible]     -3.[illegible]-02
 1                0.                -2.[illegible]-01  -9.[illegible]-02
 2                0.                 2.[illegible]     -1.[illegible]-01
 3                0.                 4.[illegible]      3.[illegible]-02
 4                0.                 1.[illegible]      7.[illegible]-03
 5                0.                 5.[illegible]      2.[illegible]-03
 6                0.                 2.[illegible]      8.[illegible]-04
 7                0.                 9.[illegible]      3.[illegible]-04
 8                0.                 4.[illegible]      1.[illegible]-04
 9                0.                 2.[illegible]      7.[illegible]-05
10                0.                 1.[illegible]      3.[illegible]-05
11                0.                 5.[illegible]      1.[illegible]-05
12                0.                 3.[illegible]      9.[illegible]-06
13                0.                 1.[illegible]      4.[illegible]-06
14                0.                 [illegible]        2.[illegible]-06
15                0.                 6.[illegible]      1.[illegible]-06
16                0.                 3.[illegible]      9.[illegible]-07
17                0.                 2.[illegible]      5.[illegible]-07
18                0.                 1.[illegible]      3.[illegible]-07
19                0.                 1.[illegible]      2.[illegible]-07
20                0.                 6.[illegible]      1.[illegible]-07
21                0.                 4.[illegible]      8.[illegible]-08
22                0.                 3.[illegible]      5.[illegible]-08
23                0.                 2.[illegible]      3.[illegible]-08
24                0.                 1.[illegible]      2.[illegible]-08
25                0.                 1.[illegible]      1.[illegible]-08
26                0.                 7.[illegible]      1.[illegible]-08
27                0.                 5.[illegible]      8.[illegible]-09
28                0.                 3.[illegible]      6.[illegible]-09
29                0.                 2.[illegible]      4.[illegible]-09
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L                        1                    1                    1
R                        3                    4                    5

EIGENVALUE       -2.71692051E+00      -3.25046821E+00      -3.78035403E+00

COEFFICIENT
 K
 0                2.41828476E-02       1.63427850E-02       1.16253887E-02
 1                5.53755023E-02       3.63403874E-02       2.54514815E-02
 2                9.27265299E-02       5.91794742E-02       4.10913595E-02
 3                1.44984584E-01       8.65328466E-02       5.93293526E-02
 4               -4.83243446E-02       1.19026395E-01       7.96256792E-02
 5               -8.61713895E-03      -5.44400248E-02       9.86706485E-02
 6               -2.70715533E-03      -9.27462361E-03      -5.89699337E-02
 7               -1.02520388E-03      -2.94039485E-03      -9.42707912E-03
 8               -4.27205654E-04      -1.12344561E-03      -2.98640002E-03
 9               -1.88820156E-04      -4.68803528E-04      -1.14110045E-03
10               -8.69251791E-05      -2.05273667E-04      -4.72577818E-04
11               -4.12658043E-05      -9.23263391E-05      -2.02712304E-04
12               -2.00864770E-05      -4.20647728E-05      -8.75464375E-05
13               -9.99289312E-06      -1.91960041E-05      -3.70830659E-05
14               -5.07295269E-06      -8.67252422E-06      -1.48491440E-05
15               -2.62662383E-06      -3.81976519E-06      -5.19648123E-06
16               -1.38746418E-06      -1.59846774E-06      -1.17879836E-06
17               -7.48296715E-07      -6.01337834E-07       3.43224918E-07
18               -4.12491527E-07      -1.70627694E-07       7.95100974E-07
19               -2.32661407E-07       1.94924178E-09       8.18650118E-07
20               -1.34400124E-07       6.03282789E-08       6.95650664E-07
21               -7.95556799E-08       7.09142536E-08       5.43522948E-07
22               -4.82548647E-08       6.36361004E-08       4.06138554E-07
23               -2.99750698E-08       5.14230557E-08       2.95763658E-07
24               -1.90478644E-08       3.94279944E-08       2.12126339E-07
25               -1.23831942E-08       2.93627159E-08       1.50810674E-07
26               -8.18141629E-09       2.15051830E-08       1.06734316E-07
27               -5.50942522E-09       1.56045566E-08       7.54190875E-08
28               -3.76826194E-09       1.12707787E-08       5.33167853E-08
29               -2.61313965E-09       8.12824062E-09       3.77659349E-08
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L                        1                  1                  1
R                        6                  7                  8

EIGENVALUE     -4,30767341E+00    -4,83305031E+00    -5,35688185E+00

COEFFICIENT
 K
 0             -8,57301211E-03     6,49593726E-03    -5,02851036E-03
 1             -1,85930564E-02     1,40003880E-02    -1,07893608E-02
 2             -2,99437514E-02     2,25422168E-02    -1,73829460E-02
 3             -4,31701833E-02     3,25593957E-02    -2,51787737E-02
 4             -5,79066671E-02     4,38489152E-02    -3,40788380E-02
 5             -7,27312986E-02     5,56716881E-02    -4,36647322E-02
 6             -8,20477441E-02     6,60693414E-02    -5,29776123E-02
 7              6,23735468E-02     6,80986113E-02    -5,97108911E-02
 8              9,20222645E-03    -6,49234744E-02    -5,61699878E-02
 9              2,88928928E-03    -8,68636633E-03     6,67969143E-02
10              1,09468511E-03    -2,68221223E-03     7,94138156E-03
11              4,45144266E-04    -9,97915093E-04     2,39074207E-03
12              1,83996213E-04    -3,92556167E-04     8,62112687E-04
13              7,39413766E-05    -1,51981106E-04     3,20147199E-04
14              2,70294820E-05    -5,29622565E-05     1,09332612E-04
15              7,44871543E-06    -1,26999576E-05     2,60268128E-05
16             -1,92746502E-07     2,53815461E-06    -5,10238380E-06
17             -2,69928427E-06     7,20675019E-06    -1,46297020E-05
18             -3,10355913E-06     7,63052168E-06    -1,55430695E-05
19             -2,74183764E-06     6,56302229E-06    -1,34188602E-05
20             -2,18154348E-06     5,16048518E-06    -1,05919459E-05
21             -1,64450528E-06     3,86635910E-06    -7,96425498E-06
22             -1,20152691E-06     2,81426114E-06    -5,81458686E-06
23             -8,61318825E-07     2,01150213E-06    -4,16525824E-06
24             -6,10269776E-07     1,42108941E-06    -2,94641461E-06
25             -4,29428953E-07     9,96689510E-07    -2,06689298E-06
26             -3,01100843E-07     6,96095521E-07    -1,44216919E-06
27             -2,10872595E-07     4,85209974E-07    -1,00312458E-06
28             -1,47768945E-07     3,38134458E-07    -6,96754453E-07
29             -1,03747814E-07     2,35900858E-07    -4,83931296E-07
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L                           1                    1                    1
R                           9                   10                   11

EIGENVALUE     -5.87944060E+00      -6.40092410E+00      -6.92148149E+00

COEFFICIENT
  K
  0             3.[illegible]       -3.[illegible]        2.[illegible]
  1             8.[illegible]       -6.[illegible]        5.[illegible]
  2             1.[illegible]       -1.[illegible]        8.[illegible]
  3             1.[illegible]       -1.[illegible]        1.[illegible]
  4             2.[illegible]       -2.[illegible]        1.[illegible]
  5             3.[illegible]       -2.[illegible]        2.[illegible]
  6             4.[illegible]       -3.[illegible]        2.[illegible]
  7             5.[illegible]       -4.[illegible]        3.[illegible]
  8             5.[illegible]       -4.[illegible]        4.[illegible]
  9             4.[illegible]       -4.[illegible]        4.[illegible]
 10            -6.[illegible]       -3.[illegible]        4.[illegible]
 11            -7.[illegible]        6.[illegible]        2.[illegible]
 12            -2.[illegible]        5.[illegible]       -6.[illegible]
 13            -6.[illegible]        1.[illegible]       -4.[illegible]
 14            -2.[illegible]        5.[illegible]       -1.[illegible]
 15            -5.[illegible]        1.[illegible]       -3.[illegible]
 16             5.[illegible]        1.[illegible]       -2.[illegible]
 17             2.[illegible]       -4.[illegible]        5.[illegible]
 18             2.[illegible]       -4.[illegible]        7.[illegible]
 19             2.[illegible]       -4.[illegible]        7.[illegible]
 20             1.[illegible]       -3.[illegible]        5.[illegible]
 21             1.[illegible]       -2.[illegible]        4.[illegible]
 22             1.[illegible]       -1.[illegible]        3.[illegible]
 23             7.[illegible]       -1.[illegible]        2.[illegible]
 24             5.[illegible]       -1.[illegible]        1.[illegible]
 25             3.[illegible]       -7.[illegible]        1.[illegible]
 26             2.[illegible]       -[illegible]          8.[illegible]
 27             1.[illegible]       -3.[illegible]        6.[illegible]
 28             1.[illegible]       -2.[illegible]        4.[illegible]
 29             9.[illegible]       -1.[illegible]        2.[illegible]
```

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L                     1              1              1
R                    12             13             14

EIGENVALUE   -7.44122898E+00  -7.96025946E+00  -8.47864870E+00

COEFFICIENT
 K
 0            2.[illegible]    1.[illegible]    1.[illegible]
 1            4.[illegible]    3.[illegible]    3.[illegible]
 2            7.[illegible]    5.[illegible]    4.[illegible]
 3            1.[illegible]    8.[illegible]    7.[illegible]
 4            1.[illegible]    1.[illegible]    1.[illegible]
 5            1.[illegible]    1.[illegible]    1.[illegible]
 6            2.[illegible]    2.[illegible]    1.[illegible]
 7            2.[illegible]    2.[illegible]    2.[illegible]
 8            3.[illegible]    2.[illegible]    2.[illegible]
 9            3.[illegible]    3.[illegible]    2.[illegible]
10            4.[illegible]    3.[illegible]    3.[illegible]
11            3.[illegible]    3.[illegible]    3.[illegible]
12            2.[illegible]    3.[illegible]    3.[illegible]
13           -6.[illegible]    1.[illegible]    2.[illegible]
14           -3.[illegible]   -6.[illegible]    9.[illegible]
15           -7.[illegible]   -2.[illegible]   -6.[illegible]
16           -9.[illegible]   -2.[illegible]   -6.[illegible]
17            8.[illegible]    1.[illegible]    2.[illegible]
18            1.[illegible]    1.[illegible]    3.[illegible]
19            1.[illegible]    1.[illegible]    3.[illegible]
20            9.[illegible]    1.[illegible]    2.[illegible]
21            7.[illegible]    1.[illegible]    1.[illegible]
22            5.[illegible]    9.[illegible]    1.[illegible]
23            4.[illegible]    6.[illegible]    1.[illegible]
24            2.[illegible]    4.[illegible]    7.[illegible]
25            2.[illegible]    3.[illegible]    5.[illegible]
26            1.[illegible]    2.[illegible]    3.[illegible]
27            1.[illegible]    1.[illegible]    2.[illegible]
28            7.[illegible]    1.[illegible]    1.[illegible]
29            5.[illegible]    8.[illegible]    1.[illegible]
```

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L                                  1                    1                    1
R                                 15                   16                   17

EIGENVALUE           -8,99645956E+00      -9,51374505E+00      -1,00305502E+01

COEFFICIENT
 K
 0                   -1,20680880E-03      -1,01849305E-03      -8,64685252E-04
 1                   -2,55383811E-03      -2,15323352E-03      -1,82649693E-03
 2                   -4,13746515E-03      -3,49024581E-03      -2,96199222E-03
 3                   -6,08908814E-03      -5,14355273E-03      -4,3703230[illegible]E-03
 4                   -8,45502824E-03      -7,15745463E-03      -6,09302541E-03
 5                   -1,12469823E-02      -9,54941012E-03      -8,15069931E-03
 6                   -1,44417487E-02      -1,23104944E-02      -1,05438327E-02
 7                   -1,79725391E-02      -1,53989752E-02      -1,32478711E-02
 8                   -2,17151684E-02      -1,87305617E-02      -1,62064852E-02
 9                   -2,54676155E-02      -2,21648576E-02      -1,93210169E-02
10                   -2,89175524E-02      -2,54856197E-02      -2,24385064E-02
11                   -3,15857365E-02      -2,83695895E-02      -2,53323679E-02
12                   -3,27155266E-02      -3,03324678E-02      -2,76728677E-02
13                   -3,10226864E-02      -3,06242252E-02      -2,89760473E-02
14                   -2,[illegible]9890861E-02      -2,79940424E-02      -2,85054150E-02
15                   -4,[illegible]4432982E-03      -2,00341014E-02      -2,50529966E-02
16                    6,83265696E-02      -5,18950399E-04      -1,63345507E-02
17                   -7,80281254E-04       6,74[illegible]7226E-02       3,41907014E-03
18                   -7,15724445E-04      -2,2740[illegible]349E-03       6,64610139E-02
19                   -5,63646530E-04      -1,19572420E-03      -3,78879836E-03
20                   -4,27448832E-04      -7,78097227E-04      -1,66618785E-03
21                   -3,18272560E-04      -5,38308983E-04      -9,86119070E-04
22                   -2,34108750E-04      -3,80796865E-04      -6,45249850E-04
23                   -1,70565673E-04      -2,71534914E-04      -4,40845785E-04
24                   -1,23263678E-04      -1,93957951E-04      -3,07325601E-04
25                   -8,84362957E-05      -1,38357755E-04      -2,16229388E-04
26                   -6,30297331E-05      -9,84035052E-05      -1,52663579E-04
27                   -4,46460574E-05      -6,97176553E-05      -1,07806919E-04
28                   -3,14417068E-05      -4,91793484E-05      -7,59979836E-05
29                   -2,20215701E-05      -3,45307308E-05      -5,34158782E-05
```

```
L                           1                 1                 1
R                          18                19                20

EIGENVALUE     -1,05469139E+01   -1.10628698E+01   -1,15784477E+01

COEFFICIENT
 K
 0             -7,38080583E-04    6,33130531E-04   -5,45570866E-04
 1             -1,55787969E-03    1,33544966E-03   -1,15005665E-03
 2             -2.52742669E-03    2,16737652E-03   -1,86712416E-03
 3             -3,73313554E-03    3,20439924E-03   -2,76287352E-03
 4             -5,21344868E-03    4,48178674E-03   -3,86946983E-03
 5             -6,99036841E-03    6,02181678E-03   -5,20875149E-03
 6             -9,07049167E-03    7,83492427E-03   -6,79342851E-03
 7             -1,14413115E-02    9,91683861E-03   -8,62485355E-03
 8             -1,40656770E-02    1,22442445E-02   -1,06895725E-02
 9             -1,68747202E-02    1,47693553E-02   -1,29550528E-02
10             -1,97587723E-02    1.74132216E-02   -1,53645602E-02
11             -2,25550853E-02    2,00571932E-02   -1,78309038E-02
12             -2,50300396E-02    2.25313879E-02   -2,02284672E-02
13             -2,68512359E-02    2.45980054E-02   -2,23824535E-02
14             -2,75396257E-02    2,59252519E-02   -2,40533572E-02
15             -2,63779795E-02    2,60428532E-02   -2,49128000E-02
16             -2,22086122E-02    2,42575428E-02   -2,45025385E-02
17             -1,28803108E-02    1,94677080E-02   -2,21570931E-02
18              6,91720717E-03    9,66152857E-03   -1,68353094E-02
19              6,52882962E-02   -1,00164352E-02   -6,66861393E-03
20             -5,31508485E-03   -6,39310877E-02    1,27525161E-02
21             -2,12313320E-03    6,84479535E-03    6,25559507E-02
22             -1,18583281E-03    2,56316984E-03   -8,37073298E-03
23             -7,47259751E-04    1,37567993E-03   -2,98341720E-03
24             -4,97833112E-04    8,43509292E-04   -1,55437948E-03
25             -3,41124629E-04    5,51279303E-04   -9,33323006E-04
26             -2,37155585E-04    3,72640823E-04   -6,00798544E-04
27             -1,66035305E-04    2.56553069E-04   -4,01640645E-04
28             -1,16549052E-04    1.78353661E-04   -2,74274971E-04
29             -8,18039120E-05    1,24550165E-04   -1,89523317E-04
```

```
L                            1                     1                     1
R                           21                    22                    23

EIGENVALUE       -1,20936735E+01       -1,26085705E+01       -1,31231593E+01

COEFFICIENT
 K
 0               -4,[illegible]         4,[illegible]        -3,[illegible]
 1               -9,[illegible]         8,[illegible]        -7,[illegible]
 2               -1,[illegible]         1,[illegible]        -1,[illegible]
 3               -2,[illegible]         2,[illegible]        -1,[illegible]
 4               -3,[illegible]         2,[illegible]        -2,[illegible]
 5               -4,[illegible]         3,[illegible]        -3,[illegible]
 6               -5,[illegible]         5,[illegible]        -4,[illegible]
 7               -7,[illegible]         6,[illegible]        -5,[illegible]
 8               -9,[illegible]         8,[illegible]        -7,[illegible]
 9               -1,[illegible]         1,[illegible]        -8,[illegible]
10               -1,[illegible]         1,[illegible]        -1,[illegible]
11               -1,[illegible]         1,[illegible]        -1,[illegible]
12               -1,[illegible]         1,[illegible]        -1,[illegible]
13               -2,[illegible]         1,[illegible]        -1,[illegible]
14               -2,[illegible]         2,[illegible]        -1,[illegible]
15               -2,[illegible]         2,[illegible]        -2,[illegible]
16               -2,[illegible]         2,[illegible]        -2,[illegible]
17               -2,[illegible]         2,[illegible]        -2,[illegible]
18               -2,[illegible]         2,[illegible]        -2,[illegible]
19               -1,[illegible]         1,[illegible]        -1,[illegible]
20               -3,[illegible]         1,[illegible]        -1,[illegible]
21                1,[illegible]         1,[illegible]        -9,[illegible]
22                6,[illegible]        -1,[illegible]         1,[illegible]
23               -9,[illegible]        -5,[illegible]         1,[illegible]
24               -3,[illegible]         1,[illegible]         5,[illegible]
25               -1,[illegible]         3,[illegible]        -1,[illegible]
26               -1,[illegible]         1,[illegible]        -4,[illegible]
27               -6,[illegible]         1,[illegible]        -2,[illegible]
28               -4,[illegible]         6,[illegible]        -1,[illegible]
29               -2,[illegible]         4,[illegible]        -7,[illegible]
```

```
L                                1                  1                  1
R                               24                 25                 26

EIGENVALUE         -1.36374586E+01    -1.41514850E+01    -1.46652539E+01

COEFFICIENT
 K
 0                 -3.12724122E-04     2.74403991E-04     2.41487109E-04
 1                 -6.57941501E-04     5.77096007E-04     5.07687353E-04
 2                 -1.06933735E-03     9.38148765E-04     8.25485116E-04
 3                 -1.58668979E-03     1.39279419E-03     1.22615159E-03
 4                 -2.23162279E-03     1.96055883E-03     1.72731760E-03
 5                 -3.02141627E-03     2.65743098E-03     2.34372103E-03
 6                 -3.97009774E-03     3.49689276E-03     3.08817565E-03
 7                 -5.08761638E-03     4.48927937E-03     3.97107670E-03
 8                 -6.37836339E-03     5.64057150E-03     4.99941346E-03
 9                 -7.83930438E-03     6.95085258E-03     6.17549106E-03
10                 -9.45779774E-03     8.41249887E-03     7.49542162E-03
11                 -1.12091141E-02     1.00081245E-02     8.94740804E-03
12                 -1.30536337E-02     1.17082794E-02     1.05098281E-02
13                 -1.49336533E-02     1.34688720E-02     1.21491122E-02
14                 -1.67696652E-02     1.52282506E-02     1.38173870E-02
15                 -1.84558702E-02     1.69038201E-02     1.54498238E-02
16                 -1.98545128E-02     1.83879801E-02     1.69615837E-02
17                 -2.07883350E-02     1.95430266E-02     1.82441738E-02
18                 -2.10298857E-02     2.01944049E-02     1.91609063E-02
19                 -2.02852732E-02     2.01212237E-02     1.95409400E-02
20                 -1.81673146E-02     1.90419549E-02     1.91709802E-02
21                 -1.41462436E-02     1.65909953E-02     1.77028847E-02
22                 -7.44555094E-03     1.22759804E-02     1.50335402E-02
23                  3.22737430E-03     5.38831433E-03     1.04685429E-02
24                  2.06466246E-02    -5.22610013E-03     3.44673329E-03
25                  5.59538145E-02    -2.19777444E-02    -7.05136314E-03
26                 -1.43199755E-02    -5.41366033E-02    -2.30922290E-02
27                 -4.42327699E-03     1.57450025E-02    -5.22727189E-02
28                 -2.13991390E-03     4.71507588E-03     1.71374855E-02
29                 -1.21927209E-03     2.25112099E-03     4.97741594E-03
```

```
L                               1                 1                 1
R                              27                28                29

EIGENVALUE        -1.51787790E+01   -1.56920730E+01   -1.62051473E+01

COEFFICIENT
 K
 0                -2.13105666E-04   -1.88548833E-04   -1.67231140E-04
 1                -4.47871764E-04   -3.96140400E-04   -3.51251569E-04
 2                -7.28365967E-04   -6.44351117E-04   -5.71431507E-04
 3                -1.08240059E-03   -9.57965657E-04   -8.49899430E-04
 4                -1.52589778E-03   -1.35136882E-03   -1.19965848E-03
 5                -2.07240606E-03   -1.83699173E-03   -1.63209917E-03
 6                -2.73400495E-03   -2.42615296E-03   -2.15777905E-03
 7                -3.52092612E-03   -3.12877099E-03   -2.78620716E-03
 8                -4.44074479E-03   -3.95270128E-03   -3.52530011E-03
 9                -5.49731826E-03   -4.90285306E-03   -4.38064592E-03
10                -6.68952359E-03   -5.98013045E-03   -5.35461395E-03
11                -8.00981615E-03   -7.18021700E-03   -6.44532698E-03
12                -9.44262048E-03   -8.49221532E-03   -7.64550606E-03
13                -1.09625570E-02   -9.89715012E-03   -8.94119749E-03
14                -1.25324973E-02   -1.13663372E-02   -1.03103892E-02
15                -1.41014222E-02   -1.28596122E-02   -1.17215201E-02
16                -1.56020300E-02   -1.43233970E-02   -1.31318774E-02
17                -1.69480018E-02   -1.56885599E-02   -1.44858652E-02
18                -1.80307658E-02   -1.68679920E-02   -1.57131085E-02
19                -1.87155046E-02   -1.77537713E-02   -1.67263326E-02
20                -1.88359705E-02   -1.82137049E-02   -1.74189154E-02
21                -1.81873452E-02   -1.80859002E-02   -1.76619514E-02
22                -1.65157005E-02   -1.71777538E-02   -1.73005583E-02
23                -1.35010788E-02   -1.52472074E-02   -1.61489584E-02
24                -8.72727248E-03   -1.19989061E-02   -1.39834635E-02
25                -1.61964923E-03   -7.05479557E-03   -1.05315776E-02
26                 8.71109102E-03    9.45009381E-05   -5.45311500E-03
27                 2.40072125E-02    1.02129909E-02    1.69761994E-03
28                 5.03707133E-02    2.47384460E-02    1.15645519E-02
29                -1.84943758E-02    4.84384433E-02    2.53004581E-02
```

Table A-2

Matrix elements for a rigid sphere gas and a Maxwellian gas.

```
MATRIX OF QUOTIENTS JRL/J02 FOR RIGID SPHERES FOR L=    0
   0.        0.        0.        0.        0.        0.        0.        0.
   0.        0.        0.        0.        0.        0.        0.        0.
   0.        0.        0.66667  -0.15430  -0.01818  -0.00433  -0.00130  -0.00044
   0.        0.       -0.15430   1.10714  -0.28200  -0.03712  -0.00982  -0.00324
   0.        0.       -0.01818  -0.28200   1.43288  -0.39006  -0.05495  -0.01557
   0.        0.       -0.00433  -0.03712  -0.39006   1.74397  -0.48438  -0.07148
   0.        0.       -0.00130  -0.00982  -0.05495  -0.48438   1.99892  -0.56863
   0.        0.       -0.00044  -0.00324  -0.01557  -0.07148  -0.56863   2.22791

MATRIX OF QUOTIENTS JMRL/JM02 FOR MAXWELLIAN MOLECULES FOR L =    0
  -0.        0.        0.        0.        0.        0.        0.        0.
   0.       -0.        0.        0.        0.        0.        0.        0.
   0.        0.        0.66667   0.        0.        0.        0.        0.
   0.        0.        0.        1.00000   0.        0.        0.        0.
   0.        0.        0.        0.        1.22814   0.        0.        0.
   0.        0.        0.        0.        0.        1.40369   0.        0.
   0.        0.        0.        0.        0.        0.        1.54745   0.
   0.        0.                  0.        0.        0.        0.        1.65980
```

```
MATRIX OF QUOTIENTS JRL/JO2 FOR RIGID SPHERES FOR L=     1
  0.         0.         0.         0.         0.         0.         0.         0.
  0.         0.66667   -0.12599   -0.01286   -0.00274   -0.00075   -0.00024   -0.00008
  0.        -0.12599    1.07143   -0.25030   -0.03057   -0.00758   -0.00237   -0.00083
  0.        -0.01286   -0.25030    1.40303   -0.35867   -0.04817   -0.01307   -0.00444
  0.        -0.00274   -0.03057   -0.35867    1.68819   -0.45413   -0.06480   -0.01868
  0.        -0.00075   -0.00758   -0.04817   -0.45413    1.94075   -0.53969   -0.08036
  0.        -0.00024   -0.00237   -0.01307   -0.06480   -0.53969    2.16905   -0.61755
  0.        -0.00008   -0.00083   -0.00444   -0.01868   -0.08036   -0.61755    2.37653

MATRIX OF QUOTIENTS JMRL/JMO2 FOR MAXWELLIAN MOLECULES FOR L =   1
 -0.         0.         0.         0.         0.         0.         0.         0.
  0.         0.66667    0.         0.         0.         0.         0.         0.
  0.         0.         1.00000    0.         0.         0.         0.         0.
  0.         0.         0.         1.22814    0.         0.         0.         0.
  0.         0.         0.         0.         1.40369    0.         0.         0.
  0.         0.         0.         0.         0.         1.54745    0.         0.
  0.         0.         0.         0.         0.         0.         1.66980    0.
  0.         0.         0.         0.         0.         0.         0.         1.77672
```

```
MATRIX OF QUOTIENTS JRL/JO2 FOR RIGID SPHERES FOR L=     2
   1.00000  -0.13363  -0.01114  -0.00206  -0.00050  -0.00014  -0.00005  -0.00002
  -0.13363   1.22024  -0.24256  -0.02629  -0.00593  -0.00171  -0.00056  -0.00020
  -0.01114  -0.24256   1.47433  -0.34443  -0.04289  -0.01092  -0.00351  -0.00127
  -0.00206  -0.02629  -0.34443   1.71982  -0.43686  -0.05914  -0.01628  -0.00562
  -0.00050  -0.00593  -0.04289  -0.43686   1.94952  -0.52098  -0.07460  -0.02169
  -0.00014  -0.00171  -0.01092  -0.05914  -0.52098   2.16361  -0.59818  -0.08920
  -0.00005  -0.00056  -0.00351  -0.01628  -0.07460  -0.59818   2.36377  -0.66967
  -0.00002  -0.00020  -0.00127  -0.00562  -0.02169  -0.08920  -0.66967   2.55181
```

```
MATRIX OF QUOTIENTS JMRL/JMO2 FOR MAXWELLIAN MOLECULES FOR L =   2
   1.00000  0.        0.        0.        0.        0.        0.        0.
   0.       1.16667   0.        0.        0.        0.        0.        0.
   0.       0.        1.34222   0.        0.        0.        0.        0.
   0.       0.        0.        1.49147   0.        0.        0.        0.
   0.       0.        0.        0.        1.61932   0.        0.        0.
   0.       0.        0.        0.        0.        1.73098   0.        0.
   0.       0.        0.        0.        0.        0.        1.83018   0.
   0.       0.        0.        0.        0.        0.        0.        1.91966
```

```
MATRIX OF QUOTIENTS JRL/J02 FOR RIGID SPHERES FOR L=     3
   1.50000  -0.22728  -0.02094  -0.00420  -0.00111  -0.00034  -0.00011  -0.00004
  -0.22728   1.64187  -0.33299  -0.03730  -0.00873  -0.00262  -0.00089  -0.00033
  -0.02094  -0.33299   1.82502  -0.42449  -0.05337  -0.01381  -0.00453  -0.00167
  -0.00420  -0.03730  -0.42449   2.01665  -0.50737  -0.06879  -0.01908  -0.00667
  -0.00111  -0.00873  -0.05337  -0.50737   2.20584  -0.58362  -0.08343  -0.02435
  -0.00034  -0.00262  -0.01381  -0.06879  -0.58362   2.38887  -0.65445  -0.09730
  -0.00011  -0.00089  -0.00453  -0.01908  -0.08343  -0.65445   2.56438  -0.72075
  -0.00004  -0.00033  -0.00167  -0.00667  -0.02435  -0.09730  -0.72075   2.73323


MATRIX OF QUOTIENTS JMRL/JM02 FOR MAXWELLIAN MOLECULES FOR L =   3
   1.50000  0.        0.        0.        0.        0.        0.        0.
   0.       1.57036   0.        0.        0.        0.        0.        0.
   0.       0.        1.66702   0.        0.        0.        0.        0.
   0.       0.        0.        1.76308   0.        0.        0.        0.
   0.       0.        0.        0.        1.85333   0.        0.        0.
   0.       0.        0.        0.        0.        1.93709   0.        0.
   0.       0.        0.        0.        0.        0.        2.01478   0.
   0.       0.        0.        0.        0.        0.        0.        2.08705
```

```
MATRIX OF QUOTIENTS JRL/J02 FOR RIGID SPHERES FOR L=     4
    1.81746  -0.28511  -0.02751  -0.00580  -0.00160  -0.00051  -0.00018  -0.00007
   -0.28511   1.95626  -0.39733  -0.04519  -0.01082  -0.00333  -0.00116  -0.00044
   -0.02751  -0.39733   2.11310  -0.48704  -0.06137  -0.01603  -0.00533  -0.00200
   -0.00580  -0.04519  -0.48704   2.27649  -0.56603  -0.07650  -0.02128  -0.00750
   -0.00160  -0.01082  -0.06137  -0.56603   2.44032  -0.63809  -0.09073  -0.02648
   -0.00051  -0.00333  -0.01603  -0.07650  -0.63809   2.60160  -0.70499  -0.10418
   -0.00018  -0.00116  -0.00533  -0.02128  -0.09073  -0.70499   2.75895  -0.76775
   -0.00007  -0.00044  -0.00200  -0.00750  -0.02648  -0.10418  -0.76775   2.91182


MATRIX OF QUOTIENTS JMRL/JM02 FOR MAXWELLIAN MOLECULES FOR L =    4
    1.87313   0.        0.        0.        0.        0.        0.        0.
    0.        1.91062   0.        0.        0.        0.        0.        0.
    0.        0.        1.86334   0.        0.        0.        0.        0.
    0.        0.        0.        2.02864   0.        0.        0.        0.
    0.        0.        0.        0.        2.09168   0.        0.        0.
    0.        0.        0.        0.        0.        2.15324   0.        0.
    0.        0.        0.        0.        0.        0.        2.21268   0.
    0.        0.        0.        0.        0.        0.        0.        2.26972
```

```
MATRIX OF QUOTIENTS JRL/JO2 FOR RIGID SPHERES FOR L=    5
   2.04365  -0.31961  -0.03134  -0.00677  -0.00193  -0.00063  -0.00023  -0.00009
  -0.31961   2.19480  -0.44098  -0.05027  -0.01216  -0.00380  -0.00136  -0.00052
  -0.03134  -0.44098   2.34576  -0.53334  -0.06693  -0.01754  -0.00587  -0.00223
  -0.00677  -0.05027  -0.53334   2.49686  -0.61222  -0.08217  -0.02284  -0.00807
  -0.00193  -0.01216  -0.06693  -0.61222   2.64679  -0.68298  -0.09633  -0.02802
  -0.00063  -0.00380  -0.01754  -0.08217  -0.68298   2.79446  -0.74811  -0.10963
  -0.00023  -0.00136  -0.00587  -0.02284  -0.09633  -0.74811   2.93917  -0.80894
  -0.00009  -0.00052  -0.00223  -0.00807  -0.02802  -0.10963  -0.80894   3.08057


MATRIX OF QUOTIENTS JMRL/JMO2 FOR MAXWELLIAN MOLECULES FOR L =   5
   2.18283  0.        0.        0.        0.        0.        0.        0.
   0.        2.20659  0.        0.        0.        0.        0.        0.
   0.        0.        2.24145  0.        0.        0.        0.        0.
   0.        0.        0.        2.28236  0.        0.        0.        0.
   0.        0.        0.        0.        2.32515  0.        0.        0.
   0.        0.        0.        0.        0.        2.37099  0.        0.
   0.        0.        0.        0.        0.        0.        2.41586  0.
   0.        0.        0.        0.        0.        0.        0.        2.46017
```

```
MATRIX OF QUOTIENTS JRL/J02 FOR RIGID SPHERES FOR L=     6
   2.22122  -0.34009  -0.03327  -0.00726  -0.00210  -0.00070  -0.00026  -0.00010
  -0.34009   2.38307  -0.46987  -0.05319  -0.01289  -0.00406  -0.00147  -0.00058
  -0.03327  -0.46987   2.53527  -0.56648  -0.07043  -0.01841  -0.00618  -0.00236
  -0.00726  -0.05319  -0.56648   2.68229  -0.64726  -0.08598  -0.02379  -0.00840
  -0.00210  -0.01289  -0.07043  -0.64726   2.82556  -0.71858  -0.10030  -0.02901
  -0.00070  -0.00406  -0.01841  -0.08598  -0.71858   2.96552  -0.78350  -0.11366
  -0.00026  -0.00147  -0.00618  -0.02379  -0.10030  -0.78350   3.10229  -0.84372
  -0.00010  -0.00058  -0.00236  -0.00840  -0.02901  -0.11366  -0.84372   3.23593


MATRIX OF QUOTIENTS JMRL/JM02 FOR MAXWELLIAN MOLECULES FOR L =   6
   2.45323   0.        0.        0.        0.        0.        0.        0.
   0.        2.47033   0.        0.        0.        0.        0.        0.
   0.        0.        2.49363   0.        0.        0.        0.        0.
   0.        0.        0.        2.52154   0.        0.        0.        0.
   0.        0.        0.        0.        2.55245   0.        0.        0.
   0.        0.        0.        0.        0.        2.58517   0.        0.
   0.        0.        0.        0.        0.        0.        2.61889   0.
   0.        0.        0.        0.        0.        0.        0.        2.65303
```

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MATRIX OF QUOTIENTS JRL/J02 FOR RIGID SPHERES FOR L=    7
   2.37148  -0.35244  -0.03401  -0.00741  -0.00216  -0.00073  -0.00027  -0.00011
  -0.35244   2.53898  -0.48883  -0.05459  -0.01317  -0.00415  -0.00151  -0.00060
  -0.03401  -0.48883   2.69343  -0.58975  -0.07235  -0.01878  -0.00630  -0.00242
  -0.00741  -0.05459  -0.58975   2.83969  -0.67319  -0.08827  -0.02423  -0.00853
  -0.00216  -0.01317  -0.07235  -0.67319   2.98016  -0.74605  -0.10285  -0.02950
  -0.00073  -0.00415  -0.01878  -0.08827  -0.74605   3.11610  -0.81176  -0.11638
  -0.00027  -0.00151  -0.00630  -0.02423  -0.10285  -0.81176   3.24820  -0.87226
  -0.00011  -0.00060  -0.00242  -0.00853  -0.02950  -0.11638  -0.87226   3.37687


MATRIX OF QUOTIENTS JMRL/JM02 FOR MAXWELLIAN MOLECULES FOR L =    7
   2.69640  0.        0.        0.        0.        0.        0.        0.
   0.        2.70979  0.        0.        0.        0.        0.        0.
   0.        0.        2.72655  0.        0.        0.        0.        0.
   0.        0.        0.        2.74542  0.        0.        0.        0.
   0.        0.        0.        0.        2.76876  0.        0.        0.
   0.        0.        0.        0.        0.        2.79291  0.        0.
   0.        0.        0.        0.        0.        0.        2.81833  0.
   0.        0.        0.        0.        0.        0.        0.        2.84459
```

```
MATRIX OF QUOTIENTS JRL/J02 FOR RIGID SPHERES FOR L=    8
   2.50540  -0.36009  -0.03404  -0.00734  -0.00214  -0.00073  -0.00027  -0.00011
  -0.36009   2.67412  -0.50135  -0.05499  -0.01313  -0.00413  -0.00150  -0.00060
  -0.03404  -0.50135   2.82965  -0.60599  -0.07312  -0.01879  -0.00627  -0.00240
  -0.00734  -0.05499  -0.60599   2.97585  -0.69213  -0.08939  -0.02428  -0.00850
  -0.00214  -0.01313  -0.07312  -0.69213   3.11514  -0.76688  -0.10424  -0.02960
  -0.00073  -0.00413  -0.01879  -0.08939  -0.76688   3.24902  -0.83388  -0.11799
  -0.00027  -0.00150  -0.00627  -0.02428  -0.10424  -0.83388   3.37845  -0.89520
  -0.00011  -0.00060  -0.00240  -0.00850  -0.02960  -0.11799  -0.89520   3.50406
```

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MATRIX OF QUOTIENTS JMRL/JM02 FOR MAXWELLIAN MOLECULES FOR L =   8
   2.91932   0.        0.        0.        0.        0.        0.        0.
   0.        2.93035   0.        0.        0.        0.        0.        0.
   0.        0.        2.94320   0.        0.        0.        0.        0.
   0.        0.        0.        2.95803   0.        0.        0.        0.
   0.        0.        0.        0.        2.97468   0.        0.        0.
   0.        0.        0.        0.        0.        2.99284   0.        0.
   0.        0.        0.        0.        0.        0.        3.01222   0.
   0.        0.        0.        0.        0.        0.        0.        3.03252
```

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MATRIX OF QUOTIENTS JRL/J02 FOR RIGID SPHERES FOR L=    9
   2.62874  -0.36506  -0.03369  -0.00716  -0.00207  -0.00070  -0.00027  -0.00011
  -0.36506   2.79574  -0.50978  -0.05475  -0.01289  -0.00402  -0.00146  -0.00058
  -0.03369  -0.50978   2.95073  -0.61737  -0.07312  -0.01854  -0.00614  -0.00234
  -0.00716  -0.05475  -0.61737   3.09647  -0.70591  -0.08964  -0.02405  -0.00835
  -0.00207  -0.01289  -0.07312  -0.70591   3.23494  -0.78255  -0.10474  -0.02939
  -0.00070  -0.00402  -0.01854  -0.08964  -0.78255   3.36758  -0.85099  -0.11871
  -0.00027  -0.00146  -0.00614  -0.02405  -0.10474  -0.85099   3.49537  -0.91339
  -0.00011  -0.00058  -0.00234  -0.00835  -0.02939  -0.11871  -0.91339   3.61905


MATRIX OF QUOTIENTS JMRL/JM02 FOR MAXWELLIAN MOLECULES FOR L =    9
   3.12640   0.        0.        0.        0.        0.        0.        0.
   0.        3.13577   0.        0.        0.        0.        0.        0.
   0.        0.        3.14613   0.        0.        0.        0.        0.
   0.        0.        0.        3.15772   0.        0.        0.        0.
   0.        0.        0.        0.        3.17[illegible]   0.        0.        0.
   0.        0.        0.        0.        0.        3.18456   0.        0.
   0.        0.        0.        0.        0.        0.        3.19957   0.
   0.        0.        0.        0.        0.        0.        0.        3.21545
```

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MATRIX OF QUOTIENTS JRL/J02 FOR RIGID SPHERES FOR L=   10
   2.74466  -0.36845  -0.03312  -0.00691  -0.00197  -0.00067  -0.00025  -0.00010
  -0.36845   2.90823  -0.51563  -0.05414  -0.01254  -0.00387  -0.00139  -0.00055
  -0.03312  -0.51563   3.08135  -0.62548  -0.07261  -0.01813  -0.00594  -0.00225
  -0.00691  -0.05414  -0.62548   3.20587  -0.71601  -0.08929  -0.02362  -0.00811
  -0.00197  -0.01254  -0.07261  -0.71601   3.34331  -0.79434  -0.10459  -0.02896
  -0.00067  -0.00387  -0.01813  -0.08929  -0.79434   3.47486  -0.86417  -0.11875
  -0.00025  -0.00139  -0.00594  -0.02362  -0.10459  -0.86417   3.60144  -0.92771
  -0.00010  -0.00055  -0.00225  -0.00811  -0.02896  -0.11875  -0.92771   3.72375


MATRIX OF QUOTIENTS JMRL/JM02 FOR MAXWELLIAN MOLECULES FOR L =  10
   3.32065  0.        0.        0.        0.        0.        0.        0.
   0.        3.32877  0.        0.        0.        0.        0.        0.
   0.        0.        3.33744  0.        0.        0.        0.        0.
   0.        0.        0.        3.34685  0.        0.        0.        0.
   0.        0.        0.        0.        3.35710  0.        0.        0.
   0.        0.        0.        0.        0.        3.36819  0.        0.
   0.        0.        0.        0.        0.        0.        3.38008  0.
   0.        0.        0.        0.        0.        0.        0.        3.39267
```

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MATRIX OF QUOTIENTS JRL/J02 FOR RIGID SPHERES FOR L=   11
   2.85493  -0.37089  -0.03247  -0.00664  -0.00187  -0.00063  -0.00024  -0.00010
  -0.37089   3.01426  -0.51984  -0.05331  -0.01212  -0.00369  -0.00132  -0.00052
  -0.03247  -0.51984   3.16460  -0.63139  -0.07178  -0.01762  -0.00570  -0.00214
  -0.00664  -0.05331  -0.63139   3.30721  -0.72351  -0.08855  -0.02306  -0.00783
  -0.00187  -0.01212  -0.07178  -0.72351   3.44319  -0.80327  -0.10397  -0.02838
  -0.00063  -0.00369  -0.01762  -0.08855  -0.80327   3.57350  -0.87435  -0.11828
  -0.00024  -0.00132  -0.00570  -0.02306  -0.10397  -0.87435   3.69891  -0.93897
  -0.00010  -0.00052  -0.00214  -0.00783  -0.02838  -0.11828  -0.93897   3.82004


MATRIX OF QUOTIENTS JMRL/JM02 FOR MAXWELLIAN MOLECULES FOR L =  11
   3.50422  0.        0.        0.        0.        0.        0.        0.
   0.        3.51135   0.        0.        0.        0.        0.        0.
   0.        0.        3.51879   0.        0.        0.        0.        0.
   0.        0.        0.        3.52669   0.        0.        0.        0.
   0.        0.        0.        0.        3.53513   0.        0.        0.
   0.        0.        0.        0.        0.        3.54417   0.        0.
   0.        0.        0.        0.        0.        0.        3.55379   0.
   0.        0.        0.        0.        0.        0.        0.        3.56398
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