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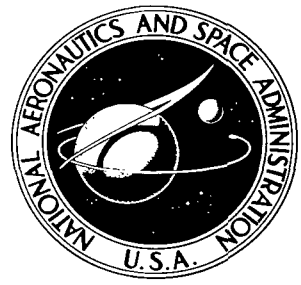

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STUDY OF A DIRECTIONAL-MEAN-FREE-PATH METHOD FOR GAS FLOW IN TRANSLATIONAL NONEQUILIBRIUM

by E. Dale Martin

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Moffett Field, Calif. 94035

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SUMMARY

A study is made of a new theoretical approach for the description of gas flows having strong deviations from local translational equilibrium (sufficient "rarefaction interaction"), when the Navier-Stokes equations become invalid. The usual approach in dealing with the limitations in the macroscopic description is to consider the kinetic level of description, governed by the Boltzmann equation, and perhaps to relate a kinetic analysis to higher approximations in the macroscopic level, by the Chapman-Enskog procedure. Because of (a) the general intractability of the Boltzmann equation or models of it, and (b) the limitation of the Chapman-Enskog theory to near-local-equilibrium flows, the present approach considers the development and possible utility of a directional level of description. Properties and equations on the directional level are obtained by integrating the molecular properties and the Boltzmann equation over all magnitudes of molecular velocity. The resulting dependent variables (properties of a class of molecules) then depend on space, time, and molecular-velocity direction, but not magnitude.

The development on the directional level, between the kinetic and macroscopic levels, is intended to exploit the significant directional aspects of translational nonequilibrium in describing the gas flow in regions of rapid variations of the flow variables. It is useful to consider a directional mean free path, defined as the average distance (measured relative to the observer) travelled by a molecule, moving in a designated direction, between collisions with other molecules. This free path is useful in formulating a physically intuitive model for approximating the "gain-term" collision integrals in the equations of change on the

directional level. The gain-term collision integrals on the directional level are replaced by terms that are related to appropriate corresponding "loss terms" evaluated at a point a directional mean free path away and at a mean collision time in the past. Several intuitive directional-average collision models are proposed for use in the directional-mean-free-path approximation.

Use of the directional-mean-free-path approximation leaves the equations on the directional level in a form where use of Lagrange's expansion for further approximation appears natural. For more than one independent variable, generalizations of Lagrange's expansion are needed, and simple forms that are directly applicable are derived. A perturbation-expansion scheme based on these generalizations is also developed. This scheme is then applied to the equations in the directional-mean-free-path method, to simplify the theory.

The use of the directional-mean-free-path method is illustrated by an outlined application to the problem of steady-flow shock-wave structure in a monatomic gas. The main value of the method would be expected to be realized only after an extension of the theory to include the effects of boundaries, for application to problems that may not be tractable by more detailed kinetic-theory methods.

FOREWORD

This report is based on a dissertation submitted to the Department of Aeronautics and Astronautics at Stanford University in May 1968 in partial fulfillment of the requirements for the Ph.D. degree. During the investigation covered by this report, the author was a member of the staff of Ames Research Center.

The author wishes to express appreciation to his adviser at Stanford, Professor Krishnamurty Karamcheti, for encouragement and many stimulating discussions during the course of the research and for helpful criticism of the manuscript. The author also sincerely appreciated inspiring discussions with, and continued interest of, Professor Maurice Rasmussen (now at the University of Oklahoma), who followed closely the progress of the research. Special thanks are due also to Professor I-Dee Chang for reading the manuscript and offering helpful comments.

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CHAPTER I

INTRODUCTION

This study introduces a new theoretical approach to the description of gas flow. This approach may eventually lead to the solution of gas-dynamic problems not accurately governed by the Navier-Stokes or higher-order continuum descriptions, and not sufficiently tractable by kinetic-theory methods.

The limitations of the Navier-Stokes equations, and of the higher-order approximations of the macroscopic-moment equations on the continuum level (obtained, e.g., by the Chapman-Enskog procedure), are well-known in the calculation of gas flows that are too far out of translational equilibrium (see, e.g., Grad 1958, 1960, 1963, 1966). The usual approach is then to consider the kinetic level of description, either by synthetic representations of the velocity distribution function, or by the theory of the Boltzmann equation or models of it. An analysis on the kinetic level may be related to higher approximations on the macroscopic level, as by the Chapman-Enskog procedure.

Synthetic methods of approximating the velocity distribution function are represented by: the bimodal-distribution method of Mott-Smith (1951); generalizations of this, including a trimodal distribution function, by Krook (1959) (see Anderson and Macomber 1965); the "two-stream" and "two-fluid" methods, which are somewhat analogous to the bimodal-distribution method, by Lees (1959) (see also Liu and Lees 1961) and Glansdorff (1961, 1962); and the ellipsoidal-distribution-function method of Holway (1965, 1967). These approximate methods are of considerable value. Some limitations have been discussed by Liepmann, Narasimha, and Chahine (1966).

Models of the Boltzmann equation, in particular the BGK, or Krook-Welander, model (Bhatnagar, Gross, and Krook 1954; Welander 1954) have been useful. Recently a more sophisticated conceptual extension and generalization (of the BGK model), the ellipsoidal-statistical model, has been presented by Holway (1966). The validity of the BGK model may be

limited in some problems by: (a) its equivalence to replacing the "gain-term" collision integral for a given point in the flow by an expression that assumes molecules come out of collisions in equilibrium with the gas at that point (cf. Liepmann, Narasimha, and Chahine 1962), or (b) its equivalence to a "first iteration" of the Boltzmann equation about a local-equilibrium velocity distribution (Gross 1954; also Rott 1964). In spite of the possible limitations, the BGK model does retain many important aspects of the Boltzmann equation for arbitrary nonequilibrium and has been, and will undoubtedly continue to be, extremely useful for kinetic-theory investigations. The noted limitations may be important in some problems, however. In addition, the model equations are still highly nonlinear integro-partial differential equations and are generally difficult to deal with.

The main purpose of the present study, then, is to investigate a new approach on what may be called the "directional level of description." The directional level deals with molecular quantities, or properties of a class of molecules, that have been integrated over, or averaged over, all magnitudes of molecular velocity; the dependent variables then all may depend on molecular-velocity direction, as well as on configuration-space coordinates and time. For each molecular property of interest, the appropriate equations are developed by one integration of the Boltzmann equation (over all molecular-velocity magnitudes). The treatment on the directional level is therefore between the kinetic level and the macroscopic level.

Theoretical analysis on the directional level may be more tractable than on the kinetic level, and may at the same time be capable of treating substantial translational nonequilibrium in gas flows, or substantial "rarefaction interaction." Detailed discussions motivating this approach are given in Chapters II and III. The basis may be noted here: that in many problems the translational nonequilibrium is essentially a directional phenomenon. Classic examples are shock waves and boundary layers, which are very thin nonequilibrium regions of rapid transition to a local-translational-equilibrium state. In those cases, the flow properties change most rapidly in a direction normal to the thin region. In

accounting for the significant directional aspects of translational nonequilibrium, the concept of a mean free path that varies with direction is useful.

In the most general form, the equations on the directional level are expected to be appropriate for approximate calculation of flows in arbitrary translational nonequilibrium because of the allowance for the variation of the flow properties with molecular-velocity direction.

This study of the new approach on the directional level may be considered to be preliminary. At various steps in the development, intuitive approximations are used; and the formulation is limited to apply only to sufficiently rarefied ("perfect") gases of similar, neutral, spherically symmetric, monatomic molecules. Also the effects of "surfaces," or condensed regions, adjacent to the gas flow have not been adequately considered. (The theory could in the future be much more highly developed, if such further developments appear justified.)

Chapters II and III include appropriate definitions and interpretations that are intended to both motivate and lay a formal rigorous foundation for the treatment on the directional level in terms of the directional mean free path.

Then in Chapter IV the directional-mean-free-path approximation for the gain-term collision integrals is introduced, along with several proposed intuitive "directional-average collision models"; and a scheme is outlined for making the system of equations on the directional level determined. The postulated intuitive models involved in the method are to be partially justified physically, but final justification for use of any model will lie in the tractability and utility it provides, in the qualitative or quantitative realism and consistency of the results it yields, and in its possible advantages over other methods.

Use of the directional-mean-free-path approximation will be seen to leave the equations on the directional level in a form amenable to treatment by vector generalizations of Lagrange's expansion, certain useful forms of which are developed in Chapter V. A perturbation-expansion scheme based on those generalizations, also developed in Chapter V, is then applied in Chapter VI to the equations for the directional-mean-free-

path method. As an illustration of the method, a description of the solution procedure for steady-flow shock-wave structure, according to a simplified first-order system of equations, is given in Chapter VII.

CHAPTER II

DISCUSSION OF MEAN-FREE-PATH CONCEPT

2.1 Definition of Mean Free Path

For proper understanding of the developments to follow, it is important to define precisely the mean free path. For a specified class of molecules, Maxwell's mean free path is defined as the average distance travelled by one molecule of that class between successive collisions with all other molecules. (Refer, e.g., to Jeans, 1954, 1952; Chapman and Cowling, 1961; or Vincenti and Kruger, 1965.) According to this definition, if ξ_{rel} is the magnitude of molecular velocity measured relative to some specified coordinate system, Maxwell's mean free path is formulated for the class of molecules under consideration as

$$\ell_{class} = \frac{\langle \xi_{rel} \rangle_{\text{average for class}}}{\Theta_{class}} \tag{2.1a}$$

$$= \text{average distance travelled per free path terminated by a molecule of the class} \tag{2.1b}$$

where

$$\langle \xi_{rel} \rangle_{\text{av for class}} \equiv \text{average distance travelled per unit time by a molecule of the class (measured in some coordinate system)} \tag{2.2a}$$

$$= \text{average } \underline{\text{velocity magnitude}} \text{ for molecules of the class, measured relative to some specified coordinate system} \tag{2.2b}$$

and where

$$\Theta_{class} \equiv \text{average number of free paths terminated per unit time by } \underline{\text{each molecule}} \text{ of the class within a very small volume (say } d\mathcal{V}_r\text{) about the point under consideration} \tag{2.3a}$$

$$= \text{average number of collisions per unit time experienced by } \underline{\text{each molecule}} \text{ of the class} \quad (2.3b)$$

$$= \frac{\left[\begin{array}{l}\text{probable number of molecules of the class} \\ \text{undergoing collisions per unit time in a} \\ \underline{\text{small volume}} \text{ about the point}\end{array}\right]}{\left[\begin{array}{l}\text{probable number of molecules of the class} \\ \text{in the small volume about the point}\end{array}\right]} \quad (2.3c)$$

which is denoted as the "average collision frequency per molecule of the class."*

In Chapter III, it will be convenient to consider various classes of molecules, to be defined. The collision frequencies, Θ_{class}, are calculated by considering velocities of molecules relative to another molecule, so concern over a specified reference frame does not enter

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*Note that for the particular class consisting of all molecules within a small differential volume $d\mathcal{V}_r$ about a point, the number of molecules undergoing collisions per unit time is twice the number of collisions per unit time, since each collision involves two molecules; thus, for this class,

$$\Theta = 2 \times \frac{\text{number of collisions per unit time in } d\mathcal{V}_r}{\text{number of molecules in } d\mathcal{V}_r}$$

However, the collision frequency of interest in eq. (2.1) is that denoted by Θ and calculated by (2.3a), (2.3b), or (2.3c), and not just the second factor in the above equation. For alternate, but similar, discussion see Vincenti and Kruger (1965), pp. 48-54. The appropriate collision frequencies will be calculated as needed, for each class considered, in a manner that does not involve concern over the factor of 2, namely by use of eqs. (2.3).

into the calculation of Θ_{class}; that is, the collision frequency per molecule of the class is not affected by the mean velocity of mass motion (e.g., see Jeans, 1954, p. 35). However, as noted in the definitions (2.2), each mean free path to be calculated will need to have the reference frame specified in which ξ_{rel} is measured. The distance travelled in unit time, or the velocity, measured in one reference frame is different from that measured relative to a reference frame moving with a different velocity. This fact is important to the discussions in the remainder of this chapter; and these discussions are important to understanding the method developed in Chapter IV.

2.2 Definitions for Calculation of Mean Free Paths

2.2.1 Configuration space, velocity space, phase space, and velocity distribution function

Consider the physical configuration space in which molecules of a gas are moving and interacting with each other, and let the reference frame of the observer be a system of Cartesian coordinates denoted by x_1, x_2, and x_3, with the orthogonal unit vectors $\vec{e}_1$, $\vec{e}_2$, and $\vec{e}_3$, respectively in the directions of the three space coordinates. A point in this space is defined by the position vector

$$\vec{r} \equiv \vec{e}_1 x_1 + \vec{e}_2 x_2 + \vec{e}_3 x_3 \tag{2.4}$$

Denote by

$$d\mathcal{V}_r \equiv dx_1\, dx_2\, dx_3 \tag{2.5}$$

a differential element of volume in the physical configuration space, and denote the range of all values of $\vec{r}$ within a certain $d\mathcal{V}_r$ by $(\vec{r}, d\mathcal{V}_r)$, which can also be thought of as the volume $d\mathcal{V}_r$ about a certain point $\vec{r}$.

Denote the velocity of a molecule, measured in this frame of reference, by

$$\vec{\xi} \equiv \vec{e}_1 \xi_1 + \vec{e}_2 \xi_2 + \vec{e}_3 \xi_3 \tag{2.6}$$

where the ξ_i are the Cartesian components of the molecular velocity. Consider molecular-velocity space (in which $\vec{\xi}$ is a "position vector") and denote a "differential volume of velocity space" by

$$d\mathcal{V}_\xi \equiv d\xi_1 \, d\xi_2 \, d\xi_3 \tag{2.7}$$

Then denote by $(\vec{\xi}, d\mathcal{V}_\xi)$ the range of all values of $\vec{\xi}$ within a certain $d\mathcal{V}_\xi$ or, equivalently, the volume $d\mathcal{V}_\xi$ about a certain point $\vec{\xi}$ in velocity space.

It is customary to speak of the "phase space" of a molecule as the six-dimensional hyper-space having coordinates $x_1, x_2, x_3, \xi_1, \xi_2, \xi_3$. A point in the molecular phase space can be defined by the six-dimensional "position vector" $\vec{x}$ with components $x_1, x_2, x_3, \xi_1, \xi_2, \xi_3$. A differential element of "volume" in this space about the point $\vec{x}$ can be denoted by $(\vec{x}, d\mathcal{V}_x)$, where

$$\begin{aligned} d\mathcal{V}_x &\equiv dx_1 \, dx_2 \, dx_3 \, d\xi_1 \, d\xi_2 \, d\xi_3 \\ &= d\mathcal{V}_r \, d\mathcal{V}_\xi \end{aligned} \tag{2.8}$$

If the total probable number of molecules in $(\vec{x}, d\mathcal{V}_x)$, (i.e., located in $(\vec{r}, d\mathcal{V}_r)$ and having molecular velocity in the range $(\vec{\xi}, d\mathcal{V}_\xi)$), at time t is denoted by $dN_{\vec{\xi}}$, then the probable number density at point $\vec{x}(\vec{r},\vec{\xi})$ in phase space at time t, called the velocity distribution function and denoted by $f(\vec{r},\vec{\xi},t)$, is defined by

$$dN_{\vec{\xi}} \equiv f(\vec{r},\vec{\xi},t) \, d\mathcal{V}_r \, d\mathcal{V}_\xi \tag{2.9}$$

If the total number of molecules in $(\vec{r},\ d\mathcal{V}_r)$ at time t is denoted by

$$dN \equiv \int_{all\,\vec{\xi}} dN_{\vec{\xi}} \tag{2.10a}$$

then the number density at point $\vec{r}$ in configuration space is

$$n(\vec{r},t) \equiv \frac{dN}{d\mathcal{V}_r} = \int_{all\,\vec{\xi}} f(\vec{r},\vec{\xi},t)\ d\mathcal{V}_\xi \tag{2.10b}$$

2.2.2 Collision frequency of a molecule

Denote by $d(\dot{N}_c)_{\vec{\xi}}$ the probable total number of molecules in $(\vec{r},\ d\mathcal{V}_r)$, $(\vec{\xi},\ d\mathcal{V}_\xi)$ that experience collisions with other molecules in unit time. Denote by $\vec{\xi}_a$ the velocity of each other molecule undergoing a collision with a molecule of velocity $\vec{\xi}$. Let $\vec{g}$ be the relative velocity before collision:

$$\vec{g} \equiv \vec{\xi}_a - \vec{\xi} \tag{2.11a}$$

and denote its magnitude by g:

$$g = |\vec{g}| = |\vec{\xi}_a - \vec{\xi}| \tag{2.11b}$$

For each $\vec{\xi}_a$, consider the plane that contains the center of the $\vec{\xi}$ molecule and that is perpendicular to the relative-velocity vector $\vec{g}$. Let b be the distance from the center of the $\vec{\xi}$ molecule in this plane, and let ε be an angle measured in this plane, centered at the $\vec{\xi}$ molecule. (Refer to Chapman and Cowling, 1961, p. 61, fig. 6. To aid understanding of the impact parameters b and ε, see also Chapman and Cowling, 1961, p. 57, fig. 3; and Vincenti and Kruger, 1965: fig. 5 in Chap. II (p. 37) and fig. 3 in Chap. IX (p. 351).) Then, as

is shown in many books on kinetic theory of gases,

$$d(\dot{N}_c)_{\vec{\xi}} = d\mathcal{V}_r \, d\mathcal{V}_\xi \int_{\text{all}\,\vec{\xi}_a} d\mathcal{V}_{\xi_a} \left[\int_0^{2\Pi} \int_0^{\sigma} f f_a \, g b db d\varepsilon \right] \tag{2.12a}$$

where σ is an effective "molecular diameter" (which in reality is infinite but which may be "truncated" at an appropriate value beyond which the effects of molecular interaction are negligible, depending on the nature of the intermolecular force potential; cf. Chapman and Cowling, 1961), and where $f = f(\vec{r},\vec{\xi},t)$ and $f_a \equiv f(\vec{r},\vec{\xi}_a,t)$. Then, since $f(\vec{r},\vec{\xi},t)$ is independent of $\vec{\xi}_a$, equation (2.12a) can be written as

$$d(\dot{N}_c)_{\vec{\xi}} = \Theta_{\vec{\xi}} \, dN_{\vec{\xi}} \tag{2.12b}$$

where $dN_{\vec{\xi}}$ is given by equation (2.9) and where

$$\Theta_{\vec{\xi}} = \Theta_{\vec{\xi}}(\vec{r},\vec{\xi},t) \equiv \frac{d(\dot{N}_c)_{\vec{\xi}}}{dN_{\vec{\xi}}} = \int_{\text{all}\,\vec{\xi}_a} d\mathcal{V}_{\xi_a} \left[\int_0^{2\Pi} \int_0^{\sigma} f_a \, g b db d\varepsilon \right] \tag{2.12c}$$

is the <u>probable fraction</u> of all the $dN_{\vec{\xi}}$ molecules in $(\vec{r},d\mathcal{V}_r)$, $(\vec{\xi},d\mathcal{V}_\xi)$ undergoing collisions per unit time. Thus $\Theta_{\vec{\xi}}$ is the collision frequency per molecule of the class of $dN_{\vec{\xi}}$, as defined by equation (2.3c)

The total number of molecules in $(\vec{r},d\mathcal{V}_r)$ undergoing collisions per unit time, denoted by $d\dot{N}_c$, is found by integrating equation (2.12a) over all $\vec{\xi}$:

$$d\dot{N}_c = \int_{\text{all}\,\vec{\xi}} \Theta_\xi \, dN_{\vec{\xi}} = d\mathcal{V}_r \int_{\text{all}\,\vec{\xi}} d\mathcal{V}_\xi \, f \int_{\text{all}\,\vec{\xi}_a} d\mathcal{V}_{\xi_a} \left[\int_0^{2\Pi} \int_0^{\sigma} f_a g b db d\varepsilon \right] \tag{2.13a}$$

This may also be written as

$$d\dot{N}_c = \theta \, dN \tag{2.13b}$$

where dN is the number in $(\vec{r}, d\mathscr{V}_r)$ (eq. 2.10)) and where, for the class of dN (all molecules in $(\vec{r}, d\mathscr{V}_r)$), θ is, according to equation (2.3c), and also from (2.13a) and (2.13b),

$$\theta = \theta(\vec{r},t) = \frac{d\dot{N}_c}{dN} = \frac{1}{n} \int_{\text{all}\vec{\xi}} \theta_{\vec{\xi}}(\vec{r},\vec{\xi},t) \, f(\vec{r},\vec{\xi},t) \, d\mathscr{V}_\xi \tag{2.13c}$$

This is the probable fraction of all the dN molecules undergoing collisions per unit time. The collision frequencies $\theta_{\vec{\xi}}$ and θ depend on the nature of the interaction potential and on the particular appropriate corresponding specification of σ.

2.2.3 Average values of molecular properties; mean mass velocity and peculiar (random) velocity

Each molecule may be said to have certain properties that may depend on its position, velocity, and time, and are denoted generally by $\phi = \phi(\vec{r},\vec{\xi},t)$. Examples are: mass/unit mass = 1; momentum/unit mass = $\vec{\xi}$; energy/unit mass = $\frac{1}{2}\xi^2$; $\vec{\xi}\vec{\xi}$; $\theta_{\vec{\xi}}$; etc. (These examples for ϕ can all be considered to be "specific" values of extensive molecular properties.) For any such molecular property, $\phi(\vec{r},\vec{\xi},t)$, one may define its average value, for the class of all molecules in $(r, d\mathscr{V}_r)$ (regardless of molecular velocity), as

$$\phi_{av}(\vec{r},t) = \left\langle \phi(\vec{r},\vec{\xi},t) \right\rangle \equiv \frac{\int_{\text{all}\vec{\xi}} \phi(\vec{r},\vec{\xi},t) \, dN_{\vec{\xi}}}{\int_{\text{all}\vec{\xi}} dN_{\vec{\xi}}}$$

$$= \frac{1}{n(\vec{r},t)} \int_{\text{all}\vec{\xi}} \phi(\vec{r},\vec{\xi},t) \, f(\vec{r},\vec{\xi},t) \, d\mathscr{V}_\xi \tag{2.14}$$

Particular examples of average values that are of concern in this chapter are found as follows: First, the mean mass velocity of the gas is defined by

$$\vec{V} \equiv \langle \vec{\xi} \rangle \tag{2.15}$$

Then the molecular velocity relative to the mean mass motion, denoted as the "random molecular velocity" or as the "peculiar velocity" is defined by

$$\vec{C} \equiv \vec{\xi} - \vec{V} \tag{2.16a}$$

$$= \vec{e}_1 C_1 + \vec{e}_2 C_2 + \vec{e}_3 C_3$$

where the C_i are the Cartesian components of $\vec{C}$. The magnitudes of the vectors $\vec{\xi}$ and $\vec{C}$ are, respectively,

$$\xi \equiv |\vec{\xi}| = (\xi_1^2 + \xi_2^2 + \xi_3^2)^{1/2} \tag{2.17}$$

$$C \equiv |\vec{C}| = (C_1^2 + C_2^2 + C_3^2)^{1/2}$$

Quantities that will be of interest below are the average values of ξ and C, found by taking $\phi = \xi$ and $\phi = C$ in equation (2.14) to obtain, respectively, $\langle \xi \rangle$ and $\langle C \rangle$. Note also that taking $\phi(\vec{r}, \vec{\xi}, t) = \Theta_{\vec{\xi}}$ (the probability of a molecule in the class $dN_{\vec{\xi}}$ undergoing a collision in unit time) one finds (cf. eq. (2.13c)):

$$\Theta = \Theta(\vec{r}, t) = \langle \Theta_{\vec{\xi}} \rangle \tag{2.19}$$

2.3 Mean Free Path for a Gas at Rest; and Mean Free Path Relative to Mean Motion of the Gas, λ

Maxwell's mean free path was originally calculated for a gas at rest, that is, with no overall mass motion, and in a uniform state (see derivations outlined by Jeans, 1952, and by Chapman and Cowling, 1961). In that case, $C = \xi$, and the average velocity magnitude measured relative to the reference frame of the observer (i.e., relative to the coordinates of $\vec{r}$ space; see § 2.2.1) is then $\langle C \rangle$. Then Maxwell's mean free path for the class of all molecules in a small volume about a point is, from (2.1a),

$$\ell_{(\vec{V}=0)} = \frac{\langle C \rangle}{\theta} \tag{2.20a}$$

For a gas composed of rigid elastic spheres, in equilibrium, and with no mean mass motion (see above references),

$$\theta = \sqrt{2}\, \pi\, n\, \sigma^2 \langle C \rangle \tag{2.20b}$$

so in that case (2.20a) becomes

$$\ell_{(\vec{V}=0)} = \frac{1}{\sqrt{2}\, \pi\, n\, \sigma^2} \tag{2.20c}$$

The notion of mean free path has been extremely useful in the extension to gases with nonvanishing mean mass motion $(\vec{V} \neq 0)$ for the calculation of transport phenomena (e.g., see especially Chapman and Cowling, 1961; Present, 1958; Lighthill, 1956; Hirschfelder, Curtiss, and Bird, 1964; Guggenheim, 1960; and Vincenti and Kruger, 1965). However, the mean free path used in that extension has been calculated from equations (2.20), or

$$\lambda \equiv \frac{\langle C \rangle}{\theta} \tag{2.21}$$

That is, the relative velocity magnitude in equations (2.1) and (2.2), or the average distance travelled by a molecule in unit time, has been measured in a reference frame that moves with the mean motion of the gas. One may therefore refer to λ, defined by equation (2.21), as the mean free path relative to the mean mass motion. As noted above (at the end of § 2.1), although θ is not affected by the mean velocity of mass motion $\vec{V}$, the calculation of the average velocity magnitude, $\langle \xi_{rel} \rangle_{av}$, does depend on the reference frame in which it is measured. This is further discussed in § 2.5.

2.4 Absolute Mean Free Path, λ^*

It will be found useful to consider what may be denoted as the absolute mean free path, defined by

$$\lambda^* \equiv \frac{\langle \xi \rangle}{\theta} \tag{2.22}$$

From the definitions (2.1) and (2.2), for the class of all molecules in $(\vec{r}, d\mathcal{V}_r)$, since ξ is the distance per unit time travelled by a molecule relative to the observer's reference frame (i.e., relative to the coordinates of the $\vec{r}$ space defined in § 2.2.1), λ^* is the average distance travelled, relative to the observer's reference frame, by a molecule between successive collisions. The significance of λ^*, and its comparison with λ, are discussed in § 2.5.

2.5 Comparison of λ^* with λ; and Significance of λ^*

In comparing λ^*, defined by equation (2.22), with λ, defined by equation (2.21), it will first be noted that if $\vec{V} = 0$, λ^* is the same as λ. However, at least for an equilibrium distribution with $\vec{V} \neq 0$, $\lambda^* > \lambda$. For example, consider a uniform flow of a gas in translational equilibrium with very large $\vec{V}$. Then within the mean collision time of a molecule,

$t_c = 1/\theta$, nearly all the molecules move a very large distance in the observer's reference frame. In fact $\lambda^* \to \infty$ as $\vec{V} \to \infty$. However, λ does not depend on $\vec{V}$. This illustration is made more precise by the calculation in the following paragraph.

Consider calculation of λ^* and λ for a gas having a Maxwellian distribution function

$$f = f_e \equiv n(\beta_e/\Pi)^{3/2} e^{-\beta_e C^2} \tag{2.23a}$$

and having mean mass velocity $\vec{V} = \langle \vec{\xi} \rangle$, with magnitude V, where

$$\beta_e \equiv \frac{m}{2kT} = \frac{1}{2RT} = \frac{\gamma/2}{a^2} \tag{2.23b}$$

and where m is the mass of a molecule, k is Boltzmann's constant, T is the gas temperature, γ is the ratio of specific heats of the gas (c_p/c_v), and $a = (\gamma RT)^{1/2}$ is the speed of sound in the gas. Without loss of generality, one can take $\vec{V} = \vec{e}_1 u$ for this calculation, since the x_1 axis can arbitrarily be aligned with the velocity vector. Then

$$C^2 = (\xi_1 - u)^2 + \xi_2^2 + \xi_3^2 \tag{2.23c}$$

It is readily found by substituting equations (2.23a-c) into equation (2.14) with $\phi = C$ that

$$\langle C \rangle = \frac{2}{\sqrt{\Pi \beta_e}} = \left(\frac{8kT}{\Pi\, m}\right)^{1/2} = \left(\frac{8}{\Pi\gamma}\right)^{1/2} a \tag{2.23d}$$

(cf. Chapman and Cowling, 1961, p. 74), and with $\phi = \xi$ that

$$\langle \xi \rangle = \frac{1}{\sqrt{\beta_e \Pi}} \left[e^{-\beta_e u^2} + \left(\frac{\Pi}{4\beta_e u^2}\right)^{1/2} (1 + 2\beta_e u^2)\ \mathrm{erf}\ (\sqrt{\beta_e}\, u) \right] \tag{2.23e}$$

where, by definition, the "error function" is

$$\operatorname{erf} \eta \equiv (2/\sqrt{\pi}) \int_0^{\eta} e^{-\zeta^2} \, d\zeta \tag{2.24}$$

With definition of the Mach number

$$M = u/a \ , \quad \text{or} \quad \sqrt{\beta_e}\, u = \sqrt{\gamma/2}\, M \equiv \bar{M} \tag{2.25}$$

and with use of the appropriate asymptotic expansions in equation (2.23e) for $M \to 0$ or $M \to \infty$, one finds: as $\sqrt{\beta_e}\, u = \bar{M} \to 0$:

$$\langle \xi \rangle = \langle C \rangle \left(1 + \frac{1}{3} \bar{M}^2 - \frac{1}{30} \bar{M}^4 + \frac{1}{210} \bar{M}^6 - + \cdots \right) \tag{2.23f}$$

and as $\sqrt{\beta_e}\, u = \bar{M} \to \infty$:

$$\langle \xi \rangle \sim u\{1 + \frac{1}{2} \bar{M}^{-2} + \pi^{-1/2} \bar{M}^{-1} e^{-\bar{M}^2} [- \frac{1}{2} \bar{M}^{-4} + O(\bar{M}^{-6})]\} \tag{2.23g}$$

Therefore, from the definitions (2.21) and (2.22), for this case of the Maxwellian distribution,

$$\frac{\lambda^*}{\lambda} \equiv \frac{\langle \xi \rangle}{\langle C \rangle} \sim 1 + \frac{1}{3} \bar{M}^2 + O(\bar{M}^4) \quad \text{as} \quad M \to 0 \tag{2.23h}$$

and

$$\frac{\lambda^*}{\lambda} \sim \frac{\pi^{1/2}}{2} \bar{M} \left[1 + \frac{1}{2} \bar{M}^{-2} + O(\bar{M}^{-5} e^{-\bar{M}^2})\right] \quad \text{as} \quad M \to \infty \tag{2.23i}$$

Hence, for small M, $\lambda^* \approx \lambda$; and for large M, $\lambda^*/\lambda = O(M)$.

One indication of the significance of λ^* is the following: Suppose we wish to consider the appropriate dimensionless parameter characterizing a molecular flow. Let L be a characteristic reference length of the problem, θ_r be a reference collision frequency per

molecule, and c_r be an appropriate reference velocity. Since $\lambda^* = \langle\xi\rangle/\theta$ is the actual mean free path relative to the observer, it is suggested that

$$Kn^* \equiv \left(\frac{\lambda^*}{L}\right)_{ref} = \left(\frac{\langle\xi\rangle}{L\,\theta}\right)_{ref} \tag{2.26a}$$

(a "Knudsen number based on the absolute mean free path") is the most appropriate characteristic dimensionless parameter, or

$$Kn^* = \frac{c_r}{L\theta_r} \tag{2.26b}$$

where

$$c_r = \langle\xi\rangle \tag{2.27}$$

The parameter $c_r/L\theta_r$ is Vincenti and Kruger's (1965, p. 380) parameter ξ or Liepmann, Narasimha, and Chahine's (1962, p. 1319) parameter $1/\alpha_o$ (the appropriate expansion parameter for the Chapman-Enskog procedure). Those writers made appropriate specifications of c_r for low speed flows and for high Mach numbers. Since, from (2.23f,g), $\langle\xi\rangle \sim \langle C\rangle$ as $M \to 0$ and $\langle\xi\rangle \sim u$ as $M \to \infty$, we see from (2.26) and (2.27) that use of λ^*, rather than λ, has led to a result for c_r (eq. (2.27)) that <u>automatically includes</u> the <u>separate</u> specifications of c_r for low-speed and high Mach number flows that were made by both Liepmann et al. (1962) and Vincenti and Kruger (1965).

The simplified calculations of the transport coefficients, from the elementary kinetic theory, treat molecules as carrying with them values of various properties (e.g., momentum) that are characteristic of the location of their last collision, a mean free path away (see references mentioned above, prior to equation (2.21)). Although λ^* is the actual mean free path relative to the observer, use of λ has been convenient, and its use is justified especially by the fact that the actual average free path of the molecules moving <u>normal</u> to the flow (used, e.g., in

calculating shear rate) is close to λ. However, for flows in which $\vec{V}$ is large and/or changes rapidly, use of λ^* (in a certain way) is suggested to be perhaps more appropriate than λ, and, in fact, use of a directional absolute mean free path (to be introduced in Chapter III) may be most appropriate in cases of significant translational nonequilibrium, where the directional mean free path of the molecules varies significantly with the direction of the molecular velocities.

CHAPTER III

THE DIRECTIONAL LEVEL OF DESCRIPTION AND ITS RELATION TO THE KINETIC AND MACROSCOPIC LEVELS

3.1 Introductory Remarks

The purpose of this chapter is to introduce the basic concepts, definitions, and formal equations that constitute the directional level of description. This formal development is to form the basis of a method for treating gas flows in translational nonequilibrium (introduced in Chapter IV). Because of the suggested importance of the directional aspects of significant translational nonequilibrium, it is proposed to treat each molecular-velocity direction separately, which is possible on the directional level. The role of the directional level of description in its relation to the kinetic and macroscopic levels is emphasized in the formulation.

It is convenient first to discuss the Boltzmann equation (§3.2), which involves both the collision frequency per molecule of the class $dN_{\vec{\xi}}$ (i.e., all molecules in $(\vec{r},d\mathscr{V}_r)$ with velocity in $(\vec{\xi},d\mathscr{V}_{\vec{\xi}})$; cf. eq. (2.9)) and the inverse collision frequency per molecule corresponding to that class. Then introduction of spherical coordinates in molecular-velocity space (§3.3) facilitates the subsequent formulation.

In Chapter II, different classes of molecules have already been mentioned. In particular were discussed: the class of all molecules in $(\vec{r},d\mathscr{V}_r)$ with velocity in $(\vec{\xi},d\mathscr{V}_\xi)$, and the class of all molecules in $(\vec{r},d\mathscr{V}_r)$ regardless of molecular velocity. In this chapter (in § 3.4) it is convenient to distinguish, and define precisely, four classes of molecules. For each of these classes, one can define certain properties and write equations of change for those properties. The Boltzmann equation applies on the kinetic level of description. One then can define the intermediate levels of description, involving marginal distributions of

molecular properties. Finally, one finds the full moment level, for which Enskog's general equation of change governs the various macroscopic properties, which are molecular properties integrated over (or averaged over) all molecular velocities. The directional level of description comprises an intermediate class, and its consideration will be found to be useful. In this connection, directional properties of the molecular motion are defined, including a mean free path that can be different for each molecular-velocity direction. Molecules with velocity in a certain direction can be thought of as constituting a "species" in a mixture of species of all directions, with each direction having its own mass density, momentum density, energy density, collision frequency per molecule, mean free path, etc. Equations of change can then be written for each of the "directional properties" (§ 3.12).

3.2 The Boltzmann Equation

The Boltzmann equation is an equation of change for the probable number of molecules in $(\vec{r},d\mathcal{V}_r),(\vec{\xi},d\mathcal{V}_\xi)$ at time t (eq. (2.9)),

$$dN_{\vec{\xi}} = f(\vec{r},\vec{\xi},t)\, d\mathcal{V}_r\, d\mathcal{V}_\xi \tag{3.1}$$

or for the probable number density, f, in phase space. Many derivations of the Boltzmann equation have been given (cf. Grad, 1958; Chapman and Cowling, 1961, pp. 46, 47, 63-66; or Hirschfelder, Curtiss, and Bird, 1964, pp. 444-452). The equation of change for $dN_{\vec{\xi}}$ in phase space involves a "net source term" owing to collisions. In writing the net source term one needs an expression for the number of molecules in $(\vec{r},d\mathcal{V}_r),(\vec{\xi},d\mathcal{V}_\xi)$ undergoing collisions per unit time, and hence the number lost from that class per unit time owing to collisions (cf. eqs. (2.12)):

$$d(\dot{N}_c)_{\vec{\xi}} = \Theta_{\vec{\xi}}\, dN_{\vec{\xi}} \tag{3.2}$$

where $\Theta_{\vec{\xi}}$, defined by (2.12c), is the fraction of the number $dN_{\vec{\xi}}$

undergoing collisions per unit time, and hence the fraction lost per unit time, and is denoted as the average collision frequency for a molecule of the class of $dN_{\vec{\xi}}$. One also needs an expression for the number of molecules undergoing "inverse collisions" per unit time that end up in $(\vec{r},d\mathcal{V}_r)$, $(\vec{\xi},d\mathcal{V}_\xi)$ after the collisions, or the probable number gained by that class per unit time owing to collisions:

$$d(\dot{N}'_c)_{\vec{\xi}} = d\mathcal{V}_r\, d\mathcal{V}_{\xi'} \int_{all\,\vec{\xi}'_a} d\mathcal{V}_{\xi'_a} \left[\int_0^{2\Pi} \int_0^{\sigma} f'f'_a\, g'b'\, db'\, d\varepsilon' \right] \tag{3.3a}$$

$$= f\, d\mathcal{V}_r\, d\mathcal{V}_\xi \int_{all\,\vec{\xi}_a} d\mathcal{V}_{\xi_a} \left[\int_0^{2\Pi} \int_0^{\sigma} \left(\frac{f'f'_a}{ff_a} \right) f_a\, g\, b\, db\, d\varepsilon \right] \tag{3.3b}$$

$$\equiv \Theta'_{\vec{\xi}}\, dN_{\vec{\xi}} \tag{3.3c}$$

where

$$\Theta'_{\vec{\xi}} \equiv \int_{all\,\vec{\xi}_a} d\mathcal{V}_{\xi_a} \left[\int_0^{2\Pi} \int_0^{\sigma} \left(\frac{f'f'_a}{ff_a} \right) f_a\, g\, b\, db\, d\varepsilon \right] \tag{3.3d}$$

is defined by equation (3.3c) as the fraction of the number $dN_{\vec{\xi}}$ that are put into $(\vec{r},d\mathcal{V}_r),(\vec{\xi},d\mathcal{V}_\xi)$ per unit time by inverse collisions. This fraction, Θ'_ξ, may be denoted as the "inverse collision frequency per molecule" for the class $dN_{\vec{\xi}}$. In equations (3.3),

$$\left.\begin{aligned} f' &\equiv f(\vec{r},\vec{\xi}',t)\ , \quad f'_a \equiv f(\vec{r},\vec{\xi}'_a,t) \\ \text{and} \\ g' &\equiv |\vec{g}'| \equiv |\vec{\xi}'_a - \vec{\xi}'| \end{aligned}\right\} \tag{3.4}$$

where $\vec{\xi}'$ and $\vec{\xi}'_a$ are the velocities of two molecules before an "inverse collision" or after a"direct collision." The velocities $\vec{\xi}'$ and $\vec{\xi}'_a$ are

not independent, but are related through the impact parameters and intermolecular potential to $\vec{\xi}$ and $\vec{\xi}_a$. In equation (3.3b) the well-known relations have been used:

$$d\mathscr{V}_{\xi'}\, d\mathscr{V}_{\xi_a'} = d\mathscr{V}_{\xi}\, d\mathscr{V}_{\xi_a} \quad ; \quad g' = g \quad ; \quad b' = b, \quad \varepsilon' = \varepsilon \tag{3.5}$$

In terms of $dN_{\vec{\xi}}$, the Boltzmann equation is written as

$$\frac{\partial}{\partial t}\left(dN_{\vec{\xi}}\right) + \nabla_r \cdot \left(\vec{\xi}\, dN_{\vec{\xi}}\right) + \nabla_\xi \cdot \left(\frac{\vec{F}_B}{m} dN_{\vec{\xi}}\right) = d(\dot{N}_c')_{\vec{\xi}} - d(\dot{N}_c)_{\vec{\xi}} \tag{3.6a}$$

$$\equiv \left(\Theta'_{\vec{\xi}} - \Theta_{\vec{\xi}}\right) dN_{\vec{\xi}} \tag{3.6b}$$

or, upon dividing by $d\mathscr{V}_r\, d\mathscr{V}_\xi$

$$\frac{\partial f}{\partial t} + \nabla_r \cdot (\vec{\xi} f) + \nabla_\xi \cdot \left(\frac{\vec{F}_B}{m} f\right) = \left(\Theta'_{\vec{\xi}} - \Theta_{\vec{\xi}}\right) f \tag{3.7}$$

where

$$\left.\begin{aligned} \nabla_r &\equiv \vec{e}_1 \frac{\partial}{\partial x_1} + \vec{e}_2 \frac{\partial}{\partial x_2} + \vec{e}_3 \frac{\partial}{\partial x_3} \\ \nabla_\xi &\equiv \vec{e}_1 \frac{\partial}{\partial \xi_1} + \vec{e}_2 \frac{\partial}{\partial \xi_2} + \vec{e}_3 \frac{\partial}{\partial \xi_3} \end{aligned}\right\} \tag{3.8}$$

and $\vec{F}_B$ is the external body force acting on a molecule.

3.3 Distribution Function in Spherical Coordinates in Molecular-Velocity Space

For subsequent developments it is convenient to transform the coordinates of velocity space to spherical coordinates.

With the molecular velocity $\vec{\xi}$ defined by equation (2.6) and its magnitude by (2.17), the transformation is

$$\left.\begin{aligned} \xi_1 &= \xi \cos \varphi \\ \xi_2 &= \xi \sin \varphi \cos \theta \\ \xi_3 &= \xi \sin \varphi \sin \theta \end{aligned}\right\} \qquad (3.9)$$

where, for a molecule located at point $\vec{r}$ and having velocity $\vec{\xi}$ (see figure 3.1), φ is the angle between the ξ_1 axis (which is parallel to the x_1 axis) and the molecular-velocity vector $\vec{\xi}$; and θ is the angle of the projection of the vector $\vec{\xi}$ on the plane of ξ_2, ξ_3 (which is parallel to the x_2, x_3 plane). The angle θ is measured from the ξ_2 axis, as shown on figure 3.1.

The unit vector in the direction of $\vec{\xi}$ is then defined by this transformation (3.9) and equation (2.6) as

$$\vec{e}_{\vec{\xi}} \equiv \frac{\vec{\xi}}{\xi} = \vec{e}_1 \cos \varphi + \vec{e}_2 \sin \varphi \cos \theta + \vec{e}_3 \sin \varphi \sin \theta \qquad (3.10a)$$

Noting that $\vec{e}_{\vec{\xi}}$ is a function only of θ and φ, we will also find it convenient to use the notation

$$\vec{e}_{\theta\varphi} = \vec{e}_{\theta\varphi}(\theta, \varphi) \equiv \vec{e}_{\vec{\xi}} \qquad (3.10b)$$

The transformation of the velocity-space volume element, $d\mathcal{V}_\xi$, is given by

$$d\mathcal{V}_\xi \equiv d\xi_1 \, d\xi_2 \, d\xi_3 = \left|\frac{\partial(\xi_1, \xi_2, \xi_3)}{\partial(\xi, \theta, \varphi)}\right| d\xi \, d\theta \, d\varphi \qquad (3.11a)$$

$$= \xi^2 \sin \varphi \, d\xi \, d\theta \, d\varphi \qquad (3.11b)$$

where $\dfrac{\partial(\xi_1, \xi_2, \xi_3)}{\partial(\xi, \theta, \varphi)}$ is the Jacobian determinant of the transformation. (From Fig. 3.1, the three edges of the volume element are $\xi d\varphi$, $\xi \sin\varphi \, d\theta$, and $d\xi$ which when multiplied together also give $d\mathcal{V}_\xi$ as eq. (3.11b).)

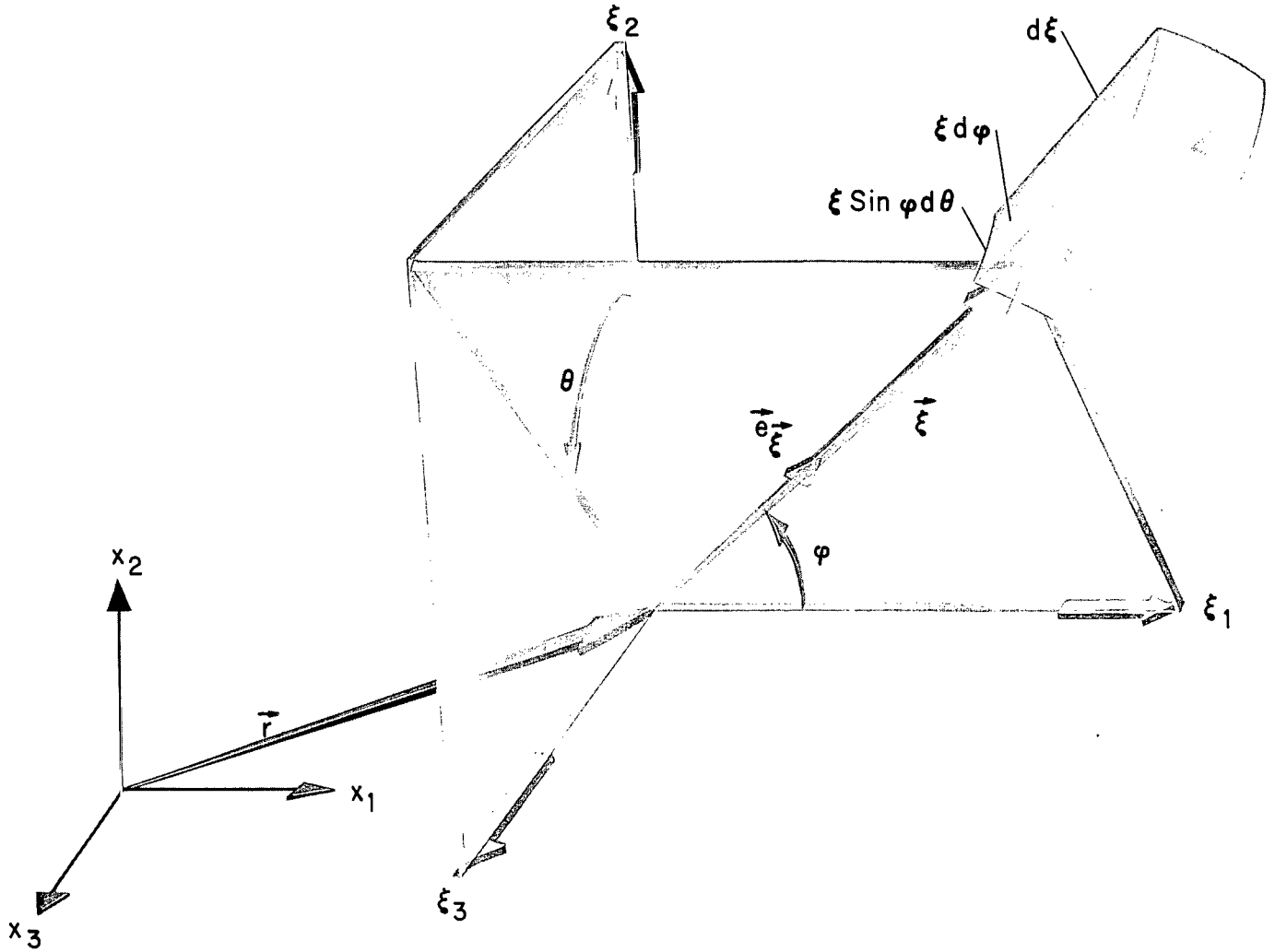

Figure 3.1 - Spherical coordinates in molecular-velocity space.

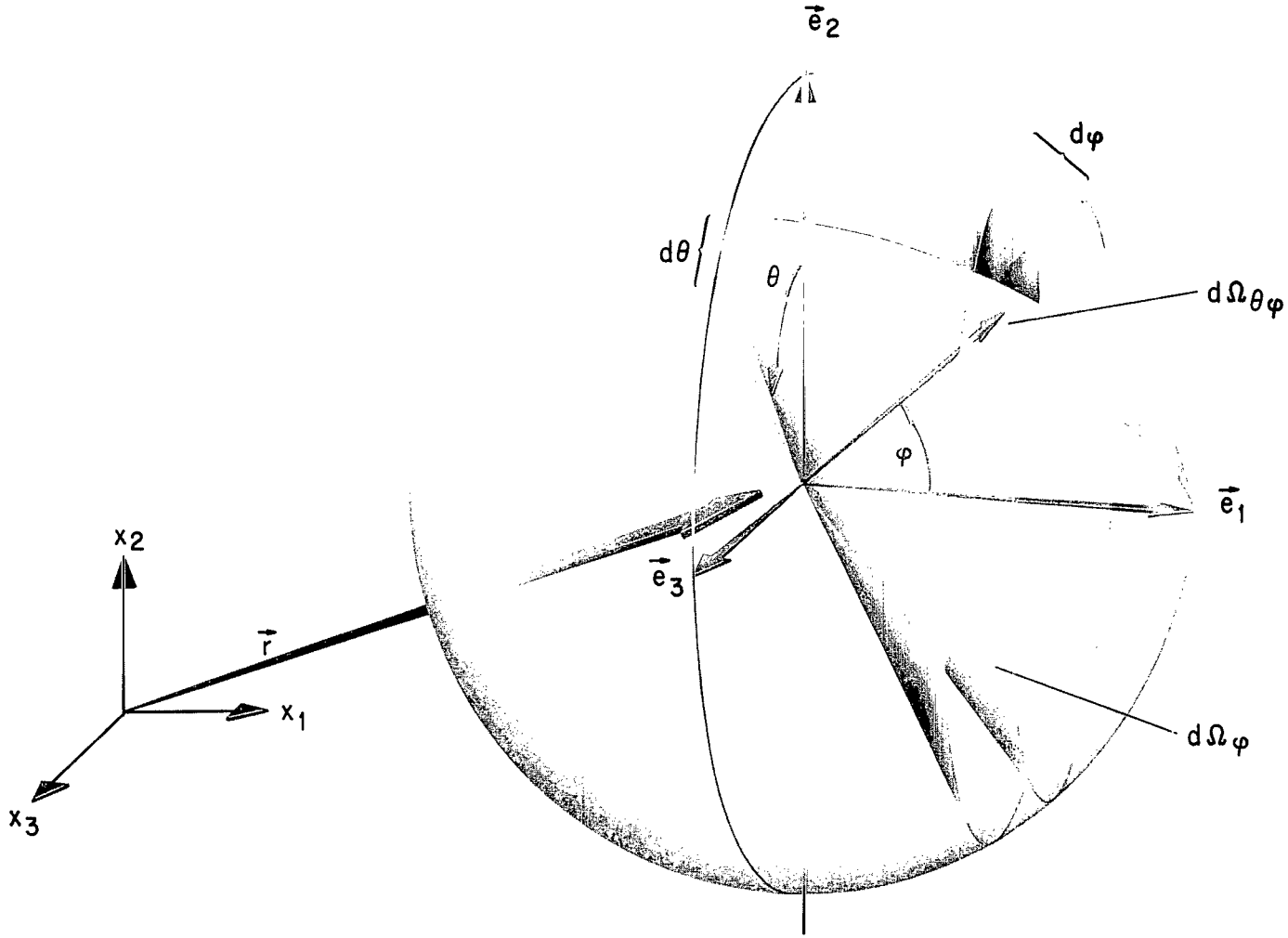

Figure 3.2 - The unit sphere and solid angles at a point $\vec{r}$.

It will be found convenient to also consider the solid angles in molecular-velocity space (see fig. 3.2):

$$d\Omega_{\theta\varphi} \equiv \sin\varphi \, d\varphi \, d\theta \tag{3.12}$$

$$d\Omega_{\varphi} \equiv \int_{\theta=-\Pi}^{\theta=\Pi} d\Omega_{\theta\varphi} = 2\Pi \sin\varphi \, d\varphi \tag{3.13}$$

in terms of which equations (3.11) may also be written as

$$d\mathcal{V}_{\xi} = \xi^2 \, d\xi \, d\Omega_{\theta\varphi} \tag{3.14a}$$

$$= \xi^2 \, d\xi \left(\frac{d\theta}{2\Pi}\right) d\Omega_{\varphi} \tag{3.14b}$$

(The significance of the subscripts $\vec{\xi}$, $\theta\varphi$, and φ is discussed in § 3.4.)

The velocity distribution function defined by equation (2.9) may be written with ξ, θ, φ as arguments. Thus define

$$f(\vec{r},\vec{\xi},t) \equiv f^*(\vec{r},\xi,\theta,\varphi,t) \tag{3.15}$$

From this point on, however, the superscript * in equation (3.15) will be dropped, with the understanding that $f(\vec{r},\xi,\theta,\varphi,t)$ is actually f^* defined in equation (3.15). Thus from equations (2.9), (3.11), (3.12), (3.13), and (3.14) we now have

$$\frac{dN_{\vec{\xi}}}{d\mathcal{V}_r} = f(\vec{r},\xi,\theta,\varphi,t) \, d\mathcal{V}_{\xi}$$

$$= f \, \xi^2 \, d\xi \, d\Omega_{\theta\varphi} \tag{3.16a}$$

$$= f \, \xi^2 \, d\xi \left(\frac{d\theta}{2\Pi}\right) d\Omega_{\varphi} \tag{3.16b}$$

$$= f \, \xi^2 \, d\xi \, d\theta \sin\varphi \, d\varphi \tag{3.16c}$$

3.4 Classes of Molecules Considered; Total Number and Notation for Each Class

The remainder of this chapter involves consideration of four classes of molecules:

(a) The class of all molecules in $(\vec{r},d\mathcal{V}_r)$ and having velocity in $(\vec{\xi},d\mathcal{V}_\xi)$ contains the number

$$dN_{\vec{\xi}} = d\mathcal{V}_r\, d\mathcal{V}_\xi\, f(\vec{r},\xi,\theta,\varphi,t) \tag{3.17a}$$

where the notation $(\vec{r},d\mathcal{V}_r),(\vec{\xi},d\mathcal{V}_\xi)$ has been defined in § 2.2.1. This class is denoted as the class $dN_{\vec{\xi}}$. The subscript $\vec{\xi}$ is to be used generally to denote quantities in this class, which can be functions of $\vec{\xi}$ (or of ξ, θ, φ), as well as of $\vec{r}$ and t.

(b) The class of all molecules in $(\vec{r},d\mathcal{V}_r)$ and having velocity direction in $(\theta, \varphi, d\Omega_{\theta\varphi})$ (regardless of the magnitude ξ) contains the total probable number

$$dN_{\theta\varphi} \equiv \int_{\xi=0}^{\xi=\infty} dN_{\vec{\xi}} = d\mathcal{V}_r\, d\Omega_{\theta\varphi} \int_0^\infty f\, \xi^2\, d\xi \tag{3.17b}$$

where $(\theta, \varphi, d\Omega_{\theta\varphi})$ indicates the range of θ and φ in the solid angle $d\Omega_{\theta\varphi}$ about the vector $\vec{e}_{\theta\varphi}(\theta,\varphi) = \vec{e}_{\vec{\xi}}$. (See fig. 3.2.) This class is denoted as the class $dN_{\theta\varphi}$. The subscript $\theta\varphi$ is to be used generally to denote quantities corresponding to this class which may be functions of θ and φ as well as of $\vec{r}$ and t (but not functions of the velocity magnitude ξ).

(c) The class of all molecules in $(\vec{r},d\mathcal{V}_r)$ and having velocity angles in $(\varphi,d\Omega_\varphi)$ (regardless of the values of ξ and θ) contains the total probable number

$$dN_\varphi \equiv \int_{\theta=-\Pi}^{\theta=\Pi} \int_{\xi=0}^{\xi=\infty} dN_{\vec{\xi}} = d\mathcal{V}_r\, d\Omega_\varphi \frac{1}{2\Pi} \int_{-\Pi}^{\Pi} d\theta \int_0^\infty f\, \xi^2\, d\xi \tag{3.17c}$$

where $(\varphi, d\Omega_\varphi)$ indicates a direction in the range $d\varphi$ about the angle φ anywhere in the solid angle $d\Omega_\varphi$ (see fig. 3.2). This class is denoted as the class dN_φ. The subscript φ is to be used generally to denote quantities corresponding to this class, which may be functions of φ, as well as of $\vec{r}$ and t (but not functions of ξ and θ).

(d) The class of all molecules in $(\vec{r}, d\mathcal{V}_r)$ (regardless of $\vec{\xi}$) contains the total probable number (cf. eqs. (2.10a,b))

$$dN \equiv \int_{\varphi=0}^{\varphi=\Pi} \int_{\theta=-\Pi}^{\theta=\Pi} \int_{\xi=0}^{\xi=\infty} dN_{\vec{\xi}} = d\mathcal{V}_r \int_0^{\Pi} d\varphi (\sin\varphi) \int_{-\Pi}^{\Pi} d\theta \int_0^{\infty} f\, \xi^2\, d\xi \qquad (3.17d)$$

This class is denoted as the class dN. Quantities corresponding to this class may be functions of $\vec{r}$ and t (but not of ξ, θ, or φ).

3.5 Total Number of Molecules Undergoing Collisions per Unit Time in Each Class of Molecules

For the class $dN_{\vec{\xi}}$, the total number of molecules undergoing collisions per unit time is given by equation (2.12b) as

$$d(\dot{N}_c)_{\vec{\xi}} = \Theta_{\vec{\xi}}\, dN_{\vec{\xi}} = d\mathcal{V}_r\, d\mathcal{V}_\xi\, \Theta_{\vec{\xi}}\, f \qquad (3.18a)$$

where $\Theta_{\vec{\xi}}$, defined by equation (2.12c), is the fraction of the number $dN_{\vec{\xi}}$ that undergo collisions per unit time (cf. eq. (2.3c)).

For the class $dN_{\theta\varphi}$, the total number of molecules undergoing collisions per unit time is

$$d(\dot{N}_c)_{\theta\varphi} \equiv \int_{\xi=0}^{\xi=\infty} d(\dot{N}_c)_{\vec{\xi}} = d\mathcal{V}_r\, d\Omega_{\theta\varphi} \int_0^{\infty} \Theta_{\vec{\xi}}\, f\, \xi^2\, d\xi$$

$$\equiv \Theta_{\theta\varphi}\, dN_{\theta\varphi} \qquad (3.18b)$$

which therefore defines $\Theta_{\theta\varphi}$ as the fraction of the number $dN_{\theta\varphi}$ that undergo collisions in unit time (cf. eq. (2.3c)).

For the class' dN_{φ}, the total number of molecules undergoing collisions per unit time is

$$d(\dot{N}_c)_{\varphi} \equiv \int_{\theta=-\Pi}^{\theta=\Pi} \int_{\xi=o}^{\xi=\infty} d(\dot{N}_c)_{\vec{\xi}} = d\mathscr{V}_r \, d\Omega_{\varphi} \frac{1}{2\Pi} \int_{-\Pi}^{\Pi} d\theta \int_{o}^{\infty} \Theta_{\vec{\xi}} \, f \, \xi^2 \, d\xi$$

$$\equiv \Theta_{\varphi} \, dN_{\varphi} \tag{3.18c}$$

which therefore defines Θ_{φ} as the fraction of the number dN_{φ} that undergo collisions in unit time (cf. eq. (2.3c)).

For the class dN, the total number of molecules undergoing collisions per unit time is

$$d\dot{N}_c \equiv \int_{\varphi=o}^{\varphi=\Pi} \int_{\theta=-\Pi}^{\theta=\Pi} \int_{\xi=o}^{\xi=\infty} d(\dot{N}_c)_{\vec{\xi}} = d\mathscr{V}_r \int_{o}^{\Pi} d\varphi (\sin\varphi) \int_{-\Pi}^{\Pi} d\theta \int_{o}^{\infty} \Theta_{\vec{\xi}} \, f \, \xi^2 \, d\xi$$

$$\equiv \Theta \, dN \tag{3.18d}$$

which defines Θ as the fraction of the number dN that undergo collisions in unit time (cf. eqs. (2.3c) and (2.13b)).

3.6 Total Number of Molecules Undergoing "Inverse Collisions" Per Unit Time Corresponding to Each Class of Molecules

For the class $dN_{\vec{\xi}}$, the total number of molecules undergoing "inverse collisions" (molecules that end up in the class $dN_{\vec{\xi}}$ after the collision) per unit time is given by equation (3.3c) as

$$d(\dot{N}'_c)_{\vec{\xi}} = \Theta'_{\vec{\xi}} \, dN_{\vec{\xi}} = d\mathscr{V}_r \, d\mathscr{V}_{\xi} \, \Theta'_{\vec{\xi}} \, f \tag{3.19a}$$

where $\Theta'_{\vec{\xi}}$, defined by equation (3.3d), is the fraction of the number $dN_{\vec{\xi}}$ that are put into the class $dN_{\vec{\xi}}$ per unit time by collisions.

For the class $dN_{\theta\varphi}$, the total number of molecules undergoing inverse collisions that end up in $(\vec{r},d\mathcal{V}_r)$ with molecular velocity in the direction range $(\theta, \varphi, d\Omega_{\theta\varphi})$ per unit time is

$$d(\dot{N}'_c)_{\theta\varphi} = \int_{\xi=o}^{\xi=\infty} d(\dot{N}'_c)_{\vec{\xi}} = d\mathcal{V}_r \, d\Omega_{\theta\varphi} \int_o^\infty \Theta'_{\vec{\xi}} \, f \, \xi^2 \, d\xi$$

$$= \Theta'_{\theta\varphi} \, dN_{\theta\varphi} \qquad (3.19b)$$

which <u>defines</u> $\Theta'_{\theta\varphi}$ as the fraction of the number $dN_{\theta\varphi}$ that are put into the class $dN_{\theta\varphi}$ per unit time owing to collisions.

For the class dN_φ, the total number of molecules undergoing inverse collisions that end up in $(\vec{r},d\mathcal{V}_r)$ with molecular velocity in the direction range $(\varphi, d\Omega_\varphi)$ per unit time is

$$d(\dot{N}'_c)_\varphi \equiv \int_{\theta=-\Pi}^{\theta=\Pi} \int_{\xi=o}^{\xi=\infty} d(\dot{N}'_c)_{\vec{\xi}} = d\mathcal{V}_r \, d\Omega_\varphi \, \frac{1}{2\Pi} \int_{-\Pi}^{\Pi} d\theta \int_o^\infty \Theta'_{\vec{\xi}} \, f \, \xi^2 \, d\xi$$

$$\equiv \Theta'_\varphi \, dN_\varphi \qquad (3.19c)$$

which <u>defines</u> Θ'_φ as the fraction of the number dN_φ that are put into the class dN_φ per unit time owing to collisions.

For the class dN, the total number of molecules undergoing inverse collisions in $(\vec{r},d\mathcal{V}_r)$ per unit time is

$$d\dot{N}'_c \equiv \int_{\varphi=o}^{\varphi=\Pi} \int_{\theta=-\Pi}^{\theta=\Pi} \int_{\xi=o}^{\xi=\infty} d(\dot{N}'_c)_{\vec{\xi}} = d\mathcal{V}_r \int_o^\Pi d\varphi \, (\sin\varphi) \int_{-\Pi}^{\Pi} d\theta \int_o^\infty \Theta'_{\vec{\xi}} \, f \, \xi^2 \, d\xi$$

$$\equiv \Theta' \, dN \qquad (3.19d)$$

which defines Θ' as the fraction of the number dN that undergo collisions per unit time, and is therefore equal to Θ, a well-known result (see § 3.12 below).

3.7 Molecular-Property-Density Distributions for Each Class of Molecules

3.7.1 Definition of property-density distributions for each class

For any molecular property $\phi(\vec{r},\vec{\xi},t)$ (cf. § 2.2.3 above and § 3.7.2 below) one can define expressions for the density distributions of the property ϕ for each class.

For the class $dN_{\vec{\xi}}$, the density of the molecular property ϕ per unit volume of configuration space and per unit volume of velocity space is defined simply as

$$\Phi_{\vec{\xi}}(\vec{r},\vec{\xi},t) \equiv \frac{\phi\, dN_{\vec{\xi}}}{d\mathcal{V}_r\, d\mathcal{V}_\xi} = \phi f \qquad (3.20a)$$

For the class $dN_{\theta\varphi}$, the density of the molecular property ϕ per unit volume of configuration space at $\vec{r}$ and per unit solid angle of velocity space at θ, φ is defined as

$$\Phi_{\theta\varphi}(\vec{r},\theta,\varphi,t) \equiv \frac{\int_{\xi=o}^{\xi=\infty} \phi\, dN_{\vec{\xi}}}{d\mathcal{V}_r\, d\Omega_{\theta\varphi}} = \int_o^\infty \phi\, f\, \xi^2\, d\xi \qquad (3.20b)$$

For the class dN_{φ}, the density of the molecular property ϕ per unit volume of configuration space at $\vec{r}$ and per unit solid angle of velocity space at angle φ (integrated over all θ) is defined as

$$\Phi_{\varphi}(\vec{r},\varphi,t) \equiv \frac{\int_{\theta=-\Pi}^{\theta=\Pi}\int_{\xi=o}^{\xi=\infty} \phi\, dN_{\vec{\xi}}}{d\mathcal{V}_r\, d\Omega_{\varphi}} = \frac{1}{2\Pi}\int_{-\Pi}^{\Pi} d\theta \int_o^\infty \phi\, f\, \xi^2\, d\xi \qquad (3.20c)$$

For the class dN, the density of the molecular property ϕ per unit volume of configuration space at $\vec{r}$ is defined as

$$\Phi(\vec{r},t) \equiv \frac{\int_{\varphi=0}^{\varphi=\Pi}\int_{\theta=-\Pi}^{\theta=\Pi}\int_{\xi=0}^{\xi=\infty} \phi \, dN_{\vec{\xi}}}{d\mathscr{V}_r} = \int_0^{\Pi} d\varphi \, (\sin\varphi) \int_{-\Pi}^{\Pi} d\theta \int_0^{\infty} \phi \, f \, \xi^2 \, d\xi \qquad (3.20d)$$

3.7.2 Specific examples of molecular properties of interest, and their density distributions in each class

Examples of molecular properties that may be of particular interest are:

$$\phi = \phi_{\vec{\xi}}^{(\ell)} \equiv \underbrace{\vec{\xi}\vec{\xi}\vec{\xi}\ldots\vec{\xi}}_{\ell \text{ times}} = \underbrace{\vec{e}_{\vec{\xi}}\vec{e}_{\vec{\xi}}\vec{e}_{\vec{\xi}}\ldots\vec{e}_{\vec{\xi}}}_{\ell \text{ times}} \xi^{\ell} \,, \quad \ell=0,1,2,\ldots \qquad (3.21a)$$

(which is a tensor of order ℓ),

$$\phi = m \, \phi_{\vec{\xi}}^{(\ell)} \,, \quad \ell=0,1,2,\ldots \qquad (3.21b)$$

$$\phi = \frac{1}{2} \mathbf{I} : m \, \phi_{\vec{\xi}}^{(\ell)} \,, \quad \ell=0,1,2,\ldots \; \dagger \qquad (3.21c)$$

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† For any two Cartesian tensors of second order or higher, say

$$\mathbf{A} \equiv \sum_{i=1}^{3}\sum_{j=1}^{3} \mathbf{A}_{ij} \vec{e}_i \vec{e}_j \quad \text{and} \quad \mathbf{B} \equiv \sum_{k=1}^{3}\sum_{\ell=1}^{3} \vec{e}_k \vec{e}_\ell \, \mathbf{B}_{k\ell}$$

the "double-dot" product is defined by

$$\mathbf{A} : \mathbf{B} = \sum_{i=1}^{3}\sum_{j=1}^{3} \mathbf{A}_{ij} \, \mathbf{B}_{ji}$$

where the components $\mathbf{A}_{ij}$ and $\mathbf{B}_{k\ell}$ may themselves be tensors of zeroth

(where $\mathbf{I} \equiv \vec{e}_1\vec{e}_1 + \vec{e}_2\vec{e}_2 + \vec{e}_3\vec{e}_3$ is the unit tensor, or "idemtensor")

$$\phi = \xi^{\ell}, \quad \ell=0,1,2,... \tag{3.21d}$$

$$\phi = f(\vec{r},\vec{\xi},t) \tag{3.21e}$$

$$\phi = \lambda^{*}_{\vec{\xi}} \qquad \text{(to be defined below in § 3.11)} \tag{3.21f}$$

$$\phi = \hat{\phi}\,\vec{\xi} \tag{3.21g}$$

$$\phi = \hat{\phi}\,\Theta_{\vec{\xi}} \tag{3.21h}$$

$$\phi = \hat{\phi}\,\Theta'_{\vec{\xi}} \tag{3.21i}$$

where $\hat{\phi}$ may be <u>any other</u> molecular property. Some of these examples are discussed and the property densities for each class indicated below.

The <u>number density</u> in each class is found by taking ϕ from equation (3.21a) with $\ell = 0$ and using equations (3.20). Thus, with $\phi = \phi^{(o)}_{\vec{\xi}} = 1$,

$$n_{\vec{\xi}}(\vec{r},\vec{\xi},t) = f(\vec{r},\vec{\xi},t) = \frac{dN_{\vec{\xi}}}{d\mathcal{V}_r\, d\mathcal{V}_{\xi}} \tag{3.22a}$$

$$n_{\theta\varphi}(\vec{r},\theta,\varphi,t) = \int_0^{\infty} f\,\xi^2\,d\xi = \frac{dN_{\theta\varphi}}{d\mathcal{V}_r\, d\Omega_{\theta\varphi}} \tag{3.22b}$$

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order or higher, i.e., scalars, vectors, or higher-order tensors. The orders of the component tensors $\mathbf{A}_{ij}$ and $\mathbf{B}_{k\ell}$ are by definition two orders lower than the orders of the tensors $\mathbf{A}$ and $\mathbf{B}$ respectively; if $\mathbf{A}$ and $\mathbf{B}$ are second-order tensors, then the components $\mathbf{A}_{ij}$ and $\mathbf{B}_{k\ell}$ are scalars.

$$n_{\varphi}(\vec{r},\varphi,t) = \frac{1}{2\Pi}\int_{-\Pi}^{\Pi} d\theta \int_{0}^{\infty} f\ \xi^2\ d\xi = \frac{dN_{\varphi}}{d\mathcal{V}_r\, d\Omega_{\varphi}} \tag{3.22c}$$

$$n(\vec{r},t) = \int_{0}^{\Pi} d\varphi(\sin\varphi) \int_{-\Pi}^{\Pi} d\theta \int_{0}^{\infty} f\ \xi^2\ d\xi = \frac{dN}{d\mathcal{V}_r} \tag{3.22d}$$

In particular, $n_{\theta\varphi}$ may be denoted as the "directional number density" (which is the same as n_{φ} if f does not vary with θ).

The mass density in each class is found by taking ϕ from equation (3.21b) with $\ell = 0$ and using equations (3.20), or by simply multiplying each of equations (3.22) by the molecular mass, m, to obtain, respectively,

$$\rho_{\vec{\xi}} = mn_{\vec{\xi}}\ ,\quad \rho_{\theta\varphi} = mn_{\theta\varphi}\ ,\quad \rho_{\varphi} = mn_{\varphi}\ ,\quad \rho = mn \tag{3.23}$$

The quantity $\rho_{\theta\varphi}$ may be denoted as the "directional mass density."

If we define $\Phi^{(\ell)}_{class} = \Phi_{class}$ with ϕ given by equation (3.21b), where the property densities Φ_{class} are defined by equations (3.20), then

$$\rho_{class} = \Phi^{(0)}_{class}$$

The momentum density (or mass flux) in each class is found by taking ϕ from equation (3.21b) with $\ell=1$ ($\phi=m\vec{\xi}$) and using equations (3.20) to obtain

$$\Phi^{(1)}_{\vec{\xi}} \equiv m\vec{\xi}f = \vec{e}_{\vec{\xi}}\, m\xi f \tag{3.24a}$$

$$\Phi^{(1)}_{\theta\varphi} \equiv \int_{0}^{\infty} m\vec{\xi}f\xi^2 d\xi = m\,\vec{e}_{\theta\varphi} \int_{0}^{\infty} f\ \xi^3\ d\xi \tag{3.24b}$$

$$\Phi^{(1)}_{\varphi} \equiv \frac{1}{2\Pi} \int_{-\Pi}^{\Pi} d\theta \int_{0}^{\infty} m\vec{\xi}f\xi^2 d\xi = \frac{m}{2\Pi} \int_{-\Pi}^{\Pi} d\theta(\vec{e}_{\theta\varphi}) \int_{0}^{\infty} f\ \xi^3\ d\xi \tag{3.24c}$$

$$\rho\vec{V} = \Phi^{(1)} \equiv \int_{0}^{\Pi} d\varphi(\sin\varphi) \int_{-\Pi}^{\Pi} d\theta \int_{0}^{\infty} m\vec{\xi}f\xi^2 d\xi = m\int_{0}^{\Pi} d\varphi(\sin\varphi) \int_{-\Pi}^{\Pi} d\theta(\vec{e}_{\theta\varphi}) \int_{0}^{\infty} f\xi^3 d\xi \tag{3.24d}$$

The quantity $\Phi^{(1)}_{\theta\varphi}$ could be denoted as the "directional momentum density" (or as the "directional flux of mass").

The energy density in each class is found by taking ϕ from equation (3.21c) with $\ell=2$ $(\Phi = \frac{1}{2} m\xi^2)$ and using equations (3.20) to obtain:

$$\tfrac{1}{2}\,\blacksquare\colon\ \Phi^{(2)}_{\vec{\xi}} \equiv \tfrac{1}{2} m\, \xi^2\, f \tag{3.25a}$$

$$\tfrac{1}{2}\,\blacksquare\colon\ \Phi^{(2)}_{\theta\varphi} \equiv \int_0^\infty \tfrac{1}{2} m\, f\, \xi^4\, d\xi = \tfrac{1}{2} m \int_0^\infty f\, \xi^4\, d\xi \tag{3.25b}$$

$$\tfrac{1}{2}\,\blacksquare\colon\ \Phi^{(2)}_{\varphi} \equiv \frac{1}{2\Pi} \int_{-\Pi}^{\Pi} d\theta \int_0^\infty \tfrac{1}{2} mf\xi^4 d\xi = \tfrac{1}{2} m \frac{1}{2\Pi} \int_{-\Pi}^{\Pi} d\theta \int_0^\infty f\, \xi^4\, d\xi \tag{3.25c}$$

$$\tfrac{1}{2}\,\blacksquare\colon\ \Phi^{(2)} \equiv \int_0^\Pi d\varphi(\sin\varphi) \int_{-\Pi}^{\Pi} d\theta \int_0^\infty \tfrac{1}{2} mf\xi^4 d\xi = \tfrac{1}{2} m \int_0^\Pi d\varphi(\sin\varphi) \int_{-\Pi}^{\Pi} d\theta \int_0^\infty f\xi^4 d\xi \tag{3.25d}$$

The quantity calculated in equation (3.25b) may be denoted as the "directional energy density."

The quantity

$$\Phi^{(2)}_{\theta\varphi} \equiv \int_0^\infty m\, \vec{\xi}\vec{\xi}\, f\, \xi^2\, d\xi = \vec{e}_{\theta\varphi}\vec{e}_{\theta\varphi}\, m \int_0^\infty f\, \xi^4\, d\xi \tag{3.26}$$

is the "directional flux of momentum." The quantity

$$\tfrac{1}{2}\,\blacksquare\colon\ \Phi^{(3)}_{\theta\varphi} \equiv \int_0^\infty \tfrac{1}{2} m\, \xi^2 \vec{\xi}\, f\, \xi^2\, d\xi = \vec{e}_{\theta\varphi}\, \tfrac{1}{2} m \int_0^\infty f\, \xi^5\, d\xi \tag{3.27}$$

is the "directional flux of energy."

By taking ϕ from equation (3.21g) and using equations (3.20) one obtains for each class the density of the molecular property ϕ or the flux of the molecular property $\hat{\phi}$. For example, the quantity

$$\Phi^{(\ell)}_{\theta\varphi} \equiv \int_0^\infty m\, \phi^{(\ell)}_{\vec{\xi}}\, f\, \xi^2\, d\xi \tag{3.28}$$

is the directional flux of the molecular property $m\, \phi^{(\ell-1)}_{\vec{\xi}}$ as defined in equation (3.21b) with (3.21a) (the directional density of the latter property being $\Phi^{(\ell-1)}_{\theta\varphi}$).

By taking ϕ from equations (3.21h) or (3.21i) and using equations (3.20) one obtains for each class the density of the property $\hat{\phi}$ respectively lost or gained per unit time by each class owing to collisions. For example, with $\hat{\phi}=1$ ($\phi=\Theta_{\vec{\xi}}$), equations (3.20) give the number density of molecules undergoing collisions per unit time for each class (respectively: $d(\dot{N}_c)_{\vec{\xi}}/d\mathcal{V}_r\, d\mathcal{V}_\xi$; $d(\dot{N}_c)_{\theta\varphi}/d\mathcal{V}_r\, d\Omega_{\theta\varphi}$; $d(\dot{N}_c)_{\varphi}/d\mathcal{V}_r\, d\Omega_{\varphi}$; and $d\dot{N}_c/d\mathcal{V}_r$; cf. eqs. (3.18)).

3.8 Average Values of Molecular Properties for Each Class of Molecules

For any molecular property $\phi(\vec{r},\vec{\xi},t)$, an average value of the property possessed by the molecules of each class is defined by

$$\langle\phi\rangle_{\text{class}} \equiv \frac{\int_{\text{class}} \phi\, dN_{\vec{\xi}}}{\int_{\text{class}} dN_{\vec{\xi}}} = \frac{\Phi_{\text{class}}}{n_{\text{class}}} \tag{3.29}$$

where the Φ_{class} are defined by equations (3.20) for each ϕ and the n_{class} are defined by equations (3.22). In § 2.23, only the averages for the class dN (all molecules in $(\vec{r},d\mathcal{V}_r)$; thus averaged over all $\vec{\xi}$) were considered. However, the definition (3.29) can apply to any of the four classes defined in § 3.4.

The subscripts $\vec{\xi}$, $\theta\varphi$, φ are used to indicate what part of the molecular velocity the resulting quantity can be a function of.

The average value of ϕ for the molecules in the class $dN_{\vec{\xi}}$ is therefore

$$\langle\phi\rangle_{\vec{\xi}} \equiv \phi = \frac{\Phi_{\vec{\xi}}}{n_{\vec{\xi}}} \tag{3.30a}$$

The average value of ϕ for the molecules in the class $dN_{\theta\varphi}$ is

$$\langle\phi\rangle_{\theta\varphi} \equiv \frac{\int_0^\infty \phi\, f\, \xi^2\, d\xi}{\int_0^\infty f\, \xi^2\, d\xi} = \frac{\Phi_{\theta\varphi}}{n_{\theta\varphi}} \tag{3.30b}$$

The average value of ϕ for the molecules in the class dN_{φ} is

$$\langle\phi\rangle_{\varphi} \equiv \frac{\int_{-\Pi}^{\Pi} d\theta \int_0^\infty \phi\, f\, \xi^2\, d\xi}{\int_{-\Pi}^{\Pi} d\theta \int_0^\infty f\, \xi^2\, d\xi} = \frac{\Phi_{\varphi}}{n_{\varphi}} \tag{3.30c}$$

The average value of ϕ for the molecules in the class dN (cf. eq. (2.14)) is

$$\langle\phi\rangle \equiv \frac{\int_0^{\Pi} d\varphi\, (\sin\varphi) \int_{-\Pi}^{\Pi} d\theta \int_0^\infty \phi\, f\, \xi^2\, d\xi}{\int_0^{\Pi} d\varphi\, (\sin\varphi) \int_{-\Pi}^{\Pi} d\theta \int_0^\infty f\, \xi^2\, d\xi} = \frac{\Phi}{n} \tag{3.30d}$$

Note that in equations (3.30) the quantity Φ_{class} corresponding to any molecular property $\phi(\vec{r},\vec{\xi},t)$ is defined by equations (3.20).

Particular average values of interest are discussed in §§ 3.9, 3.10, and 3.11. One particular average value that is convenient to use is defined by taking $\phi = \xi^\ell$ (eq. (3.21d)) and using equations (3.30); thus define

$$v_{class}^{(\ell)} \equiv \langle\xi^\ell\rangle_{class} \tag{3.31a}$$

or

$$v_{\theta\varphi}^{(\ell)} \equiv \langle \xi^{\ell} \rangle_{\theta\varphi} \equiv \frac{1}{n_{\theta\varphi}} \int_{0}^{\infty} f\, \xi^{2+\ell}\, d\xi \tag{3.31b}$$

$$v_{\varphi}^{(\ell)} \equiv \langle \xi^{\ell} \rangle_{\varphi} \equiv \frac{1}{n_{\varphi}} \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \int_{0}^{\infty} f\, \xi^{2+\ell}\, d\xi \tag{3.31c}$$

$$v^{(\ell)} \equiv \langle \xi^{\ell} \rangle \equiv \frac{1}{n} \int_{0}^{\pi} d\varphi\, (\sin\varphi) \int_{-\pi}^{\pi} d\theta \int_{0}^{\infty} f \xi^{2+\ell}\, d\xi \tag{3.31d}$$

The quantity $v^{(1)} \equiv \langle \xi \rangle$ has already found use in Chapter II. For the case $\ell=1$, it is often convenient to omit the superscript; thus

$$v_{class} \equiv v_{class}^{(1)} = \langle \xi \rangle_{class} \tag{3.31e}$$

3.9 Collision Frequency Per Molecule of Each Class

For each of the classes defined in § 3.4, the total number in the class that undergo collisions in unit time was found in § 3.5. Also defined in § 3.5 were the quantities Θ_{class}, which represent the fraction of the total number of the class that undergo collisions in unit time. Starting with $\Theta_{\vec{\xi}}$, defined in equation (2.12c), as the molecular property ϕ, one finds from equations (3.18) and (3.30) that, for each class,

$$\frac{d(\dot{N}_c)_{class}}{dN_{class}} \equiv \Theta_{class} = \langle \Theta_{\vec{\xi}} \rangle_{class} \tag{3.32}$$

Thus:

$$d(\dot{N}_c)_{\vec{\xi}} / dN_{\vec{\xi}} \equiv \Theta_{\vec{\xi}} \tag{3.33a}$$

$$d(\dot{N}_c)_{\theta\varphi} / dN_{\theta\varphi} \equiv \Theta_{\theta\varphi} = \langle \Theta_{\vec{\xi}} \rangle_{\theta\varphi} = \frac{1}{n_{\theta\varphi}} \int_{0}^{\infty} \Theta_{\vec{\xi}}\, f\, \xi^{2}\, d\xi \tag{3.33b}$$

$$d(\dot{N}_c)_{\varphi}/dN_{\varphi} \equiv \Theta_{\varphi} = \left\langle \Theta_{\vec{\xi}} \right\rangle_{\varphi} = \frac{1}{n_{\varphi}} \frac{1}{2\Pi} \int_{-\Pi}^{\Pi} d\theta \int_{0}^{\infty} \Theta_{\vec{\xi}} \, f \, \xi^2 \, d\xi \qquad (3.33c)$$

$$d\dot{N}_c/dN \equiv \Theta = \left\langle \Theta_{\vec{\xi}} \right\rangle = \frac{1}{n} \int_{0}^{\Pi} d\varphi (\sin \varphi) \int_{-\Pi}^{\Pi} d\theta \int_{0}^{\infty} \Theta_{\vec{\xi}} \, f \, \xi^2 \, d\xi \qquad (3.33d)$$

(cf. eqs. (2.13c) and (2.19)).

3.10 "Inverse Collision Frequency" Per Molecule of Each Class

For each of the classes defined in § 3.4, the total number of molecules undergoing inverse collisions in unit time that end up in the class was found in § 3.6. Also defined in § 3.6 were the "inverse collision frequencies," Θ'_{class} for each class, which represent the fraction of the total number in the class that undergo inverse collisions in unit time. Starting with $\Theta'_{\vec{\xi}}$, defined by equation (3.3d), as the molecular property ϕ, one finds from equations (3.19) and (3.30) that, for each class,

$$\frac{d(\dot{N}'_c)_{class}}{dN_{class}} \equiv \Theta'_{class} = \left\langle \Theta'_{\vec{\xi}} \right\rangle_{class} \qquad (3.34)$$

Thus:

$$d(\dot{N}'_c)_{\vec{\xi}}/dN_{\vec{\xi}} \equiv \Theta'_{\vec{\xi}} \qquad (3.35a)$$

$$d(\dot{N}'_c)_{\theta\varphi}/dN_{\theta\varphi} \equiv \Theta'_{\theta\varphi} = \left\langle \Theta'_{\vec{\xi}} \right\rangle_{\theta\varphi} \qquad (3.35b)$$

$$d(\dot{N}'_c)_{\varphi}/dN_{\varphi} \equiv \Theta'_{\varphi} = \left\langle \Theta'_{\vec{\xi}} \right\rangle_{\varphi} \qquad (3.35c)$$

$$d\dot{N}'_c/dN \equiv \Theta' = \left\langle \Theta'_{\vec{\xi}} \right\rangle \qquad (3.35d)$$

3.11 Absolute Mean Free Path for Each Class, Including Directional Mean Free Path

According to the definition (2.1a) (and with use of eq. (3.32)), the mean free path measured relative to the observer (or the "absolute mean free path"; cf. eq. (2.22)) for each class is

$$\lambda^*_{\text{class}} \equiv \frac{\langle \xi \rangle_{\text{class}}}{\Theta_{\text{class}}} = \frac{\langle \xi \rangle_{\text{class}}}{\langle \Theta_{\vec{\xi}} \rangle_{\text{class}}} \tag{3.36}$$

Thus for molecules in the class $dN_{\vec{\xi}}$, the absolute mean free path is

$$\lambda^*_{\vec{\xi}} \equiv \xi / \Theta_{\vec{\xi}} \tag{3.37a}$$

(For a gas composed of rigid elastic spheres in equilibrium, this free path is given by eq. (8) on page 95 in Chapman and Cowling (1961). Note that c in their notation is ξ in present notation.)

For molecules in the class $dN_{\theta\varphi}$, the absolute mean free path is

$$\lambda^*_{\theta\varphi} \equiv \frac{\langle \xi \rangle_{\theta\varphi}}{\Theta_{\theta\varphi}} = \frac{\langle \xi \rangle_{\theta\varphi}}{\langle \Theta_{\vec{\xi}} \rangle_{\theta\varphi}} = \frac{\int_0^\infty f\, \xi^3\, d\xi}{\int_0^\infty \Theta_{\vec{\xi}}\, f\, \xi^2\, d\xi} \tag{3.37b}$$

For molecules in the class dN_{φ}, the absolute mean free path is

$$\lambda^*_{\varphi} \equiv \frac{\langle \xi \rangle_{\varphi}}{\Theta_{\varphi}} = \frac{\langle \xi \rangle_{\varphi}}{\langle \Theta_{\vec{\xi}} \rangle_{\varphi}} = \frac{\int_{-\Pi}^{\Pi} d\theta \int_0^\infty f\, \xi^3\, d\xi}{\int_{-\Pi}^{\Pi} d\theta \int_0^\infty \Theta_{\vec{\xi}}\, f\, \xi^2\, d\xi} \tag{3.37c}$$

For molecules in the class dN (cf. eq. (2.22)), the absolute mean free path is

$$\lambda^* \equiv \frac{\langle \xi \rangle}{\Theta} = \frac{\langle \xi \rangle}{\langle \Theta_{\vec{\xi}} \rangle} = \frac{\int_0^{\Pi} d\varphi(\sin\varphi) \int_{-\Pi}^{\Pi} d\theta \int_0^{\infty} f\, \xi^3\, d\xi}{\int_0^{\Pi} d\varphi(\sin\varphi) \int_{-\Pi}^{\Pi} d\theta \int_0^{\infty} \Theta_{\vec{\xi}} f\, \xi^2\, d\xi} \tag{3.37d}$$

Note that for the classes $dN_{\vec{\xi}}$ and $dN_{\theta\varphi}$ one can define a vector mean free path by:

$$\vec{\lambda}^*_{\vec{\xi}} \equiv \frac{\vec{\xi}}{\Theta_{\vec{\xi}}} = \vec{e}_{\vec{\xi}}\, \lambda^*_{\vec{\xi}} \tag{3.38a}$$

$$\vec{\lambda}^*_{\theta\varphi} \equiv \frac{\langle \vec{\xi} \rangle_{\theta\varphi}}{\Theta_{\theta\varphi}} = \vec{e}_{\theta\varphi}\, \lambda^*_{\theta\varphi} \tag{3.38b}$$

Either the vector $\vec{\lambda}^*_{\theta\varphi}$ or its magnitude, $\lambda^*_{\theta\varphi}$, may be denoted as the directional mean free path. Note also that if f does not depend on θ, then $\lambda^*_{\theta\varphi} = \lambda^*_{\varphi}$.

It may also be convenient to define an average absolute free path calculated in a different way, defined by:

$$\Lambda_{\text{class}} \equiv \langle \lambda^*_{\vec{\xi}} \rangle_{\text{class}} \tag{3.39}$$

thus:

$$\Lambda_{\vec{\xi}} \equiv \lambda^*_{\vec{\xi}} \tag{3.40a}$$

$$\Lambda_{\theta\varphi} \equiv \langle \lambda^*_{\vec{\xi}} \rangle_{\theta\varphi} \tag{3.40b}$$

$$\Lambda_{\varphi} \equiv \langle \lambda^*_{\vec{\xi}} \rangle_{\varphi} \tag{3.40c}$$

$$\Lambda \equiv \langle \lambda^*_{\vec{\xi}} \rangle \tag{3.40d}$$

3.12 Equations of Change for Molecular-Property Distributions for Each Class of Molecules

For any molecular property $\phi(\vec{r},\vec{\xi},t)$ one can write an equation of change for the property density $\Phi_{class} = n_{class} \langle \phi \rangle_{class}$ for each of the four classes of molecules defined in § 3.4, equations (3.17). These will be of use, particularly for the class $dN_{\theta\varphi}$, in the directional level of description, in § 4.1. For convenience in the following developments it is assumed there are no external body forces acting on a molecule other than those involved in the isolated molecular encounters, that is, $\vec{F}_B = 0$.

3.12.1 Equation of change for number density in each class

For molecules in the class $dN_{\vec{\xi}}$, on the kinetic level, the equation of change for $dN_{\vec{\xi}}$ is given by (3.6b). That equation is divided by $d\mathcal{V}_r\, d\mathcal{V}_\xi$ to obtain an equation of change for the number density in phase space, $n_{\vec{\xi}} \equiv f(\vec{r},\vec{\xi},t)$ (eq. (3.7), a form of the Boltzmann equation):

$$\frac{\partial f}{\partial t} + \nabla_r \cdot (\vec{\xi} f) = (\Theta'_{\vec{\xi}} - \Theta_{\vec{\xi}})\, f \qquad (3.41a)$$

In equation (3.41a), $\Theta_{\vec{\xi}}\, f$ is the probable number density of molecules lost from $(\vec{r},d\mathcal{V}_r),(\vec{\xi},d\mathcal{V}_\xi)$ per unit time because of collisions, and $\Theta'_{\vec{\xi}}\, f$ is the probable number density of molecules gained by $(\vec{r},d\mathcal{V}_r)$, $(\vec{\xi},d\mathcal{V}_\xi)$ because of collisions (see §§ 3.5 and 3.6).

For the class $dN_{\theta\varphi}$, equation (3.6b) is integrated over all velocity magnitudes, ξ, from 0 to infinity, then divided by $d\mathcal{V}_r\, d\Omega_{\theta\varphi}$ to obtain an equation of change for the number density $n_{\theta\varphi}(\vec{r},\theta,\varphi,t)$, the probable number of molecules per unit volume of configuration space at $\vec{r}$ and per unit solid angle of molecular-velocity space, in the direction θ,φ:

$$\frac{\partial n_{\theta\varphi}}{\partial t} + \nabla_r \cdot [n_{\theta\varphi} \langle \vec{\xi} \rangle_{\theta\varphi}] = n_{\theta\varphi}(\Theta'_{\theta\varphi} - \Theta_{\theta\varphi}) \qquad (3.41b)$$

In equation (3.41b), $n_{\theta\varphi}\,\Theta_{\theta\varphi}$ is the probable number lost, owing to collisions, per unit time, per unit volume at $\vec{r}$, and per unit solid angle of velocity space in the direction θ, φ; $n_{\theta\varphi}\,\Theta'_{\theta\varphi}$ is the probable number gained, owing to collisions, per unit time, per unit volume at $\vec{r}$, and per unit solid angle of velocity space in the direction θ, φ (see §§ 3.5 and 3.6).

For the class dN_{φ}, equation (3.6b) is integrated over all velocity magnitudes ξ from 0 to infinity and over all θ from $-\Pi$ to Π, then divided by $d\mathcal{V}_r\, d\Omega_{\varphi}$ to obtain an equation of change for the number density $n_{\varphi}(\vec{r},\varphi,t)$, the probable number of molecules per unit volume at $\vec{r}$ and per unit solid angle of velocity space in the direction φ (averaged over all θ):

$$\frac{\partial n_{\varphi}}{\partial t} + \nabla_r \cdot [n_{\varphi}\langle\vec{\xi}\rangle_{\varphi}] = n_{\varphi}(\Theta'_{\varphi} - \Theta_{\varphi}) \qquad (3.41c)$$

In equation (3.41c), $n_{\varphi}\,\Theta_{\varphi}$ is the probable number lost, owing to collisions, per unit time, per unit volume at $\vec{r}$, and per unit solid angle in velocity space in the direction of φ (averaged over all θ); $n_{\varphi}\,\Theta'_{\varphi}$ is the probable number gained, owing to collisions, per unit time, per unit volume at $\vec{r}$, and per unit solid angle of velocity space in the direction φ (averaged over θ) (see §§ 3.5 and 3.6).

For the class dN, equation (3.6b) is integrated over all $\vec{\xi}$; that is, over all ξ from 0 to infinity, over all θ from $-\Pi$ to Π, and over all φ from 0 to Π; then divided by $d\mathcal{V}_r$ to obtain an equation of change for the number density $n(\vec{r},t)$, the probable number of molecules per unit volume at $\vec{r}$:

$$\frac{\partial n}{\partial t} + \nabla_r \cdot [n\langle\vec{\xi}\rangle] = n(\Theta' - \Theta) = 0 \qquad (3.41d)$$

In equation (3.41d), $n\,\Theta$ is the total number density of molecules undergoing "direct collisions" per unit time, which is the same as the total number density of molecules undergoing "inverse collisions" per unit time, $n\,\Theta'$ (see §§ 3.5 and 3.6).

3.12.2 Equations of change for other molecular-property distributions in each class

For any other molecular property, the equations of change for each class of molecules defined in § 3.4 are found as follows:

For the class $dN_{\vec{\xi}}$, the density distribution of the property $\phi(\vec{r},\vec{\xi},t)$ in phase space is (eq. (3.20a)):

$$\Phi_{\vec{\xi}} = \phi f$$

To obtain an equation of change for the distribution ϕf, multiply equation (3.41a) by ϕ (where ϕ may be a tensor of any order):

$$\phi \frac{\partial f}{\partial t} + \phi \nabla_r \cdot (\vec{\xi} f) = f \phi(\Theta'_{\vec{\xi}} - \Theta_{\vec{\xi}})$$

and rearrange in the form

$$\frac{\partial}{\partial t}(f\phi) + \nabla_r \cdot (f\vec{\xi}\phi) - f\left[\frac{\partial \phi}{\partial t} + \vec{\xi}\cdot\nabla_r\phi\right] = f[\phi(\Theta'_{\vec{\xi}} - \Theta_{\vec{\xi}})] \qquad (3.42a)$$

To obtain equations of change for the property-density distributions in each of the other three classes, multiply equation (3.42a) by $d\mathcal{V}_\xi = \xi^2\, d\xi\, d\theta \sin\varphi\, d\varphi$ and integrate first over $d\xi$, then over $d\theta$, then over $d\varphi$ to obtain respectively the results:

$$\frac{\partial}{\partial t}[n_{\theta\varphi}\langle\phi\rangle_{\theta\varphi}] + \nabla_r\cdot[n_{\theta\varphi}\langle\vec{\xi}\phi\rangle_{\theta\varphi}] - n_{\theta\varphi}\left[\left\langle\frac{\partial\phi}{\partial t}\right\rangle_{\theta\varphi} + \langle\vec{\xi}\cdot\nabla_r\phi\rangle_{\theta\varphi}\right]$$

$$= n_{\theta\varphi}[\langle\phi\Theta'_{\vec{\xi}}\rangle_{\theta\varphi} - \langle\phi\Theta_{\vec{\xi}}\rangle_{\theta\varphi}] \qquad (3.42b)$$

$$\frac{\partial}{\partial t}[n_{\varphi}\langle\phi\rangle_{\varphi}] + \nabla_r\cdot[n_{\varphi}\langle\vec{\xi}\phi\rangle_{\varphi}] - n_{\varphi}\left[\left\langle\frac{\partial\phi}{\partial t}\right\rangle_{\varphi} + \langle\vec{\xi}\cdot\nabla_r\phi\rangle_{\varphi}\right]$$

$$= n_{\varphi}[\langle\phi\Theta'_{\vec{\xi}}\rangle_{\varphi} - \langle\phi\Theta_{\vec{\xi}}\rangle_{\varphi}] \qquad (3.42c)$$

$$\frac{\partial}{\partial t}\left[n\left\langle\phi\right\rangle\right] + \nabla_r\cdot\left[n\left\langle\vec{\xi}\phi\right\rangle\right] - n\left[\left\langle\frac{\partial\phi}{\partial t}\right\rangle + \left\langle\vec{\xi}\cdot\nabla_r\phi\right\rangle\right]$$

$$= n\left[\left\langle\phi\Theta'_{\vec{\xi}}\right\rangle - \left\langle\phi\Theta_{\vec{\xi}}\right\rangle\right] \qquad (3.42d)$$

In each of equations (3.42a, b, c, d) the first term on the right side is the density, for the class, of the molecular property ϕ gained by the respective class of molecules owing to collisions, and the second term on the right side is the density, for the class, of the molecular property ϕ lost from the respective class owing to collisions.

Note that equations (3.42) all have a very similar form and that equation (3.42d) is Enskog's general equation of change (with $\vec{F}_B = 0$). (See, e.g., Hirschfelder, Curtiss, and Bird, 1964, p. 460.)

For the particular cases of $\phi=m$, $\phi=m\vec{\xi}$, and $\phi=\frac{1}{2}m\xi^2$ (the summational invariants of a collision) one obtains from (3.42d) a form of the conservation equations of gasdynamics (for which $\left\langle\phi\,(\Theta'_{\vec{\xi}} - \Theta_{\vec{\xi}})\right\rangle = 0$):

$$\frac{\partial\rho}{\partial t} + \nabla_r\cdot\left[\rho\left\langle\vec{\xi}\right\rangle\right] = \rho\left\langle\Theta'_{\vec{\xi}} - \Theta_{\vec{\xi}}\right\rangle = 0 \qquad (3.43a)$$

$$\frac{\partial}{\partial t}\left[\rho\left\langle\vec{\xi}\right\rangle\right] + \nabla_r\cdot\left[\rho\left\langle\vec{\xi}\vec{\xi}\right\rangle\right] = \rho\left\langle\vec{\xi}(\Theta'_{\vec{\xi}} - \Theta_{\vec{\xi}})\right\rangle = 0 \qquad (3.43b)$$

$$\frac{\partial}{\partial t}\left[\frac{1}{2}\rho\left\langle\xi^2\right\rangle\right] + \nabla_r\cdot\left[\frac{1}{2}\rho\left\langle\xi^2\vec{\xi}\right\rangle\right] = \rho\left\langle\frac{1}{2}\xi^2(\Theta'_{\vec{\xi}} - \Theta_{\vec{\xi}})\right\rangle = 0 \qquad (3.43c)$$

CHAPTER IV

PRELIMINARY FORMULATION OF THE

DIRECTIONAL-MEAN-FREE-PATH METHOD

4.1 Directional-Mean-Free-Path Approximation for the "Gain-Term" Collision Integrals in Flows Far From Boundaries

In this section a model for the "gain-term" collision integrals is proposed that simplifies the treatment on the directional level of description; that is, in consideration of the class $dN_{\theta\varphi}$ (cf. § 3.4), or the class of molecules in $(\vec{r}, d\mathcal{V}_r)$ with molecular velocity in the direction range $(\theta, \varphi, d\Omega_{\theta\varphi})$.

Up to this point, all developments and definitions made have been completely rigorous and formal, with no approximations made other than those involved in assuming validity of Boltzmann's equation in the form of equation (3.7), with $\vec{F}_B$ subsequently taken to be zero.

The model to be proposed here involves a physically intuitive approximation of the "gain term" of the collision integrals in equations (3.41b) and (3.42b). It makes use of the concept of the directional mean free path, introduced in § 3.11. The form of the approximations will be seen to be particularly amenable to treatment by certain generalizations of Lagrange's expansion, to be developed in Chapter V and to be applied in Chapter VI.

The equation of change for $dN_{\theta\varphi}$, or for $n_{\theta\varphi}$, can be written as

$$d\mathcal{V}_r\, d\Omega_{\theta\varphi}\left\{\frac{\partial n_{\theta\varphi}}{\partial t} + \nabla_r \cdot [n_{\theta\varphi}\langle\vec{\xi}\rangle_{\theta\varphi}]\right\} = d(\dot{N}_c')_{\theta\varphi} - d(\dot{N}_c)_{\theta\varphi}$$

$$= dN_{\theta\varphi}(\Theta'_{\theta\varphi} - \Theta_{\theta\varphi})$$

$$= d\mathcal{V}_r\, d\Omega_{\theta\varphi}\, n_{\theta\varphi}(\Theta'_{\theta\varphi} - \Theta_{\theta\varphi}) \qquad (4.1)$$

where $d(\dot{N}_c)_{\theta\varphi}$ is the total probable number of molecules undergoing collisions per unit time in $(\vec{r},d\mathcal{V}_r),(\theta, \varphi, d\Omega_{\theta\varphi})$, and hence lost from $(\vec{r},d\mathcal{V}_r)$ and the solid-angle range of velocity $(\theta, \varphi, d\Omega_{\theta\varphi})$ per unit time because of collisions; and $d(\dot{N}'_c)_{\theta\varphi}$ is the total probable number of molecules undergoing "inverse collisions" that occur elsewhere in phase space (i.e., other than in any $d\mathcal{V}_r\, d\mathcal{V}_\xi$ within $(\vec{r},d\mathcal{V}_r),(\theta, \varphi, d\Omega_{\theta\varphi})$) that are put into $(\vec{r},d\mathcal{V}_r),(\theta, \varphi, d\Omega_{\theta\varphi})$ in unit time at time t because of collisions.

4.1.1 Definitions and assumptions of the directional-mean-free-path approximation for the gain term

The aim of the directional-mean-free-path approximation is to replace the difficult gain term on the directional level by an appropriate corresponding loss term.

The inverse collisions all occur in elements of phase space, $d\mathcal{V}_r\, d\mathcal{V}_\xi$, back in the direction $-\vec{e}_{\theta\varphi}$ at locations within the solid angle opposite to $(\theta, \varphi, d\Omega_{\theta\varphi})$ from the point $\vec{r}$ (see fig. 4.1).

One may think of the gain term in equation (4.1), therefore, as resulting, on the average, from collisions occurring at a directional mean free path, $\tilde{\lambda}^*_{\theta\varphi}$, back from the point $\vec{r}$ in the solid angle equal to $d\Omega_{\theta\varphi}$ about $-\vec{e}_{\theta\varphi}$ and at a mean collision time in the past (corresponding to this direction), $1/\tilde{\Theta}_{\theta\varphi}$. Let the representative midpoint and time of the inverse collisions be denoted by $\tilde{\vec{r}}$ and $\tilde{t}$, defined implicitly by

$$\tilde{\vec{r}} + \tilde{\vec{\lambda}}^*_{\theta\varphi} = \vec{r} \tag{4.2a}$$

$$\tilde{t} + 1/\tilde{\Theta}_{\theta\varphi} = t \tag{4.2b}$$

where

$$\tilde{\vec{\lambda}}^*_{\theta\varphi} \equiv \vec{\lambda}^*_{\theta\varphi}(\tilde{\vec{r}},\theta,\varphi,\tilde{t}) \equiv \vec{e}_{\theta\varphi} \langle\tilde{\xi}\rangle_{\theta\varphi}/\tilde{\Theta}_{\theta\varphi} \tag{4.3a}$$

$$\tilde{\theta}_{\theta\varphi} \equiv \theta_{\theta\varphi}(\tilde{\vec{r}}\ \theta,\varphi,\tilde{t}) = \left\langle \tilde{\theta}_{\vec{\xi}} \right\rangle_{\theta\varphi} \tag{4.3b}$$

$$\left\langle \tilde{\xi} \right\rangle_{\theta\varphi} \equiv [\langle \xi \rangle_{\theta\varphi} \text{ evaluated at } \tilde{\vec{r}},\tilde{t}] = \frac{1}{\tilde{n}_{\theta\varphi}} \int_0^\infty f(\tilde{\vec{r}},\xi,\theta,\varphi,\tilde{t})\xi^3 d\xi \tag{4.3c}$$

$$\tilde{n}_{\theta\varphi} \equiv n_{\theta\varphi}(\tilde{\vec{r}},\theta,\varphi,\tilde{t}) \tag{4.3d}$$

in which $\tilde{\vec{\lambda}}^*_{\theta\varphi}$ and $1/\tilde{\theta}_{\theta\varphi}$ are respectively the directional absolute mean free path and mean collision time that are characteristic of the direction θ,φ at the point $\tilde{\vec{r}}$ and at time $\tilde{t}$.

The number of molecules, $d(\dot{N}'_c)_{\theta\varphi}$, put into $(\vec{r},d\mathcal{V}_r)$ with velocity direction in $(\theta,\varphi,d\Omega_{\theta\varphi})$ at time t per unit time owing to collisions is accordingly assumed to be <u>emitted</u> per unit time from collisions in $(\tilde{\vec{r}},d\mathcal{V}_r)$ with average velocity $\tilde{v}_{\theta\varphi} \equiv \left\langle \tilde{\xi} \right\rangle_{\theta\varphi}$ with direction in $(\theta,\varphi,d\Omega_{\theta\varphi})$ at time $\tilde{t}$. The appropriateness of this assumption can be seen from figure 4.2 and the following considerations: The volume $(\tilde{\vec{r}},d\mathcal{V}_r)$ is equal in size to the volume $(\vec{r},d\mathcal{V}_r)$. Let B denote the area, in the plane perpendicular to $\vec{e}_{\theta\varphi}$ at point $\tilde{\vec{r}}$, that subtends the solid angle $d\Omega_{\theta\varphi}$ from the point $\vec{r}$, with point $\tilde{\vec{r}}$ in the center of area B. Thus

$$B = (\tilde{\lambda}^*_{\theta\varphi})^2\ d\Omega_{\theta\varphi}$$

Let $d\omega$ be the solid angle, centered also at point $\vec{r}$, and subtended by the cross-sectional area of the volume $(\tilde{\vec{r}},d\mathcal{V}_r)$; denote the cross section of $(\tilde{\vec{r}},d\mathcal{V}_r)$ by dB, so that

$$dB = (\tilde{\lambda}^*_{\theta\varphi})^2\ d\omega$$

Let the ratio of $d\Omega_{\theta\varphi}$ to $d\omega$ be j; thus

$$d\Omega_{\theta\varphi} = j\ d\omega$$

$$B = j\ dB$$

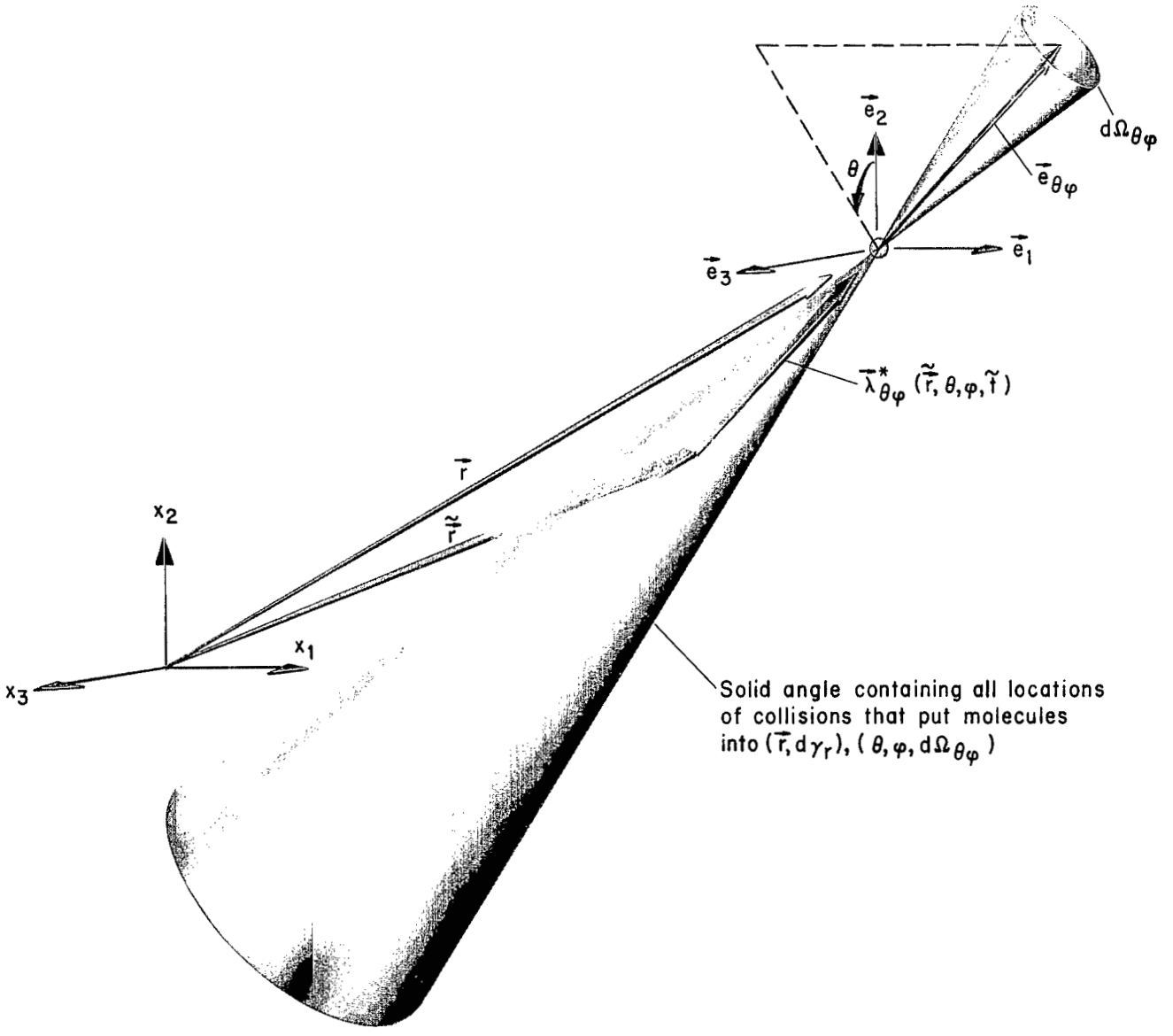

Figure 4.1 - Solid angle containing inverse-collision locations; and depiction of $\vec{\lambda}^*_{\theta\varphi}$.

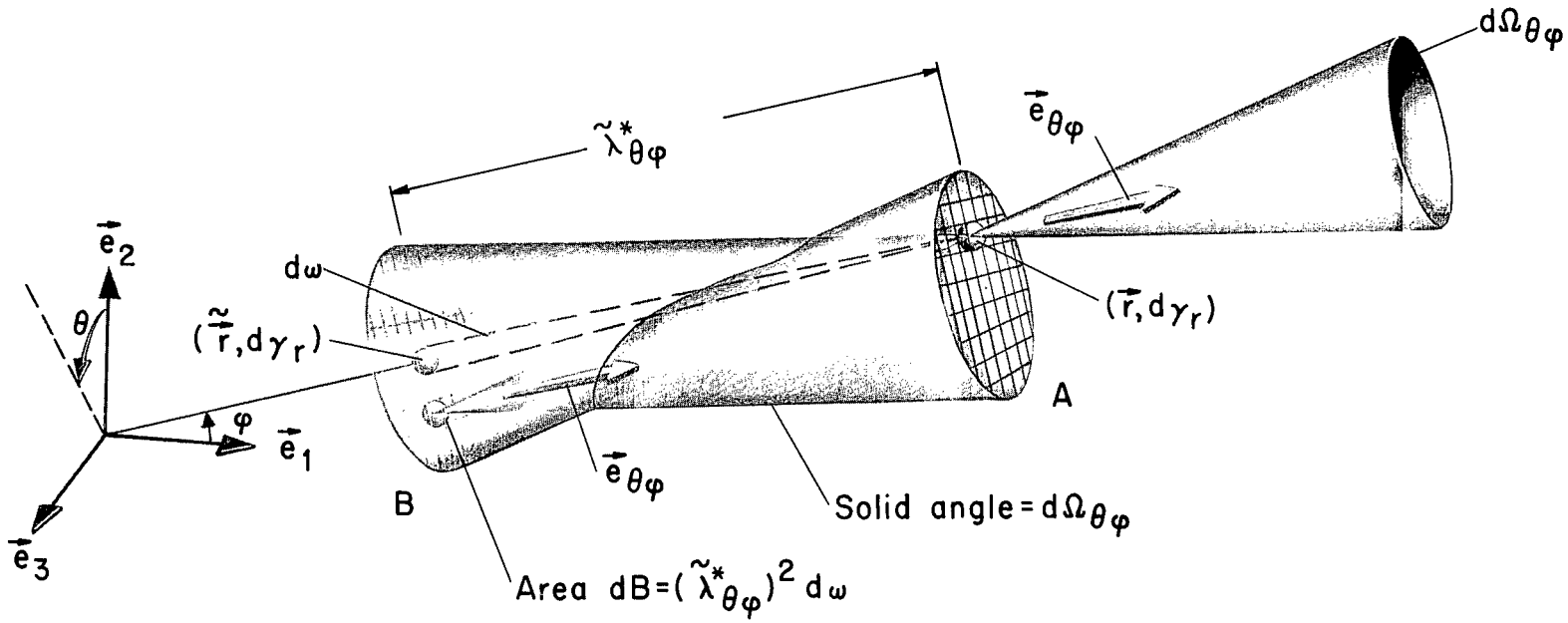

Figure 4.2 - Sketch for description of directional-mean-free-path approximation.

Now divide the area B into j equal parts, dB, so that each subtends a solid angle $d\omega$ from the point $\vec{r}$. Consider the small volume $d\mathcal{V}_r$ centered on each of the j small areas, dB. Each of these j elements has a cone of solid angle $d\Omega_{\theta\varphi}$ in the direction $\vec{e}_{\theta\varphi}$. Each of these cones is subtended by a surface A in the plane that is normal to $\vec{e}_{\theta\varphi}$ and passes through the point $\vec{r}$. Each of these areas, A, is equal to B, and each A may be divided into j equal parts, dA = dB, one of which contains the cross-section of $(\vec{r},d\mathcal{V}_r)$. The number of molecules emitted per unit time in $(\theta,\varphi,d\Omega_{\theta\varphi})$ with average velocity $\tilde{v}_{\theta\varphi}$ from each $d\mathcal{V}_r$ is assumed to be $d(\dot{N}'_c)_{\theta\varphi}$. A fraction, 1/j, of this number per unit time is received by $(\vec{r},d\mathcal{V}_r)$ at time $t = \tilde{t} + 1/\tilde{\Theta}_{\theta\varphi}$ from each of the j volume elements $d\mathcal{V}_r$ on area B. Hence $(\vec{r},d\mathcal{V}_r)$ receives $j(1/j)d(\dot{N}'_c)_{\theta\varphi} = d(\dot{N}'_c)_{\theta\varphi}$ molecules per unit time at time t with velocity direction in $(\theta,\varphi,d\Omega_{\theta\varphi})$, where $d(\dot{N}'_c)_{\theta\varphi}$ is also the number originally assumed to be emitted from $(\tilde{\vec{r}},d\mathcal{V}_r)$ by collisions per unit time at time $\tilde{t}$ with velocity direction in $(\theta,\varphi,d\Omega_{\theta\varphi})$.

It is significant that, on the average, the $d(\dot{N}'_c)_{\theta\varphi}$ molecules, assumed to be emitted from $(\tilde{\vec{r}},d\mathcal{V}_r)$ in $(\theta,\varphi,d\Omega_{\theta\varphi})$ per unit time at time $\tilde{t}$, travel the distance $\tilde{\lambda}^*_{\theta\varphi}$ to point $\vec{r}$ in the time interval $1/\tilde{\Theta}_{\theta\varphi} = \tilde{\lambda}^*_{\theta\varphi}/\tilde{v}_{\theta\varphi}$, where $1/\tilde{\Theta}_{\theta\varphi}$ is the average frequency of direct collisions at $\tilde{\vec{r}}$, $\tilde{t}$ in direction range $(\theta, \varphi, d\Omega_{\theta\varphi})$. Note that $d(\dot{N}'_c)_{\theta\varphi}$ is yet to be determined.

4.1.2 Directional-average collision models to be used with the directional-mean-free-path approximation for the gain term

For the directional-mean-free-path approximation partially introduced above, all the $d(\dot{N}'_c)_{\theta\varphi}$ molecules have been assumed, on the average, to be emitted from collisions taking place within $(\tilde{\vec{r}},d\mathcal{V}_r)$ at time $\tilde{t}$, per unit time. This number $d(\dot{N}'_c)_{\theta\varphi}$ must now be estimated in some way. For this estimate, just as $(\tilde{\vec{r}},d\mathcal{V}_r)$ was taken to be a small volume at a representative average location in which the inverse collisions occur, so there is also now assumed to be some representative average direction that the $d(\dot{N}'_c)_{\theta\varphi}$ molecules had before the "inverse collisions" in

$(\tilde{\vec{r}},d\mathcal{V}_r)$ at time $\tilde{t}$ that resulted in the final average velocity $\tilde{v}_{\theta\varphi}=\langle\tilde{\xi}\rangle_{\theta\varphi}$ in the direction range $(\theta,\varphi,d\Omega_{\theta\varphi})$. The number $d(\dot{N}'_c)_{\theta\varphi}$ is estimated in terms of a representative average direction (θ',φ') (see fig. 4.3) for the $d(\dot{N}'_c)_{\theta\varphi}$ molecules before collision in $(\tilde{\vec{r}},d\mathcal{V}_r)$ at time $\tilde{t}$, per unit time, according to one of several "directional-average collision models" for the gain term, as described below in §§ 4.1.2.1, 4.1.2.2, and 4.1.2.3. These models for the gain term simply represent approximate ways of evaluating the representative direction θ',φ' and of relating the gain term collision integral, in the directional-mean-free-path approximation, to a corresponding loss term, which is easier to deal with. The resulting collision integrals must then still be evaluated in terms of some process of molecular interaction, with some assumed representation of a molecular-interaction potential, to be considered in §§ 4.1.3 and 4.3.3. Thus, the number per unit time, $d(\dot{N}'_c)_{\theta\varphi}$, is to be related to $d(\dot{\tilde{N}}_c)_{\theta'\varphi'}$, the number of molecules undergoing direct collisions per unit time in $(\tilde{\vec{r}},d\mathcal{V}_r)$ at time $\tilde{t}$ and having initial velocities in the solid angle range $d\Omega_{\theta'\varphi'}$ about $\vec{e}_{\theta'\varphi'}$, where (cf. eqs. (3.10))

$$\vec{e}_{\theta'\varphi'} \equiv \vec{e}_{\theta\varphi}(\theta',\varphi') \tag{4.4}$$

is the unit vector in the direction θ',φ'.

For any directional-average collision model to be discussed, one will first need to consider the number of molecules in $(\tilde{\vec{r}},d\mathcal{V}_r)$ at time $\tilde{t}$ with velocity direction in $(\theta',\varphi',d\Omega_{\theta'\varphi'})$ (see fig. 4.3):

$$d\tilde{N}_{\theta'\varphi'} \equiv \tilde{n}_{\theta'\varphi'}\, d\mathcal{V}_r\, d\Omega_{\theta'\varphi'} \tag{4.5a}$$

$$\equiv n_{\theta\varphi}(\tilde{\vec{r}},\theta',\varphi',\tilde{t})\, d\mathcal{V}_r\, d\Omega_{\theta'\varphi'} \tag{4.5b}$$

(where the direction θ',φ' is yet to be defined for the particular directional-average collision models). During the time interval dt after time $\tilde{t}$, a fraction,

$$\tilde{\Theta}_{\theta'\varphi'}\, dt \equiv \Theta_{\theta\varphi}(\tilde{\vec{r}},\theta',\varphi',\tilde{t})\, dt \tag{4.6}$$

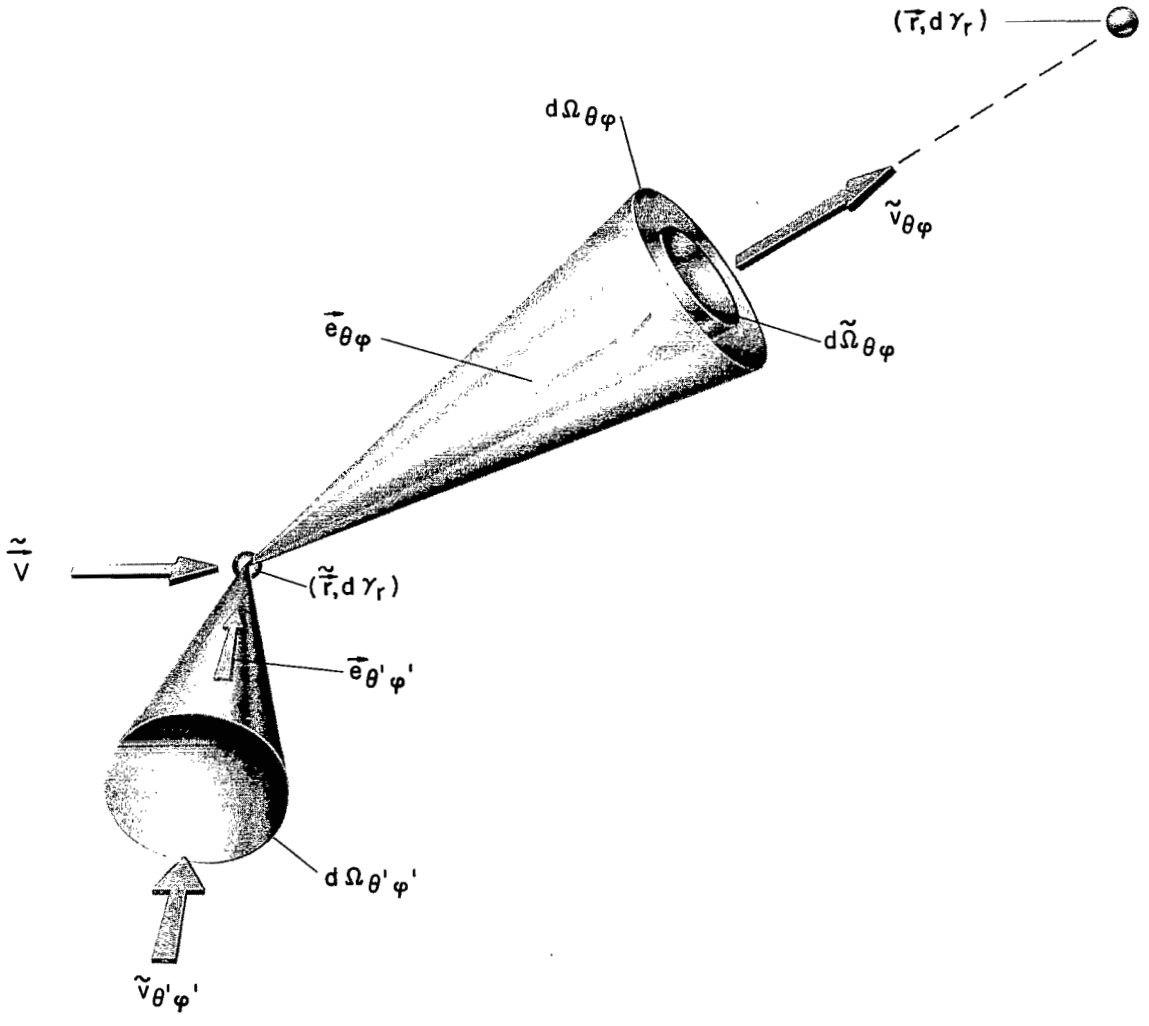

Figure 4.3 - Illustration for directional-average collision models

of this number $d\tilde{N}_{\theta'\varphi'}$ undergo collisions with other molecules that have average velocity $\vec{\tilde{V}} \equiv \vec{V}(\vec{\tilde{r}},\tilde{t})$, where $\vec{V}(\vec{r},t) \equiv \langle \vec{\xi} \rangle$. Thus, the number, out of the original $d\tilde{N}_{\theta'\varphi'}$, that undergo collisions in time dt is

$$d(\dot{\tilde{N}}_c)_{\theta'\varphi'}\, dt = \tilde{\Theta}_{\theta'\varphi'}\, d\tilde{N}_{\theta'\varphi'}\, dt \tag{4.7a}$$

$$= \tilde{n}_{\theta'\varphi'}\, \tilde{\Theta}_{\theta'\varphi'}\, d\mathscr{V}_r\, d\Omega_{\theta'\varphi'}\, dt \tag{4.7b}$$

This number is scattered in all directions and with all velocities by the collisions. (In the center-of-mass frame of reference of each pair of colliding molecules, at least for hard elastic spheres, they are scattered isotropically; cf. Jeans, 1952. This has been a useful concept in the formulation and interpretation of the BGK collision model; see Liepmann, Narasimha, and Chahine, 1962, p.1318.)

For any directional-average collision model to be considered, it is convenient to define certain "inverse-collision factors," $Z(\vec{r},\theta,\varphi,t)$, by

$$n_{\theta\varphi} \langle \phi\Theta'_{\vec{\xi}} \rangle_{\theta\varphi} \equiv Z\, \tilde{n}_{\theta'\varphi'} \widetilde{\langle \phi\Theta_{\vec{\xi}} \rangle}_{\theta'\varphi'} \tag{4.8a}$$

and in particular

$$n_{\theta\varphi} \langle \phi^{(\ell)}\Theta'_{\vec{\xi}} \rangle_{\theta\varphi} \equiv {}^{(\ell)}Z\, \tilde{n}_{\theta'\varphi'} \widetilde{\langle \phi^{(\ell)}\Theta_{\vec{\xi}} \rangle}_{\theta'\varphi'} \tag{4.8b}$$

where $\phi^{(\ell)} = \xi^{\ell}$, $\ell = 0,1,2,\ldots$. For various collision models (I, II, III) one can denote $Z = Z_I$, $Z = Z_{II}$, or $Z = Z_{III}$.

In terms of these defined inverse collision factors, equations (3.41b) and (3.42b) become

$$\frac{\partial n_{\theta\varphi}}{\partial t} + \vec{e}_{\theta\varphi} \cdot \nabla_r [n_{\theta\varphi} \langle \xi \rangle_{\theta\varphi}]$$

$$= {}^{(0)}Z\, \tilde{n}_{\theta'\varphi'} \widetilde{\langle \Theta_{\vec{\xi}} \rangle}_{\theta'\varphi'} - n_{\theta\varphi} \langle \Theta_{\vec{\xi}} \rangle_{\theta\varphi} \tag{4.9a}$$

$$\frac{\partial}{\partial t}\left[n_{\theta\varphi}\left\langle\phi^{(\ell)}\right\rangle_{\theta\varphi}\right] + \vec{e}_{\theta\varphi}\cdot\nabla_r\left[n_{\theta\varphi}\left\langle\phi^{(\ell+1)}\right\rangle_{\theta\varphi}\right]$$

$$= {}^{(\ell)}Z\,\tilde{n}_{\theta'\varphi'}\left\langle\widetilde{\phi^{(\ell)}\Theta_{\vec{\xi}}}\right\rangle_{\theta'\varphi'} - n_{\theta\varphi}\left\langle\phi^{(\ell)}\Theta_{\vec{\xi}}\right\rangle_{\theta\varphi} \qquad (4.9b)$$

and for any other $\phi(\vec{r},\vec{\xi},t)$,

$$\frac{\partial}{\partial t}\left[n_{\theta\varphi}\left\langle\phi\right\rangle_{\theta\varphi}\right] + \vec{e}_{\theta\varphi}\cdot\nabla_r\left[n_{\theta\varphi}\left\langle\xi\phi\right\rangle_{\theta\varphi}\right] - n_{\theta\varphi}\left[\left\langle\frac{\partial\phi}{\partial t}\right\rangle_{\theta\varphi} + \vec{e}_{\theta\varphi}\cdot\left\langle\nabla_r(\xi\phi)\right\rangle_{\theta\varphi}\right]$$

$$= Z\,\tilde{n}_{\theta'\varphi'}\left\langle\widetilde{\phi\Theta_{\vec{\xi}}}\right\rangle_{\theta'\varphi'} - n_{\theta\varphi}\left\langle\phi\Theta_{\vec{\xi}}\right\rangle_{\theta\varphi} \qquad (4.9c)$$

where, for any function $F(\vec{r},\theta,\varphi,t)$, the notation $\tilde{F}$ indicates:

$$\tilde{F} \equiv F(\tilde{\vec{r}},\theta,\varphi,\tilde{t})$$

where

$$\left.\begin{aligned}\tilde{\vec{r}} &\equiv \vec{r} - \vec{\lambda}^{*}_{\theta\varphi}(\tilde{\vec{r}},\theta,\varphi,\tilde{t}) = \vec{r} - \vec{e}_{\theta\varphi}\,\frac{\left\langle\widetilde{\xi}\right\rangle_{\theta\varphi}}{\left\langle\widetilde{\Theta_{\vec{\xi}}}\right\rangle_{\theta\varphi}}\\ \tilde{t} &\equiv t - 1/\left\langle\widetilde{\Theta_{\vec{\xi}}}\right\rangle_{\theta\varphi}\end{aligned}\right\} \qquad (4.10)$$

and where the particular collision model considered determines the direction θ',φ' corresponding to each θ,φ and determines the factors Z, to be considered below.

A particular constraint to be satisfied by the collision models should be noted: Since in local translational equilibrium (with a local Maxwellian molecular-velocity distribution function) the sum of the collision terms on the right side of the Boltzmann equation (e.g., in the form (3.41a)) vanishes, the right side of each of the <u>integrals</u> of that equation, equations (4.9), must also vanish in equilibrium. It is evident then that the specification of the collision models should allow, in the limiting condition of equilibrium, $\vec{e}_{\theta'\varphi'}$ to become coincident with $\vec{e}_{\theta\varphi}$

and each Z to become unity. The task in the remainder of this section is to consider various directional-average collision models for determining $\vec{e}_{\theta'\varphi'}$ and the corresponding factors Z that satisfy these conditions.

4.1.2.1 The simplest directional-average collision model, I

The molecules whose number is given by equations (4.7), scattered out of $d\Omega_{\theta'\varphi'}$ in all directions during dt by collisions in $(\tilde{\vec{r}}, d\mathscr{V}_r)$, tend to favor the original direction before collision (even though the colliding molecules may be scattered isotropically in the frame of reference fixed relative to the center of mass of each pair of colliding molecules) because of the effect of persistence of velocities (cf. Chapman and Cowling, 1961; Jeans, 1952; and Present, 1958). We therefore take, for the simplest model to consider, that the representative direction before the collisions (θ',φ') is approximately the same as (θ,φ). Then take as a reasonable intuitive assumption that, on the average, this number $d(\tilde{\dot{N}}_c)_{\theta\varphi}$, scattered out of $(\tilde{\vec{r}}, d\mathscr{V}_r)$, $(\theta,\varphi,d\Omega_{\theta\varphi})$ per unit time, can represent approximately the number put into a volume $d\mathscr{V}_r$ of the same size a directional mean free path away at $\vec{r} = \tilde{\vec{r}} + \vec{\lambda}^*_{\theta\varphi}(\tilde{\vec{r}},\theta,\varphi,\tilde{t})$ per unit time at time $t = \tilde{t}+1/\Theta_{\theta\varphi}(\tilde{\vec{r}},\theta,\varphi,\tilde{t})$, with final velocity in the solid angle $(\theta,\varphi,d\Omega_{\theta\varphi})$ at $\vec{r}$, owing to collisions at point $\tilde{\vec{r}}$ at time $\tilde{t}$. Thus we assume for the model that

$$\vec{e}_{\theta'\varphi'} = \vec{e}_{\theta\varphi} \qquad \text{(model I)} \qquad (4.11a)$$

and that

$$(0)_{Z_I} = 1 \qquad (4.11b)$$

in equation (4.9a) (so that the right side of (4.9a) would become $\tilde{n}_{\theta\varphi}\,\tilde{\Theta}_{\theta\varphi} - n_{\theta\varphi}\,\Theta_{\theta\varphi}$).

Furthermore, assume that certain other molecular properties $\phi(\tilde{\vec{r}},\vec{\xi},\tilde{t})$, which are characteristic properties of the molecules at point $\tilde{\vec{r}}$ at time

$\tilde{t}$, are carried with this number of molecules, $d(\dot{\tilde{N}}_c)_{\theta\varphi}$, that has been assumed to be put into $(\vec{r},d\mathcal{V}_r)$, $(\theta,\varphi,d\Omega_{\theta\varphi})$ in unit time at time t. Thus it will be assumed for this model that, for certain $\phi(\vec{r},\vec{\xi},t)$ in equations (4.8) and (4.9):

$$Z_I = 1 \tag{4.11c}$$

The number and nature of the properties assumed to satisfy (4.11c) would be specified as required to make a determined system of equations and to provide most realistic results from the model in problems where it can be used.

It is assumed that the main justification for use of this model in any given problem would be determined by the realism and consistency of the quantitative or qualitative results it yields and by the tractability it provides in solving the equations of gas flow where significant translational nonequilibrium is present.

4.1.2.2 Directional-average collision model II

The next simplest directional-average collision model to be considered, denoted here as II, corresponds in a sense to the BGK model of the Boltzmann equation (cf. Liepmann, Narasimha, and Chahine, 1962) (also called the Krook-Welander model; cf. Bhatnagar, Gross, and Krook, 1954, and Welander, 1954).

An important aspect of the BGK kinetic model is its interpretation of molecules being emitted from collisions in local equilibrium with the state of the gas at the point of collision (see Liepmann, Narasimha, and Chahine, 1962). In the BGK model, the gain-term collision integral of the Boltzmann equation is replaced by the local Maxwellian distribution function times the local collision frequency; that is, the term $\Theta'_{\vec{\xi}}\, f$ in equation (3.41) is replaced by $\Theta\, f_e$ where f_e is the local Maxwellian (eq. (2.23a)).

This same notion is used here to define collision model II, except that here the molecules are assumed to be emitted from collisions in equilibrium with the local state at point $\tilde{\vec{r}}$ when considering the gain term for the point $\vec{r}$. For this model, the initial direction $\vec{e}_{\theta'\varphi'}$ at point $\tilde{\vec{r}}$ is immaterial, so we take:

$$\vec{e}_{\theta'\varphi'} = \vec{e}_{\theta\varphi} \qquad \text{(model II)} \qquad (4.12a)$$

and assume that the right side of each of equations (4.9) is

$$(\tilde{n}_{\theta\varphi})_e \left[\widetilde{\langle \phi\Theta_{\vec{\xi}} \rangle_{\theta\varphi}}\right]_e - n_{\theta\varphi}\langle \phi\Theta_{\vec{\xi}} \rangle_{\theta\varphi}$$

where subscript e indicates a local-equilibrium value, evaluated using a local-Maxwellian velocity distribution function (to be described in § 4.3.2 and to be used in Chapter VII). This is equivalent to defining, for each ${}^{(\ell)}Z$ in equations (4.9):

$$ {}^{(\ell)}Z_{II} \equiv \frac{n_{\theta\varphi}\langle \phi^{(\ell)}\Theta'_{\vec{\xi}} \rangle_{\theta\varphi}}{\tilde{n}_{\theta'\varphi'}\widetilde{\langle \phi^{(\ell)}\Theta_{\vec{\xi}} \rangle_{\theta'\varphi'}}} = \frac{(\tilde{n}_{\theta\varphi})_e\left[\widetilde{\langle \phi^{(\ell)}\Theta_{\vec{\xi}} \rangle_{\theta\varphi}}\right]_e}{\tilde{n}_{\theta'\varphi'}\widetilde{\langle \phi^{(\ell)}\Theta_{\vec{\xi}} \rangle_{\theta'\varphi'}}} \qquad (4.12b)$$

It will be seen that the first approximation in a scheme described in Chapter VI gives a result on the directional level for this model, II, that corresponds to direct integration of the BGK kinetic equation.

4.1.2.3 Directional-average collision model III

The following-described model, denoted as III, estimates a direction $\vec{e}_{\theta'\varphi'}$ that is different from $\vec{e}_{\theta\varphi}$ in regions of spatially varying flow. The corresponding evaluation of the inverse-collision factor, Z_{III}, follows directly.

For estimating $\vec{e}_{\theta'\varphi'}$, the number per unit time coming out of collisions, $d(\tilde{N}_c)_{\theta'\varphi'}$, given by (4.7), is assumed to have average velocity $\vec{e}_{\theta'\varphi'}\,\tilde{v}_{\theta'\varphi'}$ within $d\Omega_{\theta'\varphi'}$ before collision and average velocity $\vec{e}_{\theta\varphi}\,\tilde{v}_{\theta\varphi}$ within $d\tilde{\Omega}_{\theta\varphi}$ after collision (see fig. 4.3). (The relationship between $d\tilde{\Omega}_{\theta\varphi}$ and $d\Omega_{\theta\varphi}$ will be given below.) Assume that the average velocity of all the other molecules with which this number collides is $\tilde{\vec{V}}'$ before collision and $\tilde{\vec{V}}$ after collision. An equation that could be interpreted as a momentum-conservation equation between "pairs of average molecules", one with original velocity $\vec{e}_{\theta'\varphi'}\,\tilde{v}_{\theta'\varphi'}$ and final velocity $\vec{e}_{\theta\varphi}\tilde{v}_{\theta\varphi}$, the other with respective initial and final velocities $\tilde{\vec{V}}'$ and $\tilde{\vec{V}}$, is

$$\vec{e}_{\theta'\varphi'}\,\tilde{v}_{\theta'\varphi'} + \tilde{\vec{V}}' = \vec{e}_{\theta\varphi}\,\tilde{v}_{\theta\varphi} + \tilde{\vec{V}} \tag{4.13a}$$

The quantity

$$\vec{V}_c(\tilde{\vec{r}},\tilde{t},\theta,\varphi) \equiv \tilde{\vec{V}}' - \tilde{\vec{V}} = \vec{e}_{\theta\varphi}\,\tilde{v}_{\theta\varphi} - \vec{e}_{\theta'\varphi'}\,\tilde{v}_{\theta'\varphi'} \tag{4.13b}$$

could be called a "relative overall collision velocity change for the direction (θ,φ) at $(\tilde{\vec{r}},\tilde{t})$." It is a measure of the degree of spatial nonequilibrium, since it vanishes when $\vec{e}_{\theta'\varphi'} = \vec{e}_{\theta\varphi}$. One could represent $\vec{V}_c$ by any appropriate quantity that is known to vanish in equilibrium. As a special case that appears particularly appropriate, which we may denote as <u>model IIIa</u>, it is taken as a reasonable assumption that

$$\vec{V}_c \equiv \tilde{\vec{V}}' - \tilde{\vec{V}} = \tilde{\vec{V}} - \vec{V} \qquad \text{(model IIIa)} \tag{4.14}$$

that is, that the average change in the overall mass velocity of the "other molecules" colliding with the $d(\tilde{N}_c)_{\theta'\varphi'}$ molecules can be represented approximately by $\tilde{\vec{V}}-\vec{V}$, the change in overall mass velocity in one directional mean free path in the direction $\vec{e}_{\theta\varphi}$. The approximate validity of this model, IIIa, or of any other model for $\vec{V}_c$ in (4.13b),

could be tested by solving the resulting flow equations for a given problem.

Refer now to figure 4.4, which: (a) represents the vector addition of equations (4.13), and (b) illustrates the construction of the solid angles for estimating $d(\dot{N}_c')_{\theta\varphi}$ (and consequently Z_{III}), to be discussed in the following.

Note first that the vector equation (4.13b), along with the trigonometric law of cosines:

$$V_c^2 = \tilde{v}_{\theta\varphi}^2 + \tilde{v}_{\theta'\varphi'}^2 - 2\,\tilde{v}_{\theta\varphi}\tilde{v}_{\theta'\varphi'}\,\vec{e}_{\theta\varphi}\cdot\vec{e}_{\theta'\varphi'} \tag{4.15}$$

can be solved for the direction $\vec{e}_{\theta'\varphi'}$ and the magnitude $\tilde{v}_{\theta'\varphi'}$ in terms of $\vec{e}_{\theta\varphi}$, $\vec{e}_c$, $\tilde{v}_{\theta\varphi}$, and V_c, where

$$V_c \equiv |\vec{V}_c| \quad \text{and} \quad \vec{e}_c \equiv \vec{V}_c/V_c \tag{4.16}$$

and in particular,

$$V_c = |\vec{V}-\tilde{\vec{V}}| \qquad \text{(model IIIa)} \tag{4.17}$$

Thus, taking the dot product of $\vec{e}_{\theta\varphi}$ with equation (4.13b) gives an expression which, when substituted into equation (4.15), yields

$$\tilde{v}_{\theta'\varphi'} = [V_c^2 + \tilde{v}_{\theta\varphi}^2 - 2\,\tilde{v}_{\theta\varphi}\,V_c\,(\vec{e}_{\theta\varphi}\cdot\vec{e}_c)]^{1/2} \tag{4.18a}$$

Then substitution of (4.18a) back into (4.13b) gives

$$\vec{e}_{\theta'\varphi'} = \frac{\vec{e}_{\theta\varphi}\,\tilde{v}_{\theta\varphi} - \vec{e}_c\,V_c}{[V_c^2 + \tilde{v}_{\theta\varphi}^2 - 2\,\tilde{v}_{\theta\varphi}\,V_c\,(\vec{e}_{\theta\varphi}\cdot\vec{e}_c)]^{1/2}} \tag{4.18b}$$

The direction (θ',φ') is therefore defined explicitly in terms of $\vec{V}_c \equiv \vec{e}_c V_c$. (Note that model IIIa could be regarded as a first approximation

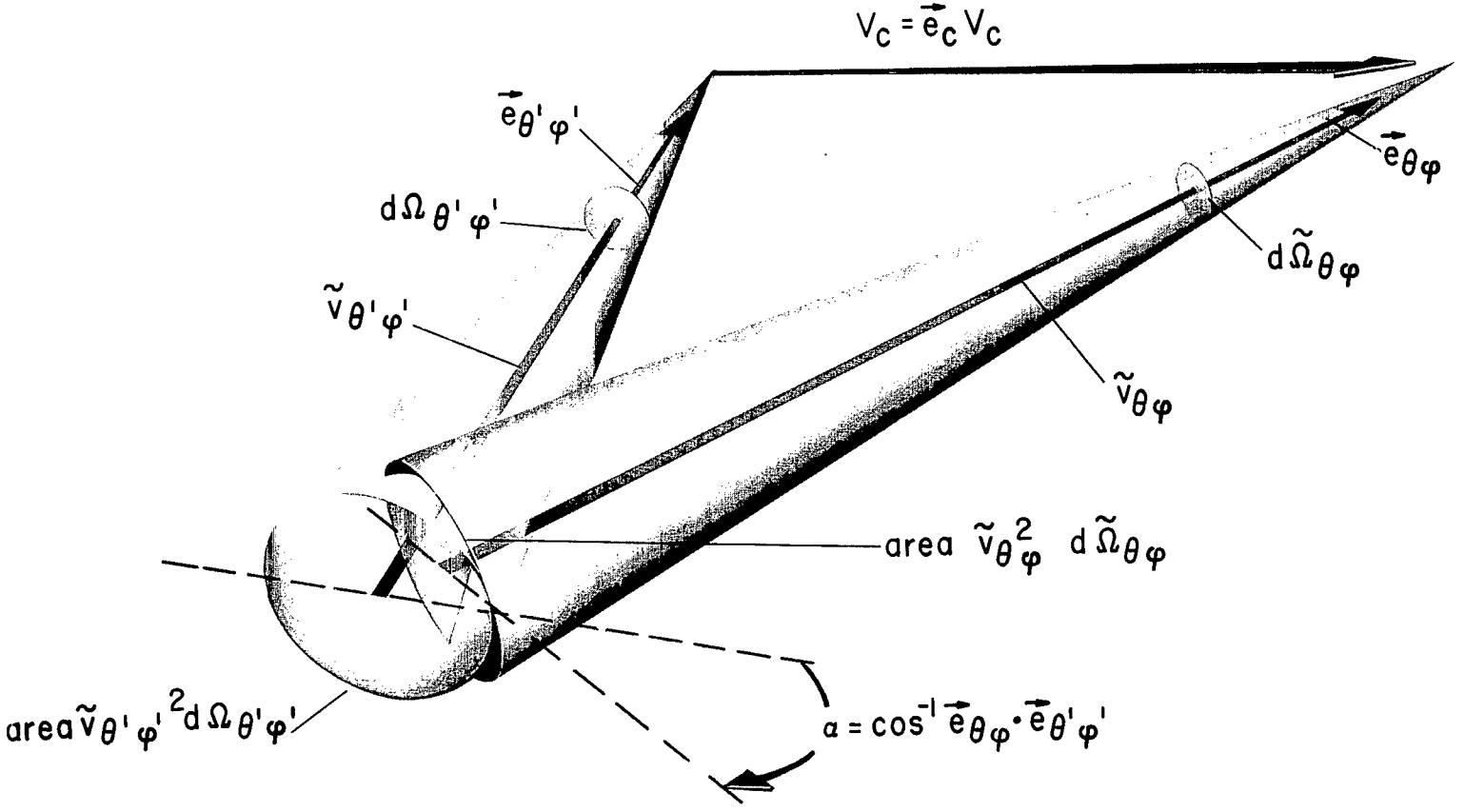

Figure 4.4 - Vector addition, and construction of solid angles, in directional-average collision model III.

for $\vec{V}_c$, and then higher order corrections made to ensure that

$$\vec{V}_c = \vec{e}_{\theta\varphi}\,\tilde{v}_{\theta\varphi} - \vec{e}_{\theta'\varphi'}\,\tilde{v}_{\theta'\varphi'} \qquad)$$

The factor $Z = Z_{III}$ for this model is now found by the following procedure. If each possible vector of magnitude $\tilde{v}_{\theta'\varphi'}$, and having any direction within $(\theta',\varphi',d\Omega_{\theta'\varphi'})$ is added to $\vec{V}_c$ (see fig. 4.4), all the resultant vectors would fill a solid angle, denoted above as $d\tilde{\Omega}_{\theta\varphi}$. In general $d\tilde{\Omega}_{\theta\varphi}$ is not the same as $d\Omega_{\theta\varphi}$. The magnitude of $d\tilde{\Omega}_{\theta\varphi}$ is found as indicated by the construction in figure 4.4:

The ratio of the area $\tilde{v}^2_{\theta\varphi}\,d\tilde{\Omega}_{\theta\varphi}$ on figure 4.4 to the area $\tilde{v}^2_{\theta'\varphi'} \times d\Omega_{\theta'\varphi'}$ is $|\cos\alpha| = |\vec{e}_{\theta\varphi}\cdot\vec{e}_{\theta'\varphi'}|$. Therefore

$$d\tilde{\Omega}_{\theta\varphi} = \left(\frac{\tilde{v}_{\theta'\varphi'}}{\tilde{v}_{\theta\varphi}}\right)^2 |\vec{e}_{\theta\varphi}\cdot\vec{e}_{\theta'\varphi'}|\; d\Omega_{\theta'\varphi'} \qquad (4.19)$$

The number of the molecules emitted from collisions per unit time in $(\tilde{\vec{r}},d\mathscr{V}_r)$ at time $\tilde{t}$ in the angle range $(\theta,\varphi,d\Omega_{\theta\varphi})$ is $d\Omega_{\theta\varphi}/d\tilde{\Omega}_{\theta\varphi}$ times the number emitted in $(\theta,\varphi,d\tilde{\Omega}_{\theta\varphi})$. Thus, from above assumptions (with use of (4.7b) and (4.19)),

$$d(\dot{N}'_c)_{\theta\varphi} = \frac{d\Omega_{\theta\varphi}}{d\tilde{\Omega}_{\theta\varphi}}\; d(\tilde{\dot{N}}_c)_{\theta'\varphi'} = \left(\frac{d\Omega_{\theta'\varphi'}}{d\tilde{\Omega}_{\theta\varphi}}\right)\left(\frac{d\Omega_{\theta\varphi}}{d\Omega_{\theta'\varphi'}}\right) d(\tilde{\dot{N}}_c)_{\theta'\varphi'}$$

$$= \left(\frac{\tilde{v}_{\theta\varphi}}{\tilde{v}_{\theta'\varphi'}}\right)^2 \frac{\tilde{n}_{\theta'\varphi'}\;\tilde{\Theta}_{\theta'\varphi'}\;d\mathscr{V}_r\;d\Omega_{\theta\varphi}}{|\vec{e}_{\theta\varphi}\cdot\vec{e}_{\theta'\varphi'}|} \qquad (4.20)$$

Now substitution of (4.18a) and of the scalar product of $\vec{e}_{\theta\varphi}$ with equation (4.18b) into equation (4.20) gives for collision model III:

$$d(\dot{N}'_c)_{\theta\varphi} \equiv n_{\theta\varphi}\, \Theta'_{\theta\varphi}\, d\mathscr{V}_r\, d\Omega_{\theta\varphi} \tag{4.21a}$$

$$= \frac{\tilde{n}_{\theta'\varphi'}\, \tilde{\Theta}_{\theta'\varphi'}\, d\mathscr{V}_r\, d\Omega_{\theta\varphi}}{\left[\left(\frac{V_c}{\tilde{v}_{\theta\varphi}}\right)^2 + 1 - 2(\vec{e}_{\theta\varphi}\cdot\vec{e}_c)\frac{V_c}{\tilde{v}_{\theta\varphi}}\right]^{1/2} \left|1-(\vec{e}_{\theta\varphi}\cdot\vec{e}_c)\frac{V_c}{\tilde{v}_{\theta\varphi}}\right|} \tag{4.21b}$$

Comparison of equations (4.21) and use of the definitions in (4.8) give for collision model III:

$$(0)_{Z_{III}} = \left[\left(\frac{V_c}{\tilde{v}_{\theta\varphi}}\right)^2 + 1 - 2(\vec{e}_{\theta\varphi}\cdot\vec{e}_c)\frac{V_c}{\tilde{v}_{\theta\varphi}}\right]^{-1/2} \left|1-(\vec{e}_{\theta\varphi}\cdot\vec{e}_c)\frac{V_c}{\tilde{v}_{\theta\varphi}}\right|^{-1} \tag{4.22}$$

where model IIIa can be used to estimate:

$$V_c = |\vec{V}-\tilde{\vec{V}}| \quad \text{and} \quad \vec{e}_c = \frac{\vec{V}-\tilde{\vec{V}}}{|\vec{V}-\tilde{\vec{V}}|} \quad \text{(model IIIa)} \tag{4.23}$$

It may be assumed that certain molecular properties $\phi(\tilde{\vec{r}},\vec{\xi}',\tilde{t})$, which are characteristic properties of the molecules at point $\tilde{\vec{r}}$ and time $\tilde{t}$, with velocity $\vec{\xi}'$ having direction (θ',φ'), are carried with the number per unit time, $d(\dot{N}'_c)_{\theta\varphi}$, on the average, as estimated by equation (4.21b) and therefore that

$$(\ell)_{Z_{III}} = (0)_{Z_{III}} \tag{4.24}$$

for use in equation (4.9b).

Further reduction of this model, and its use, are illustrated below. It is assumed that the main justification for use of this intuitive collision model would be determined by the results it yields.

4.1.3 Assumption on the collision frequency per molecule, and results

Since $\Lambda_{\theta\varphi}$, defined by equation (3.40b), could reasonably play the same role as $\lambda^*_{\theta\varphi}$ (defined by (3.37b)) in the development of the directional-mean-free-path approximation above, it is regarded as consistent with the rest of the development to consider $\Theta_{\vec{\xi}}$ (cf. eqs. (2.12c) and (3.33a)) to be <u>independent</u> of the molecular-velocity <u>magnitude</u>, ξ. The results are that

$$\Theta_{\vec{\xi}} = \Theta_{\theta\varphi}(\vec{r},\theta,\varphi,t) \tag{4.25}$$

and therefore that (cf. eqs. (3.37) to (3.40))

$$\Lambda_{\theta\varphi} = \lambda^*_{\theta\varphi} \tag{4.26}$$

In addition to the above argument, another indication that the assumption of $\Theta_{\vec{\xi}}$ independent of ξ is realistic is the fact that for <u>Maxwell</u> molecules $\Theta_{\vec{\xi}}$ does not vary with <u>any</u> part of the molecular velocity. Equation (4.25) still allows variation with θ and φ, as well as with $\vec{r}$, and t.

The assumption leading to (4.25) and (4.26) leads to further very convenient results, mainly embodied in the form taken by the directional equations of change (eqs. (3.41b) and (3.42b) or eqs. (4.9)) which, with the directional-mean-free-path approximation described above in §4.1.1 and with any of the proposed directional-average collision models (§4.1.2), become

$$\frac{\partial}{\partial t}\left[n_{\theta\varphi}\langle\phi\rangle_{\theta\varphi}\right] + \vec{e}_{\theta\varphi}\cdot\nabla_r\left[n_{\theta\varphi}\langle\xi\phi\rangle_{\theta\varphi}\right] - n_{\theta\varphi}\left[\left\langle\frac{\partial\phi}{\partial t}\right\rangle_{\theta\varphi} + \vec{e}_{\theta\varphi}\cdot\langle\nabla_r(\xi\phi)\rangle_{\theta\varphi}\right]$$

$$= Z\,\tilde{n}_{\theta'\varphi'}\langle\tilde{\phi}\rangle_{\theta'\varphi'}\,\tilde{\Theta}_{\theta'\varphi'} - n_{\theta\varphi}\langle\phi\rangle_{\theta\varphi}\,\Theta_{\theta\varphi} \tag{4.27}$$

where for any function $F(\vec{r},\theta,\varphi,t)$:

$$\left.\begin{aligned} \tilde{F} &\equiv F(\tilde{\vec{r}},\theta,\varphi,\tilde{t}) \\ \tilde{\vec{r}} &= \vec{r} - \vec{e}_{\theta\varphi}\langle\tilde{\xi}\rangle_{\theta\varphi}/\tilde{\Theta}_{\theta\varphi} \\ \tilde{t} &= t - 1/\tilde{\Theta}_{\theta\varphi} \end{aligned}\right\} \quad (4.28)$$

where $\vec{e}_{\theta\varphi}$ is defined by equations (3.10) and where the molecular properties $\phi = \phi(\vec{r},\vec{\xi},t)$ are to be appropriately chosen (see § 4.2 below).

4.2 Directional Equations and Some "Boundary Conditions" in Terms of Dimensionless Integrals of Directional Property Distributions

If one chooses to work on the directional level, as described above, one should still ensure satisfaction of the conservation equations on the macroscopic (full moment) level. A proposed method for accomplishing this is described here and is used in the following sections (§§ 4.3 and 4.4), as well as in Chapter VII. The procedure amounts to defining new dimensionless dependent variables, on the directional level, that are certain integrals of the previously defined directional property distributions. These new variables are defined in a form such that: (a) the directional equations of change can be written in terms of derivatives of the new variables, and (b) the macroscopic conservation principles can be prescribed as certain boundary conditions on the new variables on the directional level. The procedure also provides a convenient means for evaluating all the macroscopic variables of interest.

Since the macroscopic conservation equations, (3.43), are integrals of the directional equations of change (eq. (3.42d), represented approximately by (4.27) and (4.28)), with ϕ respectively m, $m\vec{\xi}$, and $\frac{1}{2}m\xi^2$, it is appropriate to use these choices for ϕ in equation (4.27). In writing the resulting equations it is convenient to use the following definitions (cf. §§ 3.7 and 3.8):

Mass density:

$$\Phi^{(0)}_{\theta\varphi} \equiv \rho_{\theta\varphi}(\vec{r},\theta,\varphi,t) = m \int_0^\infty f\, \xi^2 d\xi \tag{4.29a}$$

$$\Phi^{(0)} \equiv \rho(\vec{r},t) = \int_0^\Pi d\varphi\, (\sin\varphi) \int_{-\Pi}^{\Pi} d\theta [\rho_{\theta\varphi}(\vec{r},\theta,\varphi,t)] \tag{4.29b}$$

Mass flux, or momentum density:

$$\Phi^{(1)}_{\theta\varphi} \equiv \vec{J}_{\theta\varphi}(\vec{r},\theta,\varphi,t) \equiv \rho_{\theta\varphi} \langle \vec{\xi} \rangle_{\theta\varphi}$$

$$= \vec{e}_{\theta\varphi}\, \rho_{\theta\varphi}\, v^{(1)}_{\theta\varphi} = \vec{e}_{\theta\varphi}\, m \int_0^\infty f\, \xi^3\, d\xi \tag{4.29c}$$

$$\Phi^{(1)} \equiv \vec{J}(\vec{r},t) \equiv \rho \langle \vec{\xi} \rangle = \int_0^\Pi d\varphi\, (\sin\varphi) \int_{-\Pi}^{\Pi} d\theta [\vec{J}_{\theta\varphi}(\vec{r},\theta,\varphi,t)] \tag{4.29d}$$

Momentum flux:

$$\Phi^{(2)}_{\theta\varphi} \equiv \mathbf{P}_{\theta\varphi}(\vec{r},\theta,\varphi,t) \equiv \rho_{\theta\varphi} \langle \vec{\xi}\vec{\xi} \rangle_{\theta\varphi}$$

$$= \vec{e}_{\theta\varphi}\vec{e}_{\theta\varphi}\, \rho_{\theta\varphi}\, v^{(2)}_{\theta\varphi} = \vec{e}_{\theta\varphi}\vec{e}_{\theta\varphi}\, m \int_0^\infty f\, \xi^4\, d\xi \tag{4.29e}$$

$$\Phi^{(2)} \equiv \mathbf{P}(\vec{r},t) \equiv \rho \langle \vec{\xi}\vec{\xi} \rangle = \int_0^\infty d\varphi\, (\sin\varphi) \int_{-\Pi}^{\Pi} d\theta [\mathbf{P}_{\theta\varphi}(\vec{r},\theta,\varphi,t)] \tag{4.29f}$$

Energy density:†

$$\tfrac{1}{2}\mathbf{I}: \Phi^{(2)}_{\theta\varphi} \equiv \mathbf{E}_{\theta\varphi}(\vec{r},\theta,\varphi,t) \equiv \rho_{\theta\varphi} \left\langle \tfrac{1}{2}\xi^2 \right\rangle_{\theta\varphi} = \tfrac{1}{2}\rho_{\theta\varphi}\, v^{(2)}_{\theta\varphi} = \tfrac{1}{2} m \int_0^\infty f\, \xi^4\, d\xi \tag{4.29g}$$

†See footnote on pp. 32 and 33.

$$\frac{1}{2}\,\mathbf{I}:\ \Phi^{(2)} \equiv E(\vec{r},t) \equiv \rho\,\frac{1}{2}\langle\xi^2\rangle = \int_0^{\Pi} d\varphi\,(\sin\varphi)\int_{-\Pi}^{\Pi} d\theta[E_{\theta\varphi}(\vec{r},\theta,\varphi,t)] \qquad (4.29h)$$

Energy Flux:†

$$\frac{1}{2}\,\mathbf{I}:\ \Phi^{(3)}_{\theta\varphi} \equiv \vec{Q}_{\theta\varphi}(\vec{r},\theta,\varphi,t) \equiv \rho_{\theta\varphi}\ \frac{1}{2}\langle\xi^2\vec{\xi}\rangle_{\theta\varphi}$$

$$= \vec{e}_{\theta\varphi}\,\frac{1}{2}\,\rho_{\theta\varphi}\,v^{(3)}_{\theta\varphi} = \vec{e}_{\theta\varphi}\,\frac{1}{2}\,m\int_0^{\infty} f\,\xi^5\,d\xi \qquad (4.29i)$$

$$\frac{1}{2}\,\mathbf{I}:\ \Phi^{(3)} \equiv \vec{Q}(\vec{r},t) \equiv \rho\left\langle\frac{1}{2}\,\xi^2\vec{\xi}\right\rangle = \int_0^{\Pi} d\varphi\,(\sin\varphi)\int_{-\Pi}^{\Pi} d\theta[\vec{Q}_{\theta\varphi}(\vec{r},\theta,\varphi,t)] \qquad (4.29j)$$

Then the macroscopic conservation equations, (3.43), are

$$\partial\rho/\partial t + \nabla_r\cdot\vec{J} = 0 \qquad (4.30a)$$

$$\partial\vec{J}/\partial t + \nabla_r\cdot\mathbf{P} = 0 \qquad (4.30b)$$

$$\partial E/\partial t + \nabla_r\cdot\vec{Q} = 0 \qquad (4.30c)$$

and for $\phi = m$, $m\vec{\xi}$, and $\frac{1}{2}m\xi^2$ the corresponding forms of equation (4.27) are:

$$\partial\rho_{\theta\varphi}/\partial t + \nabla_r\cdot\vec{J}_{\theta\varphi} = {}^{(0)}Z\,\tilde{\rho}_{\theta'\varphi'}\,\tilde{\Theta}_{\theta'\varphi'} - \rho_{\theta\varphi}\,\Theta_{\theta\varphi} \qquad (4.31a)$$

$$\partial\vec{J}_{\theta\varphi}/\partial t + \nabla_r\cdot\mathbf{P}_{\theta\varphi} = {}^{(1)}Z\,\tilde{\vec{J}}_{\theta'\varphi'}\,\tilde{\Theta}_{\theta'\varphi'} - \vec{J}_{\theta\varphi}\,\Theta_{\theta\varphi} \qquad (4.31b)$$

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†See footnote on pp. 32 and 33.

$$\partial E_{\theta\varphi}/\partial t + \nabla_r \cdot \vec{Q}_{\theta\varphi} = {}^{(2)}Z\ \tilde{E}_{\theta'\varphi'}\ \tilde{\Theta}_{\theta'\varphi'} - E_{\theta\varphi}\ \Theta_{\theta\varphi} \tag{4.31c}$$

where

$$\tilde{\vec{r}} = \vec{r} - \tilde{\vec{\lambda}}^*_{\theta\varphi} = \vec{r} - \tilde{\vec{J}}_{\theta\varphi}/\tilde{\rho}_{\theta\varphi}\ \tilde{\Theta}_{\theta\varphi} \tag{4.31d}$$

$$\tilde{t} = t - 1/\tilde{\Theta}_{\theta\varphi} \tag{4.31e}$$

4.2.1 Dimensionless variables and equations of change

For the purpose of defining dimensionless variables that will facilitate solution of the equations, consider the constant reference values: arbitrary length L, density ρ_α, velocity u_α, and characteristic collision frequency Θ_α. Define the dimensionless constant:

$$\varepsilon \equiv u_\alpha/L\ \Theta_\alpha \tag{4.32}$$

It is convenient (here and in succeeding chapters) to consider time as a fourth dimension, with unit vector $\vec{e}_4$ that is orthogonal to $\vec{e}_1$, $\vec{e}_2$, and $\vec{e}_3$; that is

$$\left.\begin{aligned} \vec{e}_i \cdot \vec{e}_j &= \delta_{ij} \quad (i,j = 1,2,3,4) \\ &= 1 \quad \text{if} \quad i=j \\ &= 0 \quad \text{if} \quad i\neq j \end{aligned}\right\} \tag{4.33}$$

(All the three-dimensional vectors and tensors discussed above can be considered as four-dimensional with zero component in the $\vec{e}_4$ direction.) Then define the dimensionless four-component (space-time) position vectors (e.g., see Karamcheti, 1967):

$$\vec{\zeta} \equiv \sum_{i=1}^{4} \vec{e}_i \zeta_i \equiv \frac{1}{L}\vec{r} + \vec{e}_4 \frac{u_\alpha t}{L}$$

$$= \vec{e}_1 \frac{x_1}{L} + \vec{e}_2 \frac{x_2}{L} + \vec{e}_3 \frac{x_3}{L} + \vec{e}_4 \frac{u_\alpha t}{L} \qquad (4.34a)$$

$$\vec{z} \equiv \sum_{i=1}^{4} \vec{e}_i z_i \equiv \frac{1}{L}\vec{\tilde{r}} + \vec{e}_4 \frac{u_\alpha \tilde{t}}{L}$$

$$= \vec{e}_1 \frac{\tilde{x}_1}{L} + \vec{e}_2 \frac{\tilde{x}_2}{L} + \vec{e}_3 \frac{\tilde{x}_3}{L} + \vec{e}_4 \frac{u_\alpha \tilde{t}}{L} \qquad (4.34b)$$

and the dimensionless vector partial derivative (holding θ and φ constant in a function of $\vec{\zeta}$, θ, and φ):

$$\nabla_\zeta \equiv \sum_{i=1}^{4} \vec{e}_i \frac{\partial}{\partial \zeta_i} \equiv L \nabla_r + \vec{e}_4 \frac{L}{u_\alpha} \frac{\partial}{\partial t} \qquad (4.35)$$

Also define (for $-\Pi < \theta \leq \Pi$, $0 \leq \varphi \leq \Pi$, with ν and η, respectively, "dummy variables" for θ and φ):

$$F^{(0)}(\vec{\zeta},\theta,\varphi,\varepsilon) \equiv \int_{\varphi}^{\Pi} d\eta\, (\sin\eta) \int_{-\Pi}^{\theta} d\nu \left[\frac{\rho_{\theta\varphi}(\vec{r},\nu,\eta,t)}{\rho_\alpha}\right] \qquad (4.36a)$$

$$\vec{F}^{(1)}(\vec{\zeta},\theta,\varphi,\varepsilon) \equiv \int_{\varphi}^{\Pi} d\eta\, (\sin\eta) \int_{-\Pi}^{\theta} d\nu \left[\frac{\vec{J}_{\theta\varphi}(\vec{r},\nu,\eta,t)}{\rho_\alpha u_\alpha}\right] \qquad (4.36b)$$

$$\mathbf{F}^{(2)}(\vec{\zeta},\theta,\varphi,\varepsilon) \equiv \int_{\varphi}^{\Pi} d\eta\, (\sin\eta) \int_{-\Pi}^{\theta} d\nu \left[\frac{\mathbf{P}_{\theta\varphi}(\vec{r},\nu,\eta,t)}{\rho_\alpha u_\alpha^2}\right] \qquad (4.36c)$$

$$G^{(0)}(\vec{\zeta},\theta,\varphi,\varepsilon) \equiv \int_{\varphi}^{\Pi} d\eta\, (\sin\eta) \int_{-\Pi}^{\theta} d\nu \left[\frac{E_{\theta\varphi}(\vec{r},\nu,\eta,t)}{\rho_\alpha u_\alpha^2}\right] \qquad (4.36d)$$

$$\vec{G}^{(1)}(\vec{\zeta},\theta,\varphi,\varepsilon) \equiv \int_{\varphi}^{\Pi} d\eta\ (\sin\eta) \int_{-\Pi}^{\theta} d\nu \left[\frac{\vec{Q}_{\theta\varphi}(\vec{r},\nu,\eta,t)}{\rho_\alpha u_\alpha^3} \right] \tag{4.36e}$$

$$H(\vec{\zeta},\theta,\varphi,\varepsilon) \equiv \Theta_{\theta\varphi}(\vec{r},\theta,\varphi,t)/\Theta_\alpha \tag{4.37}$$

so that:

$$\frac{\rho_{\theta\varphi}(\vec{r},\theta,\varphi,t)}{\rho_\alpha} = -\frac{1}{\sin\varphi} \frac{\partial^2 F^{(0)}(\vec{\zeta},\theta,\varphi,\varepsilon)}{\partial\varphi\,\partial\theta} \tag{4.38a}$$

$$\frac{\vec{J}_{\theta\varphi}(\vec{r},\theta,\varphi,t)}{\rho_\alpha u_\alpha} = \frac{\vec{e}_{\theta\varphi}\rho_{\theta\varphi} v^{(1)}_{\theta\varphi}}{\rho_\alpha u_\alpha} = -\frac{1}{\sin\varphi} \frac{\partial^2 \vec{F}^{(1)}(\vec{\zeta},\theta,\varphi,t)}{\partial\varphi\partial\theta} \tag{4.38b}$$

$$\left.\begin{aligned} \frac{\mathbf{P}_{\theta\varphi}(\vec{r},\theta,\varphi,t)}{\rho_\alpha u_\alpha^2} &= \frac{\vec{e}_{\theta\varphi}\vec{e}_{\theta\varphi}\rho_{\theta\varphi} v^{(2)}_{\theta\varphi}}{\rho_\alpha u_\alpha^2} = \frac{-1}{\sin\varphi} \frac{\partial^2 \mathbf{F}^{(2)}(\vec{\zeta},\theta,\varphi,\varepsilon)}{\partial\varphi\,\partial\theta} \\ &= 2\,\vec{e}_{\theta\varphi}\vec{e}_{\theta\varphi} \frac{E_{\theta\varphi}}{\rho_\alpha u_\alpha^2} \end{aligned}\right\} \tag{4.38c}$$

$$\frac{E_{\theta\varphi}(\vec{r},\theta,\varphi,t)}{\rho_\alpha u_\alpha^2} = \frac{\frac{1}{2}\rho_{\theta\varphi} v^{(2)}_{\theta\varphi}}{\rho_\alpha u_\alpha^2} = \frac{-1}{\sin\varphi} \frac{\partial^2 G^{(0)}(\vec{\zeta},\theta,\varphi,\varepsilon)}{\partial\varphi\,\partial\theta} \tag{4.38d}$$

$$\frac{\vec{Q}_{\theta\varphi}(\vec{r},\theta,\varphi,t)}{\rho_\alpha u_\alpha^3} = \frac{\vec{e}_{\theta\varphi}\frac{1}{2}\rho_{\theta\varphi} v^{(3)}_{\theta\varphi}}{\rho_\alpha u_\alpha^3} = \frac{-1}{\sin\varphi} \frac{\partial^2 \vec{G}^{(1)}(\vec{\zeta},\theta,\varphi,\varepsilon)}{\partial\varphi\,\partial\theta} \tag{4.38e}$$

(where $\vec{e}_{\theta\varphi}$ is given by (3.10)).

For any function $f(\vec{\zeta},\theta,\varphi,\varepsilon)$, denote

$$\tilde{f} \equiv f(\vec{z},\theta,\varphi,\varepsilon) \tag{4.39}$$

Then define the four-component dimensionless vector

$$\left.\begin{aligned}
\vec{\mu}(\vec{\zeta},\theta,\boldsymbol{\varphi},\varepsilon) &\equiv \sum_{i=1}^{4} \vec{e}_i\, \mu_i(\vec{\zeta},\theta,\boldsymbol{\varphi},\varepsilon) \\
&\equiv \frac{-\vec{\lambda}^{*}_{\theta\boldsymbol{\varphi}}(\vec{r},\theta,\boldsymbol{\varphi},t)}{u_\alpha/\Theta_\alpha} - \vec{e}_4\, \frac{\Theta_\alpha}{\Theta_{\theta\boldsymbol{\varphi}}(\vec{r},\theta,\boldsymbol{\varphi},t)} \\
&= -\vec{e}_{\theta\boldsymbol{\varphi}}\left(\frac{v^{(1)}_{\theta\boldsymbol{\varphi}}}{u_\alpha}\right)\left(\frac{\Theta_\alpha}{\Theta_{\theta\boldsymbol{\varphi}}}\right) - \vec{e}_4\left(\frac{\Theta_\alpha}{\Theta_{\theta\boldsymbol{\varphi}}}\right) \\
&= -(1/H)\left[\left(\frac{\partial^2\vec{F}^{(1)}}{\partial\boldsymbol{\varphi}\partial\theta} \Big/ \frac{\partial^2 F^{(0)}}{\partial\boldsymbol{\varphi}\partial\theta}\right) + \vec{e}_4\right]
\end{aligned}\right\} \qquad (4.40)$$

with which equations (4.31d) and (4.31e) become

$$\vec{z} \equiv \vec{\zeta} + \varepsilon\, \tilde{\vec{\mu}} \qquad (4.41)$$

where

$$\tilde{\vec{\mu}} \equiv \vec{\mu}(\vec{z},\theta,\boldsymbol{\varphi},\varepsilon) = -\frac{1}{\tilde{H}}\left[\frac{\left(\frac{\partial^2\tilde{\vec{F}}^{(1)}}{\partial\boldsymbol{\varphi}\partial\theta}\right)}{\left(\frac{\partial^2\tilde{F}^{(0)}}{\partial\boldsymbol{\varphi}\partial\theta}\right)} + \vec{e}_4\right] \qquad (4.42)$$

The directional equations of change, (4.31a,b,c), are now:

$$\frac{\partial^3 F^{(0)}}{\partial\zeta_4\,\partial\boldsymbol{\varphi}\partial\theta} + \nabla_\zeta \cdot \frac{\partial^2\vec{F}^{(1)}}{\partial\boldsymbol{\varphi}\partial\theta} = \frac{1}{\varepsilon}\left[(0)_{Z\tilde{H}'}\, \frac{\sin\boldsymbol{\varphi}}{\sin\boldsymbol{\varphi}'}\, \widetilde{\left(\frac{\partial^2 F^{(0)}}{\partial\boldsymbol{\varphi}\partial\theta}\right)}' - H\,\frac{\partial^2 F^{(0)}}{\partial\boldsymbol{\varphi}\partial\theta}\right] \qquad (4.43a)$$

$$\frac{\partial^3\vec{F}^{(1)}}{\partial\zeta_4\,\partial\boldsymbol{\varphi}\partial\theta} + \nabla_\zeta \cdot \frac{\partial^2\mathbf{F}^{(2)}}{\partial\boldsymbol{\varphi}\partial\theta} = \frac{1}{\varepsilon}\left[(1)_{Z\tilde{H}'}\, \frac{\sin\boldsymbol{\varphi}}{\sin\boldsymbol{\varphi}'}\, \widetilde{\left(\frac{\partial^2\vec{F}^{(1)}}{\partial\boldsymbol{\varphi}\partial\theta}\right)}' - H\,\frac{\partial^2\vec{F}^{(1)}}{\partial\boldsymbol{\varphi}\partial\theta}\right] \qquad (4.43b)$$

$$\frac{\partial^3 G^{(0)}}{\partial \zeta_4 \, \partial \varphi \partial \theta} + \nabla_\zeta \cdot \frac{\partial^2 \vec{G}^{(1)}}{\partial \varphi \partial \theta} = \frac{1}{\varepsilon}\left[{}^{(2)}Z\tilde{H}' \, \frac{\sin \varphi}{\sin \varphi'} \left(\widetilde{\frac{\partial^2 G^{(0)}}{\partial \varphi \partial \theta}}\right)' - H \frac{\partial^2 G^{(0)}}{\partial \varphi \partial \theta}\right] \quad (4.43c)$$

where

$$\frac{\partial^2 \mathbf{F}^{(2)}}{\partial \varphi \partial \theta} = 2 \, \vec{e}_{\theta\varphi} \, \vec{e}_{\theta\varphi} \, \frac{\partial^2 G^{(0)}}{\partial \varphi \partial \theta} \quad (4.43d)$$

and where $(\,)'$ indicates a function evaluated at θ', φ', according to the collision model. We note from the definitions (4.36) that:

<u>when either $\theta = -\Pi$ or $\varphi = \Pi$</u>:

$$F^{(0)} = \vec{F}^{(1)} = \mathbf{F}^{(2)} = G^{(0)} = \vec{G}^{(1)} = 0 \quad (4.44)$$

and (cf. eqs. (4.29)): <u>when $\theta = \Pi$ and $\varphi = 0$</u>:

$$F^{(0)} = F^{(0)}(\vec{\zeta}, \Pi, 0, \varepsilon) = \rho(\vec{r},t)/\rho_\alpha \quad (4.45a)$$

$$\vec{F}^{(1)} = \vec{F}^{(1)}(\vec{\zeta}, \Pi, 0, \varepsilon) = \vec{J}(\vec{r},t)/\rho_\alpha u_\alpha \quad (4.45b)$$

$$\mathbf{F}^{(2)} = \mathbf{F}^{(2)}(\vec{\zeta}, \Pi, 0, \varepsilon) = \mathbf{P}(\vec{r},t)/\rho_\alpha u_\alpha^2 \quad (4.45c)$$

$$G^{(0)} = G^{(0)}(\vec{\zeta}, \Pi, 0, \varepsilon) = E(\vec{r},t)/\rho_\alpha u_\alpha^2 \quad (4.45d)$$

$$\vec{G}^{(1)} = \vec{G}^{(1)}(\vec{\zeta}, \Pi, 0, \varepsilon) = \vec{Q}(\vec{r},t)/\rho_\alpha u_\alpha^3 \quad (4.45e)$$

Thus, either one can regard equations (4.45) as boundary conditions on the integral functions defined in (4.36), where the macroscopic moments $(\rho, \vec{J}, \mathbf{P}, E, \vec{Q})$ must satisfy the conservation equations, (4.30); or the macroscopic conservation equations (4.30) can themselves be expressed as boundary conditions at $\theta = \Pi$, $\varphi = 0$ on the integral functions

(using eqs. (4.45)) in the form:

$$\frac{\partial F^{(0)}(\vec{\zeta},\Pi,0,\varepsilon)}{\partial \zeta_4} + \nabla_\zeta \cdot \vec{F}^{(1)}(\vec{\zeta},\Pi,0,\varepsilon) = 0 \tag{4.46a}$$

$$\frac{\partial \vec{F}^{(1)}(\vec{\zeta},\Pi,0,\varepsilon)}{\partial \zeta_4} + \nabla_\zeta \cdot \mathbf{F}^{(2)}(\vec{\zeta},\Pi,0,\varepsilon) = 0 \tag{4.46b}$$

$$\frac{\partial G^{(0)}(\vec{\zeta},\Pi,0,\varepsilon)}{\partial \zeta_4} + \nabla_\zeta \cdot \vec{G}^{(1)}(\vec{\zeta},\Pi,0,\varepsilon) = 0 \tag{4.46c}$$

Before attempting to solve a given problem using the above formulation, one needs yet to: evaluate, or relate in some manner to the other variables, the collision frequency $\theta_{\theta\varphi}$ (or H); obtain a determined system of equations by some other independent means of relating the dependent variables; and prescribe sufficient boundary conditions in the $\vec{\zeta}$ domain. These will be considered in later sections.

4.2.2 Relationships of flow-property distributions and new dimensionless variables to the more conventional macroscopic flow variables

To facilitate application of boundary conditions for solving a given problem by the above formulation, and also to enhance physical understanding, it is desired to relate the macroscopic flow properties in equations (4.29) or (4.45) to the more conventional macroscopic flow variables.

With the mean mass velocity of the gas $(\vec{V})$ defined by equation (2.15), the molecular velocity relative to the mean motion $(\vec{C})$ defined by equation (2.16), and the velocity magnitudes defined by

$$\left.\begin{aligned} \xi &= |\vec{\xi}| = (\vec{\xi}\cdot\vec{\xi})^{1/2} \\ V &= |\vec{V}| = (\vec{V}\cdot\vec{V})^{1/2} \\ C &= |\vec{C}| = (\vec{C}\cdot\vec{C})^{1/2} \end{aligned}\right\} \tag{4.47}$$

one has

$$\vec{J} \equiv \rho\langle\vec{\xi}\rangle = \rho\vec{V} \tag{4.48a}$$

$$\mathbf{P} \equiv \rho\langle\vec{\xi}\vec{\xi}\rangle = \rho\vec{V}\vec{V} + \rho\langle\vec{C}\vec{C}\rangle \tag{4.48b}$$

$$E \equiv \rho\left\langle\frac{1}{2}\vec{\xi}\cdot\vec{\xi}\right\rangle = \frac{1}{2}\rho\langle C^2\rangle + \frac{1}{2}\rho V^2 \tag{4.48c}$$

$$\vec{Q} \equiv \rho\left\langle\frac{1}{2}\vec{\xi}\cdot\vec{\xi}\vec{\xi}\right\rangle = \frac{1}{2}\rho\langle C^2\vec{C}\rangle + \vec{V}\cdot\rho\langle\vec{C}\vec{C}\rangle$$

$$+ \frac{1}{2}\langle C^2\rangle\rho\vec{V} + \frac{1}{2}\rho V^2\vec{V} \tag{4.48d}$$

The energy per unit mass relative to the mean motion, or the specific internal energy, is

$$e \equiv \frac{1}{2}\langle C^2\rangle \tag{4.49}$$

Since in equilibrium the internal energy is $\frac{1}{2}kT$ per degree of freedom of a molecule, where k is Boltzmann's constant, the temperature of a monatomic gas of neutral spherically-symmetric molecules in arbitrary translational nonequilibrium is defined by

$$me \equiv 3\left(\frac{1}{2}kT\right)$$

or

$$RT \equiv \frac{2}{3}e = \frac{1}{3}\langle C^2\rangle \tag{4.50}$$

where $R \equiv k/m$ is the gas constant.

For a perfect (sufficiently rarefied) gas (implicitly assumed in the use of the Boltzmann equation), the "collisional transfer" of momentum or energy due to finite size of molecules is neglected in comparison to the flux of momentum or energy due simply to the "flow of molecules" (e.g., see Hirschfelder, Curtiss, and Bird, 1964), so that the stress tensor and heat-flux vector are simply:

$$\boldsymbol{\sigma} = -\rho\langle\vec{C}\vec{C}\rangle \tag{4.51}$$

$$\vec{q} = \frac{1}{2}\rho\langle C^2\vec{C}\rangle \tag{4.52}$$

The hydrostatic pressure is defined by

$$p^* \equiv -\frac{1}{3}\mathbf{I}:\boldsymbol{\sigma} = \frac{1}{3}\rho\langle C^2\rangle \tag{4.53}$$

so that from equation (4.50) we have

$$p^* = \rho RT \tag{4.54}$$

The viscous-stress tensor, $\boldsymbol{\tau}$, is defined by

$$\boldsymbol{\sigma} \equiv -p\mathbf{I} + \boldsymbol{\tau} \tag{4.55}$$

where p is the thermodynamic pressure. Far from translational equilibrium, the "thermodynamic pressure" has no meaning. Therefore, since sufficiently close to equilibrium the Chapman-Enskog theory for a perfect monatomic gas gives a zero bulk viscosity, κ, defined by

$$\kappa \equiv \frac{p-p^*}{\nabla_r\cdot\vec{V}} \tag{4.56}$$

it is assumed that the "pressure" in (4.55) is

$$p = p^* = \rho RT = \frac{1}{3}\rho\langle C^2\rangle \tag{4.57}$$

and therefore that the viscous stress tensor is

$$\boldsymbol{\tau} = -\rho\langle\vec{C}\vec{C}\rangle + \mathbf{I}\frac{1}{3}\rho\langle C^2\rangle \tag{4.58}$$

With the definitions in equations (4.49) to (4.58), equations (4.48) become

$$\vec{J} = \rho\vec{V} \tag{4.59a}$$

$$\left.\begin{aligned} \mathbf{P} &= \rho\vec{V}\vec{V} - \boldsymbol{\sigma} \\ &= \rho\vec{V}\vec{V} + \mathbf{I}p - \boldsymbol{\tau} \end{aligned}\right\} \tag{4.59b}$$

$$E = \rho(e + \tfrac{1}{2}V^2) \tag{4.59c}$$

$$\left.\begin{aligned} \vec{Q} &= \rho\vec{V}(e + \tfrac{1}{2}V^2) + \vec{q} - \vec{V}\cdot\boldsymbol{\sigma} \\ &= \rho\vec{V}(e + \tfrac{1}{2}V^2) + \vec{q} - \vec{V}\cdot\boldsymbol{\tau} + p\vec{V} \end{aligned}\right\} \tag{4.59d}$$

(With equations (4.59), equations (4.30) give more familiar forms of the macroscopic conservation equations.) Equations (4.59) will be useful in determining boundary conditions on the functions in (4.45).

The common macroscopic variables of interest can then be calculated in terms of ρ, $\vec{J}$, $\mathbf{P}$, E, and $\vec{Q}$ as:

$$\vec{V} = \vec{J}/\rho \tag{4.60a}$$

$$p = (2/3)\rho e = \frac{2}{3}(E - \tfrac{1}{2}\rho V^2) \tag{4.60b}$$

$$RT = (2/3)e = p/\rho = \frac{2}{3}(E/\rho - \tfrac{1}{2}V^2) \tag{4.60c}$$

$$\boldsymbol{\sigma} = -\mathbf{P} + \rho\vec{V}\vec{V} \tag{4.60d}$$

$$\left.\begin{aligned} \boldsymbol{\tau} &= -\mathbf{P} + \rho\vec{V}\vec{V} + p\mathbf{I} \\ &= -\mathbf{P} + \rho\vec{V}\vec{V} + \frac{2}{3}(E - \tfrac{1}{2}V^2)\mathbf{I} \end{aligned}\right\} \tag{4.60e}$$

$$\vec{q} = \vec{Q} - \rho\vec{V}(e + \frac{1}{2}V^2) + \vec{V}\cdot\boldsymbol{\sigma}$$

$$= \vec{Q} - E\vec{V} - \vec{V}\cdot\mathbf{P} + \rho V^2\vec{V} \qquad (4.60f)$$

Other macroscopic variables of interest are the specific enthalpy, h, and the Mach number, M, defined by

$$h \equiv e + p/\rho = \frac{5}{3}e = \frac{5}{2}p/\rho = \frac{5}{2}RT$$

$$= \frac{5}{3}(E/\rho - \frac{1}{2}V^2) \qquad (4.60g)$$

and

$$M^2 = \frac{V^2}{(5/3)RT} = \frac{9}{5}\left(\frac{\frac{1}{2}\rho V^2}{E - \frac{1}{2}\rho V^2}\right) \qquad (4.60h)$$

(where the ratio of specific heats for the perfect monatomic gas is 5/3).

4.3 Indeterminacy of the Equations of Change, and a Proposed Method of Closure using Integrals of a Local-Directional Gaussian Distribution Function

It is well known that the conservation equations on the macroscopic level are an indeterminate system, containing more unknowns than the number of equations. In the directional-mean-free-path method introduced above, the equations on the directional level of description contain one more unknown quantity than the number of equations if the collision frequency is appropriately specified.

The purposes of this section are to: (a) propose a method of closure, on the directional level, that emphasizes the molecular-directional aspects of translational nonequilibrium and that is compatible with the known local-Maxwellian distributions of molecular velocities in limiting regions of local translational equilibrium; (b) determine the expressions for the

directional property distributions in local translational equilibrium for applying local-equilibrium boundary conditions; and (c) consider representations of the collision frequencies.

It is useful to consider what may be called a "local-directional Gaussian distribution function." First the property distributions on the directional level are to be expressed by integrating such an assumed distribution function, for use in an "integral method," to be described. As a special case, these property distributions are then found in terms of a local Maxwellian distribution of molecular velocity for use in applying boundary conditions in regions of local translational equilibrium.

4.3.1 Assumed local-directional Gaussian distribution function, and resulting directional-property distributions

For making the directional equations of change a determined system, one additional equation that relates the variables appearing in those equations((4.31) or (4.43)) may be found by what may be called an "integral method." Integral methods entail assuming the form of a certain function, and then using integrals of that function to advantage, without necessarily implying that the original precise variation, in the assumed form of the function integrated, is physically significant. In this same sense, a "local-directional Gaussian distribution" is now chosen in the form

$$f = \alpha(\vec{r},\theta,\varphi,t)\, e^{-\beta(\vec{r},\theta,\varphi,t)[\vec{\xi}-\vec{U}(\vec{r},\theta,\varphi,t)]^2} \tag{4.61a}$$

$$\equiv a\, e^{-c^2\xi^2 + 2\,b\,c\,\xi} \tag{4.61b}$$

where

$$\left.\begin{aligned} a &= a(\vec{r},\theta,\varphi,t) \equiv \alpha\, e^{-\beta\vec{U}\cdot\vec{U}} \\ b &= b(\vec{r},\theta,\varphi,t) \equiv \beta^{1/2}\, \vec{e}_{\theta\varphi}\cdot\vec{U} \\ c &= c(\vec{r},\theta,\varphi,t) \equiv \beta^{1/2} \end{aligned}\right\} \tag{4.62}$$

are unknown functions of θ and φ as well as of $\vec{r}$ and t. Note that $\vec{U}$ here is an unknown vector function having the dimensions of velocity. The form (4.61b) is especially convenient. This form for f is specified only for the purpose of integrating it to obtain an appropriate relation among the directional property distributions. Its use (as in other integral-approximation techniques) does not imply that the molecular-velocity distribution at any $(\vec{r},\theta,\varphi,t)$ is thought to be Gaussian. However, the assumed directional-Gaussian distribution is especially convenient in that it becomes the correct local Maxwellian distribution in any limiting region of local translational equilibrium, where α, β, and $\vec{U}$ become independent of θ and φ ($\vec{U}$ becomes $\vec{V}(\vec{r},t)$, β becomes $\beta_e \equiv m/2kT(\vec{r},t)$, and α becomes $n(\vec{r},t)[m/2\Pi\ kT(\vec{r},t)]^{3/2}$). A usual procedure in studying nonequilibrium phenomena (e.g., see Vincenti and Kruger, 1965, p. 225) is to use to advantage certain relations that are known to be true in equilibrium and assume that they hold approximately in arbitrary non-equilibrium; one may then ascertain that the use of such assumptions does not adversely affect the nonequilibrium results obtained; in other words that the relationship between the mathematics and the physics of the problem is not overly sensitive to the arbitrary assumptions made.

If one defines the dimensionless quantities;

$$A = A(\vec{r},\theta,\varphi,t) \equiv \frac{2\ \rho_\alpha (cu_\alpha)^3}{a\ m\ u_\alpha^3} \left(\frac{\rho_{\theta\varphi}}{\rho_\alpha} \right) \tag{4.63a}$$

$$\bar{c} = \bar{c}(\vec{r},\theta,\varphi,t) \equiv cu_\alpha \tag{4.63b}$$

and (cf. eq. (2.24))

$$B(b) \equiv \frac{1}{2}\Pi^{1/2}\ e^{b^2}(1 + \text{erf}\ b) \tag{4.63c}$$

and puts equation (4.61b) into the definitions of directional property distributions in equations (4.29), one obtains

$$A(\vec{r},\theta,\varphi,t) = (1+2b^2)\,B(b) + b \tag{4.64a}$$

$$A\,\frac{v^{(1)}_{\theta\varphi}(\vec{r},\theta,\varphi,t)}{u_\alpha} = \frac{1}{\bar{c}}\left[b(3+2b^2)\,B(b) + 1 + b^2\right] \tag{4.64b}$$

$$A\,\frac{v^{(2)}_{\theta\varphi}(\vec{r},\theta,\varphi,t)}{u_\alpha^2} = \frac{1}{2\bar{c}^2}\left[(3+12b^2+4b^4)\,B(b) + b(5+2b^2)\right] \tag{4.64c}$$

$$A\,\frac{v^{(3)}_{\theta\varphi}(\vec{r},\theta,\varphi,t)}{u_\alpha^3} = \frac{1}{2\bar{c}^3}\left[b(15+20b^2+4b^4)\,B(b) + (4+9b^2+2b^4)\right] \tag{4.64d}$$

One could regard equations (4.64a,b,c) as three equations for the three unknowns: A, b, and $\bar{c}$. "In principle", the three equations could be solved for A, b, and $\bar{c}$ as functions of $v^{(1)}_{\theta\varphi}/u_\alpha$ and $v^{(2)}_{\theta\varphi}/u_\alpha^2$. These results could then be substituted into equation (4.64d) to give $v^{(3)}_{\theta\varphi}/u_\alpha^3$ in terms of $v^{(1)}_{\theta\varphi}/u_\alpha$ and $v^{(2)}_{\theta\varphi}/u_\alpha^2$. Then one could find, from equation (4.63a),

$$\left(\frac{\frac{1}{2}mu_\alpha^3}{\rho_\alpha}\right)a = \frac{(\rho_{\theta\varphi}/\rho_\alpha)\bar{c}^3}{A} \tag{4.65}$$

In this way, two things would be accomplished in principle:

(a) A relationship among $v^{(1)}_{\theta\varphi}$, $v^{(2)}_{\theta\varphi}$, and $v^{(3)}_{\theta\varphi}$ would be determined; and

(b) The quantities a, b, and c would be determined in terms of $\rho_{\theta\varphi}$, $v^{(1)}_{\theta\varphi}$, and $v^{(2)}_{\theta\varphi}$

A perhaps less obvious, but more tractable, procedure for determining equivalent relationships is the following: By considering the four equations, (4.64), all at once, one can first determine b and $\bar{c}$ explicitly in terms of $v^{(1)}_{\theta\varphi}$, $v^{(2)}_{\theta\varphi}$, and $v^{(3)}_{\theta\varphi}$; then find A and B also explicitly in terms of $v^{(1)}_{\theta\varphi}$, $v^{(2)}_{\theta\varphi}$, and $v^{(3)}_{\theta\varphi}$. Then the expressions

for both b and B in terms of $v^{(1)}_{\theta\varphi}$, $v^{(2)}_{\theta\varphi}$, and $v^{(3)}_{\theta\varphi}$, along with the definition (4.63c), provide an implicit equation relating $v^{(1)}_{\theta\varphi}$, $v^{(2)}_{\theta\varphi}$, and $v^{(3)}_{\theta\varphi}$ (cf. the statement (a) above). Again, since A and $\bar{c}$ are determined, equations (4.65) could again be used to determine a in terms of $\rho_{\theta\varphi}$, $v^{(1)}_{\theta\varphi}$, and $v^{(2)}_{\theta\varphi}$ (since $v^{(3)}_{\theta\varphi}$ is implicitly related to $v^{(1)}_{\theta\varphi}$ and $v^{(2)}_{\theta\varphi}$), so that a, b, and c are all determined (cf. the statement (b) above). Following are the details of this more tractable procedure just described:

Combining equations (4.64a,b,c), one finds

$$\bar{c}^2 \frac{v^{(2)}_{\theta\varphi}}{u_\alpha^2} - b\bar{c} \frac{v^{(1)}_{\theta\varphi}}{u_\alpha} = \frac{3}{2} \tag{4.66a}$$

and combining equations (4.64b,c, and d), one finds

$$\bar{c}^2 \frac{v^{(3)}_{\theta\varphi}}{u_\alpha^3} - b\bar{c} \frac{v^{(2)}_{\theta\varphi}}{u_\alpha^2} = 2 \frac{v^{(1)}_{\theta\varphi}}{u_\alpha} \tag{4.66b}$$

From equations (4.64a and b) one finds

$$\left(\bar{c} \frac{v^{(1)}_{\theta\varphi}}{u_\alpha} - b\right)A - 2bB = 1 \tag{4.66c}$$

and it is convenient to write equation (4.64a) as

$$A - (1 + 2b^2)B = b \tag{4.66d}$$

If now b is eliminated from equations (4.66a and b) to obtain

$$\bar{c} = u_\alpha \left[\frac{2\left(v^{(1)}_{\theta\varphi}\right)^2 - \frac{3}{2} v^{(2)}_{\theta\varphi}}{v^{(1)}_{\theta\varphi} v^{(3)}_{\theta\varphi} - \left(v^{(2)}_{\theta\varphi}\right)^2} \right]^{1/2} \tag{4.67a}$$

then (4.66a) gives

(4.67b)

$$b = \frac{\bar{c}^2(v^{(2)}_{\theta\varphi}/u^2_\alpha)-3/2}{\bar{c}(v^{(1)}_{\theta\varphi}/u_\alpha)} = \frac{2\, v^{(1)}_{\theta\varphi}\, v^{(2)}_{\theta\varphi} - \frac{3}{2}\, v^{(3)}_{\theta\varphi}}{\left\{\left[2\left(v^{(1)}_{\theta\varphi}\right)^2 - \frac{3}{2}\, v^{(2)}_{\theta\varphi}\right]\left[v^{(1)}_{\theta\varphi} v^{(3)}_{\theta\varphi} - \left(v^{(2)}_{\theta\varphi}\right)^2\right]\right\}^{1/2}}$$

Equations (4.66c and d) are easily solved to obtain

$$A = \frac{b}{1 - (1+2b^2)(1 + b^2 - b\bar{c}\, v^{(1)}_{\theta\varphi}/u_\alpha)} \tag{4.67c}$$

and

$$B = \frac{b(1 + b^2 - b\bar{c}\, v^{(1)}_{\theta\varphi}/u_\alpha)}{1 - (1+2b^2)(1 + b^2 - b\bar{c}\, v^{(1)}_{\theta\varphi}/u_\alpha)} \tag{4.67d}$$

where b and $\bar{c}$ are given by (4.67a and b). Now if we define:

$$\psi^{(3)} = \psi^{(3)}(\vec{r},\theta,\varphi,t) \equiv v^{(3)}_{\theta\varphi}/(v^{(1)}_{\theta\varphi})^3 \tag{4.68a}$$

$$\psi^{(2)} = \psi^{(2)}(\vec{r},\theta,\varphi,t) \equiv v^{(2)}_{\theta\varphi}/(v^{(1)}_{\theta\varphi})^2 \tag{4.68b}$$

we can, as described above, use equation (4.63c) with (4.67d) to obtain the following convenient form of the desired relationship among the directional property distributions that is used to close the system of equations on the directional level:

$$B(b) \equiv \frac{1}{2}\Pi^{1/2}\, e^{b^2}(1 + \text{erf } b) = \frac{b(1 + b^2 - bs)}{1 - (1+2b^2)(1 + b^2 - bs)} \tag{4.69a}$$

where (from (4.67a) and (4.67b)):

$$b = \frac{2\,\psi^{(2)} - \frac{3}{2}\,\psi^{(3)}}{\left\{\left[2 - \frac{3}{2}\,\psi^{(2)}\right]\left[\psi^{(3)} - \left(\psi^{(2)}\right)^2\right]\right\}^{1/2}} \tag{4.69b}$$

and

$$s \equiv \overline{c}\,\frac{v_{\theta\varphi}^{(1)}}{u_\alpha} = \left[\frac{2 - \frac{3}{2}\,\psi^{(2)}}{\psi^{(3)} - \left(\psi^{(2)}\right)^2}\right]^{1/2} \tag{4.69c}$$

Implicitly, equations (4.69) define a direct functional relationship between $\psi^{(3)}$ and $\psi^{(2)}$, which may be written in the following form that will be found convenient for later use:

$$\psi^{(2)} = \Psi(\psi) \tag{4.70a}$$

where

$$\psi \equiv \left(\psi^{(2)}\right)^2 \Big/ \psi^{(3)} \tag{4.70b}$$

This relationship can be computed from (4.69) and tabulated, once and for all, for use in the method described above. One method for computing and tabulating the functional relationship (4.70) would be to specify various values of b ranging from $-\infty$ to $+\infty$ and, for each of these values of b, calculate s from (4.69a) as

$$s = \frac{1 + b^2 + (3b+2b^3)B(b)}{b + (1+2b^2)B(b)} \tag{4.71}$$

then find both $\psi^{(2)}$ and $\psi^{(3)}$ by solving (4.69b) and (4.69c) to obtain

$$\begin{aligned} \psi^{(2)} &= \frac{3}{2s^2} + \frac{b}{s} \\ \psi^{(3)} &= \frac{2}{s^2} + \frac{b}{s}\left(\frac{3}{2s^2} + \frac{b}{s}\right) \end{aligned} \tag{4.72}$$

and evaluate ψ from (4.70b).

Other relationships that are equivalent, but more convenient for later use, are found as follows: From the definition of the function B(b) in (4.63c),

$$dB(b)/db = 1 + 2b\,B(b) \tag{4.73}$$

and

$$\overline{N}(b) \equiv \frac{d}{db}[b\,B(b)] = 2\int_0^\infty e^{-\nu^2}\, e^{2b\nu}\, \nu^2\, d\nu$$

$$= b + (1+2b^2)B(b) \tag{4.74a}$$

$$\overline{N}'(b) \equiv \frac{d}{db}\overline{N}(b) = 4\int_0^\infty e^{-\nu^2}\, e^{2b\nu}\, \nu^3\, d\nu$$

$$= 2[1 + b^2 + (3b+2b^3)B(b)] \tag{4.74b}$$

$$\overline{N}''(b) \equiv \frac{d^2}{db^2}\overline{N}(b) = 4\left[\frac{5}{2}\,b + b^3 + \left(\frac{3}{2} + 6b^2+2b^4\right)B(b)\right] \tag{4.74c}$$

$$\overline{N}^{(k)}(b) \equiv \frac{d^k}{db^k}[\overline{N}(b)] = 2^{1+k}\int_0^\infty e^{-\nu^2}\, e^{2b\nu}\, \nu^{2+k}\, d\nu, \quad k=0,1,2,\ldots \tag{4.74d}$$

from which can be found the differential equations:

$$\overline{N}''(b) = 2b\,\overline{N}'(b) + 6\,\overline{N}(b) \tag{4.75a}$$

and

$$\overline{N}^{(k)}(b) = 2b\,\overline{N}^{(k-1)}(b) + 2(k+1)\,\overline{N}^{(k-2)}(b), \quad (k=2,3,4,\ldots,) \tag{4.75b}$$

Thus, it is seen that equation (4.71) is simply

$$s = \overline{N}'(b)/2\,\overline{N}(b) \tag{4.76}$$

for use in (4.72), or in fact, from (4.64), (4.68), and (4.70), that

$$\psi^{(2)} = \bar{N}(b)\,\bar{N}''(b)\Big/[\bar{N}'(b)]^2 \tag{4.77a}$$

$$\psi^{(3)} = [\bar{N}(b)]^2\,\bar{N}'''(b)\Big/[\bar{N}'(b)]^3 \tag{4.77b}$$

$$\psi = [\bar{N}''(b)]^2\Big/\bar{N}'(b)\,\bar{N}'''(b) \tag{4.77c}$$

For large negative b, it is extremely difficult to calculate B(b) to sufficient accuracy to obtain $\psi^{(2)}$, $\psi^{(3)}$, and ψ. In that case, the functions can be calculated simultaneously by numerical integration of the ordinary differential equations (4.73) and (4.75), starting at large negative b with values of the functions found from the asymptotic expansions: as $b \to -\infty$:

$$B(b) \sim \sum_{n=0}^{\infty} \frac{(-1)^{n+1}\,(2n)!}{n!\,(2b)^{2n+1}} \tag{4.78a}$$

$$\frac{d^k\bar{N}(b)}{db^k} \sim \sum_{n=1}^{\infty} \frac{(-1)^{n+k}\,(2n+k)!}{(2)^{2n}\,(n-1)!\,b^{2n+k+1}}\,, \quad (k=0,1,2,\ldots) \tag{4.78b}$$

The accuracy of this evaluation of the functions B(b) and $d^k\bar{N}(b)/db^k$ is then easily checked by comparing the values obtained at b=0 with the exact values:

$$B(0) = \sqrt{\pi}/2\,, \quad \bar{N}(0) = \sqrt{\pi}/2\,, \quad \bar{N}'(0) = 2 \tag{4.79}$$

and with the values of the higher derivatives of $\bar{N}$ at b=0 found directly from (4.75b)

The variation of $\psi^{(2)}$ and $\psi^{(3)}$ with b can be examined locally by asymptotic expansions. For example, one finds:

as $b \to -\infty$:

$$\psi^{(2)} \sim \frac{4}{3}\left[1 - 1/2b^2 + 15/4b^4 + O(1/b^6)\right] \tag{4.80a}$$

$$\psi^{(3)} \sim \frac{20}{9}\left[1 - 3/2b^2 + O(1/b^4)\right] \tag{4.80b}$$

as $b \to 0$:

$$\psi^{(2)} = (3\Pi/8)\left[1 - (3\Pi^{1/2} - 28/3\Pi^{1/2})\, b + O(b^2)\right] \tag{4.80c}$$

$$\psi^{(3)} = (\Pi/2)\left[1 - (21\Pi^{1/2}/8 - 8/\Pi^{1/2})\, b + O(b^2)\right] \tag{4.80d}$$

as $b \to +\infty$:

$$\psi^{(2)} \sim 1 + 1/2b^2 - 3/2b^4 + 15/4b^6 - + \cdots \tag{4.80e}$$

$$\psi^{(3)} \sim 1 + 3/2b^2 - 9/2b^4 + 14/b^6 - + \cdots \tag{4.80f}$$

Use of equations (4.68) through (4.80) is illustrated later. Figure 4.5 shows $\psi^{(2)}$, $\psi^{(3)}$, and ψ versus b.

4.3.2 Special case of local Maxwellian velocity-distribution function

In order to apply boundary conditions in regions of local translational equilibrium, it is convenient to express the directional property distributions in terms of the macroscopic variables. If it is assumed that in regions of local translational equilibrium the assumed directional Gaussian distribution, (4.61), becomes the local Maxwellian distribution function, (2.23a), then the functions α, β, and $\vec{U}$ in equations (4.61) and (4.62) become independent of θ and φ. Comparison of equation (4.61a) with (2.23a) then shows that, as a region of local translational equilibrium is approached, we have the asymptotic relations:

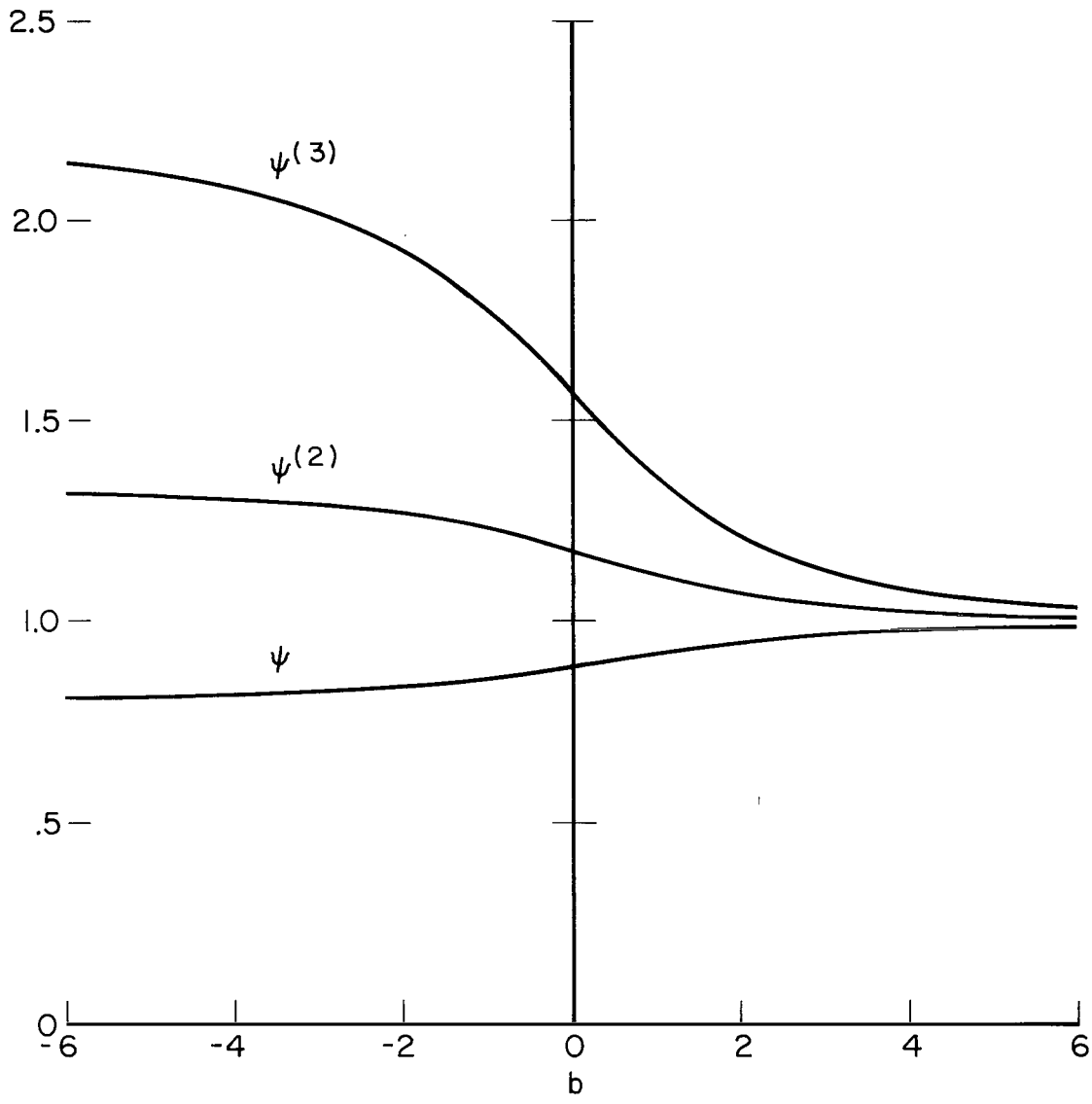

Figure 4.5 - Functions in the closure equation.

$$\alpha(\vec{r},\theta,\varphi,t) \sim n(\vec{r},t)\left[\frac{m}{2\Pi\ kT\ (\vec{r},t)}\right]^{3/2} \tag{4.81a}$$

$$\vec{U}(\vec{r},\theta,\varphi,t) \sim \vec{V}(\vec{r},t) \tag{4.81b}$$

$$\beta(\vec{r},\theta,\varphi,t) \sim m/2kT(\vec{r},t) \tag{4.81c}$$

Then, with $\beta_e = \beta_e(\vec{r},t)$ defined by equation (2.23b) and with unit vector $\vec{e} = \vec{e}(\vec{r},t) \equiv \vec{V}/V$ (eq. (4.13)), equations (4.62) and (4.81) give, as local equilibrium is approached:

$$a(\vec{r},\theta,\varphi,t) \sim n(\beta_e/\Pi)^{3/2}\ e^{-\beta_e V^2} \tag{4.82a}$$

$$b(\vec{r},\theta,\varphi,t) \sim \beta_e^{1/2}\ (\vec{e}_{\theta\varphi} \cdot \vec{e})\ V \tag{4.82b}$$

$$c(\vec{r},\theta,\varphi,t) \sim \beta_e^{1/2} \tag{4.82c}$$

and the definitions (4.63a) and (4.63b) give, as equilibrium is approached:

$$A(\vec{r},\theta,\varphi,t) \sim 2\Pi^{3/2}\ e^{\beta_e V^2}\ (\rho_{\theta\varphi}/\rho) \tag{4.82d}$$

$$\overline{c}(\vec{r},\theta,\varphi,t) \sim \beta_e^{1/2}\ u_\alpha \tag{4.82e}$$

With equations (4.82), equations (4.63c) and (4.64a,b) now give <u>as equilibrium is approached</u>:

$$\rho_{\theta\varphi}(\vec{r},\theta,\varphi,t)/\rho_\alpha \sim (\rho/\rho_\alpha)(1/2\Pi^{3/2})\ e^{-\beta_e V^2}\{\beta_e^{1/2}\ \vec{e}_{\theta\varphi} \cdot \vec{e}\ V + [1 + 2\beta_e(\vec{e}_{\theta\varphi}\cdot\vec{e})^2V^2]\ B(\beta_e^{1/2}\ \vec{e}_{\theta\varphi}\cdot\vec{e}\ V)\} \tag{4.83a}$$

and

$$\rho_{\theta\varphi} v_{\theta\varphi}^{(1)}(\vec{r},\theta,\varphi,t)/\rho_\alpha u_\alpha \sim (\rho/\rho_\alpha)(1/2\Pi^{3/2}\ \beta_e^{1/2}\ u_\alpha)\ e^{-\beta_e V^2}\ \{1$$

$$+ \beta_e(\vec{e}_{\theta\varphi}\cdot\vec{e})^2V^2 + \beta_e^{1/2}\ \vec{e}_{\theta\varphi}\cdot\vec{e}\ V[3+2\ \beta_e(\vec{e}_{\theta\varphi}\cdot\vec{e})^2V^2]\ B(\beta_e^{1/2}\ \vec{e}_{\theta\varphi}\cdot\vec{e}V)\} \qquad (4.83b)$$

where the function B(b) is defined by (4.63c). Equations (4.66a) and (4.66b) then give also:

$$\frac{\rho_{\theta\varphi} v_{\theta\varphi}^{(2)}(\vec{r},\theta,\varphi,t)}{\rho_\alpha u_\alpha^2} \sim \frac{3\ (\rho_{\theta\varphi}/\rho_\alpha)}{2\ \beta_e u_\alpha^2} + \frac{\vec{e}_{\theta\varphi}\cdot\vec{e}V}{u_\alpha}\left(\frac{\rho_{\theta\varphi} v_{\theta\varphi}^{(1)}}{\rho_\alpha u_\alpha}\right) \qquad (4.83c)$$

$$\frac{\rho_{\theta\varphi} v_{\theta\varphi}^{(3)}(\vec{r},\theta,\varphi,t)}{\rho_\alpha u_\alpha^3} \sim \frac{2}{\beta_e u_\alpha^2}\left(\frac{\rho_{\theta\varphi} v_{\theta\varphi}^{(1)}}{\rho_\alpha u_\alpha}\right) + \frac{\vec{e}_{\theta\varphi}\cdot\vec{e}V}{u_\alpha}\left(\frac{\rho_{\theta\varphi} v_{\theta\varphi}^{(2)}}{\rho_\alpha u_\alpha^2}\right) \qquad (4.83d)$$

4.3.3 Estimated or assumed forms of collision frequencies

In § 4.1.3 it was assumed that $\Theta_{\vec{\xi}}$ is independent of velocity magnitude ξ, so that $\Theta_{\vec{\xi}} = \Theta_{\theta\varphi}$. To calculate both $\Theta_{\theta\varphi}$ for use in the directional equations of change (4.31) (or in (4.37) and (4.40) - (4.43)), and Θ for the characteristic value Θ_α in (4.32) and (4.37), one now needs expressions of assumed or estimated forms of these collision frequencies per molecule of the respective classes (cf. § 3.9).

For Maxwell molecules (with the intermolecular force assumed to vary inversely as the fifth power of distance between molecules) one finds

$$\Theta_{\vec{\xi}} = \Theta_{\theta\varphi} = \Theta_{\varphi} = \Theta = k'\ \rho(\vec{r},t) \qquad (4.84)$$

If one takes k' to be a constant, then (cf. eq. (4.37))

$$H \equiv \frac{\Theta_{\theta\varphi}}{\Theta_\alpha} = \frac{\rho(\vec{r},t)}{\rho_\alpha} \qquad (4.85a)$$

This relation could be assumed as qualitatively appropriate for use in the directional-mean-free-path method. It may be more realistic, however, to use a relation equivalent to what has been used in the BGK model (see Liepmann, Narasimha, and Chahine, 1962, pp. 1319 and 1321, where their A is proportional to our k' ; see also discussion by Vincenti and Kruger, 1965, p. 384):

$$H \equiv \frac{\Theta_{\theta\varphi}}{\Theta_\alpha} \approx \frac{\Theta_e}{\Theta_\alpha} \approx \left[\frac{T/\eta}{(T/\eta)_\alpha}\right] \frac{\rho}{\rho_\alpha} \qquad (4.85b)$$

where η is a coefficient of viscosity to be evaluated from some appropriate temperature-dependent viscosity law. For Maxwell molecules, the bracketed factor in (4.85b) is unity, to give (4.85a). For rigid spheres, the factor is $(T/T_\alpha)^{1/2}$, which is obtainable also by use of equation (2.20b) with (2.23d). Liepmann, Narasimha, and Chahine (1962) used the Sutherland viscosity law for η. In (1966) they used $\eta \propto T^{0.816}$. The latter is appropriate for argon gas up to $4000°K$ (see Camac, 1965, p. 248).

Any other appropriate calculation of $\Theta_{\theta\varphi}$ from equation (3.33b), where $\Theta_{\vec{\xi}}$ is given by (2.12c), could also be used.

4.4 A Determined System of Equations in a Simplified Form of the Directional-Mean-Free-Path Method for One-Dimensional Flow

Flow in one dimension is simplified by the fact that the velocity-distribution function depends on only one configuration-space variable, x_1, and time t, as well as on ξ and φ but is independent of θ. The resulting directional-level and full-macroscopic-level equations can then be written simply in scalar form. (There is only one non-zero velocity component and one non-zero component of heat flux on the macroscopic level; and only one component of the viscous-stress tensor is of particular interest.) In that case it is convenient to reformulate part of the method described above in somewhat simpler terms, as described in the following.

4.4.1 Dimensionless variables for one-dimensional flow

Let

$$\omega \equiv \cos \varphi \tag{4.86}$$

Then, in one-dimensional flow, where the distribution function f is independent of θ (and where the velocity vector is $\vec{V} = \vec{e}_1 u$), we have

$$\vec{e}_{\theta\varphi} \cdot \vec{e}_c = \vec{e}_{\theta\varphi} \cdot \vec{e}_1 = \cos \varphi = \omega \tag{4.87}$$

If the one-dimensional flow is allowed to be time-dependent, the components of $\vec{\zeta}$ that are of concern are

$$\zeta_1 = x_1/L \qquad \text{and} \qquad \zeta_4 = u_\alpha t/L$$

(see § 4.2.1). We now define the new dimensionless dependent variables (with η now as a dummy integration variable for ω):

$$\overline{\rho}(\vec{\zeta},\omega,\varepsilon) \equiv 2\Pi \int_{-1}^{\omega} \left(\frac{\rho_\varphi}{\rho_\alpha} \right) d\eta \tag{4.88a}$$

$$\overline{J}(\vec{\zeta},\omega,\varepsilon) \equiv 2\Pi \int_{-1}^{\omega} \left(\frac{\rho_\varphi v_\varphi^{(1)}}{\rho_\alpha u_\alpha} \right) \eta \, d\eta \tag{4.88b}$$

$$\overline{P}(\vec{\zeta},\omega,\varepsilon) \equiv 2\Pi \int_{-1}^{\omega} \left(\frac{\rho_\varphi v_\varphi^{(2)}}{\rho_\alpha u_\alpha^2} \right) \eta^2 \, d\eta \tag{4.88c}$$

$$\overline{E}(\vec{\zeta},\omega,\varepsilon) \equiv 2\Pi \int_{-1}^{\omega} \frac{1}{2} \left(\frac{\rho_\varphi v_\varphi^{(2)}}{\rho_\alpha u_\alpha^2} \right) d\eta \tag{4.88d}$$

$$\overline{Q}(\vec{\zeta},\omega,\varepsilon) \equiv 2\Pi \int_{-1}^{\omega} \frac{1}{2} \left(\frac{\rho_\varphi v_\varphi^{(3)}}{\rho_\alpha u_\alpha^3} \right) \eta \, d\eta \tag{4.88e}$$

which are related to the functionsdefined in equations (4.36), evaluated at $\theta = \Pi$, by:

$$F^{(0)}(\vec{\zeta},\Pi,\varphi,\varepsilon) = \overline{\rho}(\vec{\zeta},\omega,\varepsilon) \tag{4.89a}$$

$$\vec{F}^{(1)}(\vec{\zeta},\Pi,\varphi,\varepsilon) = \vec{e}_1\,\overline{J}(\vec{\zeta},\omega,\varepsilon) \tag{4.89b}$$

$$\mathbf{F}^{(2)}(\vec{\zeta},\Pi,\varphi,\varepsilon) = \vec{e}_1\vec{e}_1\,\overline{P}(\vec{\zeta},\omega,\varepsilon) + (\vec{e}_2\vec{e}_2 + \vec{e}_3\vec{e}_3)\,[\overline{E}(\vec{\zeta},\omega,\varepsilon) - \tfrac{1}{2}\,\overline{P}(\vec{\zeta},\omega,\varepsilon)] \tag{4.89c}$$

$$G^{(0)}(\vec{\zeta},\Pi,\varphi,\varepsilon) = \overline{E}(\vec{\zeta},\omega,\varepsilon) \tag{4.89d}$$

$$\vec{G}^{(1)}(\vec{\zeta},\Pi,\varphi,\varepsilon) = \vec{e}_1\,\overline{Q}(\vec{\zeta},\omega,\varepsilon) \tag{4.89e}$$

We then have:

$$\rho_\varphi/\rho_\alpha = (1/2\Pi)\,\partial\overline{\rho}/\partial\omega \tag{4.90a}$$

$$\rho_\varphi v_\varphi^{(1)}/\rho_\alpha u_\alpha = (1/2\Pi\,\omega)\,\partial\overline{J}/\partial\omega \tag{4.90b}$$

$$\rho_\varphi v_\varphi^{(2)}/\rho_\alpha u_\alpha^2 = (1/2\Pi\,\omega^2)\,\partial\overline{P}/\partial\omega \tag{4.90c}$$

$$= (1/2\Pi)(2\,\partial\overline{E}/\partial\omega) \tag{4.90d}$$

$$\rho_\varphi v_\varphi^{(3)}/\rho_\alpha u_\alpha^3 = (1/2\Pi\,\omega)(2\,\partial\overline{Q}/\partial\omega) \tag{4.90e}$$

We note from equations (4.88) that

<u>for $\omega = -1$, all $\vec{\zeta}$</u>:

$$\overline{\rho} = \overline{J} = \overline{P} = \overline{E} = \overline{Q} = 0 \tag{4.91}$$

and from equations (4.89), (4.45), and (4.59),

for $\omega = +1$, all $\vec{\zeta}$:

$$\overline{\rho} = \overline{\rho}(\vec{\zeta},1,\varepsilon) = \rho(x,t)/\rho_\alpha \tag{4.92a}$$

$$\overline{J} = \overline{J}(\vec{\zeta},1,\varepsilon) = (1/\rho_\alpha u_\alpha)\ \rho u(x,t) \tag{4.92b}$$

$$\overline{P} = \overline{P}(\vec{\zeta},1,\varepsilon) = (1/\rho_\alpha u_\alpha^2)[\rho u^2 + p(x,t) - \tau_{11}(x,t)]$$

$$= (1/\rho_\alpha u_\alpha^2)[\rho u^2 - \sigma_{11}(x,t)] \tag{4.92c}$$

$$\overline{E} = \overline{E}(\vec{\zeta},1,\varepsilon) = (1/\rho_\alpha u_\alpha^2)[\rho e(x,t) + \tfrac{1}{2}\rho u^2] \tag{4.92d}$$

$$\overline{Q} = \overline{Q}(\vec{\zeta},1,\varepsilon) = (1/\rho_\alpha u_\alpha^3)[\rho u(e + \tfrac{1}{2}u^2) + q(x,t) - u(\tau_{11}-p)] \tag{4.92e}$$

From equations (4.92) one finds (cf. eqs. (4.60)):

$$\frac{\rho(x,t)}{\rho_\alpha} = \overline{\rho}(\vec{\zeta},1,\varepsilon) \tag{4.93a}$$

$$\frac{u(x,t)}{u_\alpha} = \left(\frac{\rho_\alpha}{\rho}\right)\ \overline{J}(\vec{\zeta},1,\varepsilon) \tag{4.93b}$$

$$\frac{p(x,t)}{\rho_\alpha u_\alpha^2} = \frac{2}{3}\left(\frac{\rho}{\rho_\alpha}\right)\left(\frac{e}{u_\alpha^2}\right) = \frac{2}{3}\left[\overline{E}(\vec{\zeta},1,\varepsilon) - \frac{1}{2}\left(\frac{\rho}{\rho_\alpha}\right)\left(\frac{u}{u_\alpha}\right)^2\right] \tag{4.93c}$$

$$\frac{RT(x,t)}{u_\alpha^2} = \frac{2}{3}\ \frac{e(x,t)}{u_\alpha^2} = \frac{2}{3}\left(\frac{\rho_\alpha}{\rho}\right)\left[\overline{E}(\vec{\zeta},1,\varepsilon) - \frac{1}{2}\left(\frac{\rho}{\rho_\alpha}\right)\left(\frac{u}{u_\alpha}\right)^2\right] \tag{4.93d}$$

$$\frac{\sigma_{11}(x,t)}{\rho_\alpha u_\alpha^2} = \left(\frac{\rho}{\rho_\alpha}\right)\left(\frac{u}{u_\alpha}\right)^2 - \overline{P}(\vec{\zeta},1,\varepsilon) \tag{4.93e}$$

$$\frac{\tau_{11}(x,t)}{\rho_\alpha u_\alpha^2} = \frac{2}{3}\left(\frac{\rho}{\rho_\alpha}\right)\left(\frac{u}{u_\alpha}\right)^2 + \frac{2}{3}\overline{E}(\vec{\zeta},1,\varepsilon) - \overline{P}(\vec{\zeta},1,\varepsilon) \tag{4.93f}$$

$$\frac{q(x,t)}{\rho_\alpha u_\alpha^3} = \overline{Q}(\vec{\zeta},1,\varepsilon) - \left(\frac{u}{u_\alpha}\right)\ [\overline{E}(\vec{\zeta},1,\varepsilon) + \overline{P}(\vec{\zeta},1,\varepsilon)] + \left(\frac{\rho}{\rho_\alpha}\right)\left(\frac{u}{u_\alpha}\right)^3 \tag{4.93g}$$

$$\frac{h(x,t)}{u_\alpha^2} = \frac{5}{2}\frac{RT}{u_\alpha^2} \tag{4.93h}$$

$$\frac{5}{3}M^2 = \frac{u^2}{RT} = \left(\frac{u}{u_\alpha}\right)^2 \Big/ \left(\frac{RT}{u_\alpha^2}\right) \tag{4.93i}$$

which can be used to evaluate the conventional macroscopic variables after $\overline{\rho}$, $\overline{J}$, $\overline{P}$, $\overline{E}$, and $\overline{Q}$ are determined.

For use in the directional equations of change for one-dimensional flow, in which for any function $F(\vec{\zeta},\omega,\varepsilon)$, we denote (cf. eq. (4.39))

$$\tilde{F} \equiv F(\vec{z},\omega,\varepsilon) \tag{4.94}$$

where

$$\vec{z} = \vec{\zeta} + \varepsilon\,\tilde{\vec{\mu}} \tag{4.95}$$

we have now (cf. eqs. (4.40)):

$$\vec{\mu}(\vec{\zeta},\omega,\varepsilon) = \vec{e}_1\left(\frac{-\partial\overline{J}/\partial\omega}{H\,\partial\overline{\rho}/\partial\omega}\right) + \vec{e}_2\mu_2 + \vec{e}_3\mu_3 + \vec{e}_4\left(-\frac{1}{H}\right) \tag{4.96}$$

(The components μ_2 and μ_3 are not significant, since there are no variations in the x_2 and x_3 directions.)

4.4.2 Equations of change for one-dimensional flow

The directional equations of change (4.31a,b,c), for one-dimensional flow in terms of the functions in equations (4.90) (with use of eqs. (4.38)), become (cf. eqs. (4.43))

$$\varepsilon\left(\frac{\partial^2 \overline{\rho}}{\partial \zeta_4 \partial \omega} + \frac{\partial^2 \overline{J}}{\partial \zeta_1 \partial \omega}\right) = {}^{(0)}\overline{\widetilde{ZH}}' \left(\frac{\partial \widetilde{\overline{\rho}}}{\partial \omega}\right)' - H \frac{\partial \overline{\rho}}{\partial \omega} \tag{4.97a}$$

$$\varepsilon\left(\frac{\partial^2 \overline{J}}{\partial \zeta_4 \partial \omega} + \frac{\partial^2 \overline{P}}{\partial \zeta_1 \partial \omega}\right) = {}^{(1)}\overline{\widetilde{ZH}}' \left(\frac{\partial \widetilde{\overline{J}}}{\partial \omega}\right)' - H \frac{\partial \overline{J}}{\partial \omega} \tag{4.97b}$$

$$\varepsilon\left(\frac{\partial^2 \overline{E}}{\partial \zeta_4 \partial \omega} + \frac{\partial^2 \overline{Q}}{\partial \zeta_1 \partial \omega}\right) = {}^{(2)}\overline{\widetilde{ZH}}' \left(\frac{\partial \widetilde{\overline{E}}}{\partial \omega}\right)' - H \frac{\partial \overline{E}}{\partial \omega} \tag{4.97c}$$

where

$$\frac{\partial \overline{E}}{\partial \omega} = \frac{1}{2\omega^2} \frac{\partial \overline{P}}{\partial \omega} \tag{4.97d}$$

where $(\ )'$ indicates a function evaluated at $\omega' = \cos \varphi'$ according to the directional-average collision models discussed in § 4.1.2; where $\widetilde{(\ )}$ is defined by equations (4.94) - (4.96); and where $\overline{Z} = \overline{Z}(\vec{\zeta},\omega,\varepsilon) \equiv Z(\vec{r},\theta,\varphi,t)$ for one-dimensional flow.

The macroscopic conservation equations (4.30) become, in terms of the functions in equations (4.88) evaluated at $\omega = 1$ (cf. eqs. (4.46) and (4.89)):

$$\frac{\partial}{\partial \zeta_4} \overline{\rho}(\vec{\zeta},1,\varepsilon) + \frac{\partial}{\partial \zeta_1} \overline{J}(\vec{\zeta},1,\varepsilon) = 0 \tag{4.98a}$$

$$\frac{\partial}{\partial \zeta_4} \overline{J}(\vec{\zeta},1,\varepsilon) + \frac{\partial}{\partial \zeta_1} \overline{P}(\vec{\zeta},1,\varepsilon) = 0 \tag{4.98b}$$

$$\frac{\partial}{\partial \zeta_4} \overline{E}(\vec{\zeta},1,\varepsilon) + \frac{\partial}{\partial \zeta_1} \overline{Q}(\vec{\zeta},1,\varepsilon) = 0 \tag{4.98c}$$

4.4.3 Directional-Gaussian closure equation

The equation used to close the system, derived in § 4.3 by relating various integrals of a local directional-Gaussian distribution function, is given by equations (4.69) and expressed implicitly by equations (4.70).

The quantities $\psi^{(2)}$, $\psi^{(3)}$, and ψ defined by equations (4.68) and (4.70b) are written in terms of the one-dimensional-flow variables as

$$\psi^{(2)} \equiv v_{\varphi}^{(2)}/(v_{\varphi}^{(1)})^2 = \frac{(\partial\overline{P}/\partial\omega)(\partial\overline{\rho}/\partial\omega)}{(\partial\overline{J}/\partial\omega)^2} \tag{4.99a}$$

$$\psi^{(3)} \equiv v_{\varphi}^{(3)}/(v_{\varphi}^{(1)})^3 = \frac{2\omega^2(\partial\overline{Q}/\partial\omega)(\partial\overline{\rho}/\partial\omega)^2}{(\partial\overline{J}/\partial\omega)^3} \tag{4.99b}$$

$$\psi \equiv (\psi^{(2)})^2/\psi^{(3)} = \frac{(\partial\overline{P}/\partial\omega)^2}{2\omega^2(\partial\overline{Q}/\partial\omega)(\partial\overline{J}/\partial\omega)} \tag{4.99c}$$

Note in particular that ψ does not contain $\partial\overline{\rho}/\partial\omega$, so that if the quantities on the right side of (4.99c) are known, one can: calculate ψ from (4.99c); obtain $\psi^{(2)}$ from (4.70a); then obtain $\partial\overline{\rho}/\partial\omega$ from (4.99a). This procedure will be used later.

4.4.4 Local-equilibrium property distributions

In regions of local translational equilibrium, where the molecular-velocity distribution function, f, is Maxwellian, the directional property distributions (eqs. (4.83)) for one-dimensional flow are simplified. The quantity $\beta_e^{1/2}V$ for a monatomic gas is $\sqrt{5/6}\,M$, and $\vec{e}_{\theta\varphi}\cdot\vec{e} = \cos\varphi = \omega$. Then (cf. eqs. (4.62) and (4.82)),

$$b = b_e = \overline{M}\omega \equiv \overline{\omega} \tag{4.100a}$$

where

$$\overline{M} \equiv \sqrt{5/6}\,M \tag{4.100b}$$

and equations (4.64), or (4.83), (with the definitions (4.63c) and (4.47)) become

$$\frac{\partial \overline{\rho}_e}{\partial \overline{\omega}} = \left[\left(\frac{\rho}{\rho_\alpha}\right) \frac{e^{-\overline{M}^2}}{\Pi^{1/2}\overline{M}}\right] \overline{N}(\overline{\omega}) \tag{4.101a}$$

$$\frac{\partial \overline{J}_e}{\partial \overline{\omega}} = \left[\frac{e^{-\overline{M}^2}}{\Pi^{1/2}\overline{M}^3}\right] \frac{\overline{\omega}}{2} \overline{N}'(\overline{\omega}) \tag{4.101b}$$

$$\frac{\partial \overline{P}_e}{\partial \overline{\omega}} = \left[\left(\frac{\rho_\alpha}{\rho}\right) \frac{e^{-\overline{M}^2}}{\Pi^{1/2}\overline{M}^5}\right] \frac{\overline{\omega}^2}{4} \overline{N}''(\overline{\omega}) \tag{4.101c}$$

$$\frac{\partial \overline{E}_e}{\partial \overline{\omega}} = \frac{\overline{M}^2}{2\overline{\omega}^2} \frac{\partial \overline{P}_e}{\partial \overline{\omega}} = \left[\left(\frac{\rho_\alpha}{\rho}\right) \frac{e^{-\overline{M}^2}}{\Pi^{1/2}\overline{M}^3}\right] \frac{1}{8} \overline{N}''(\overline{\omega}) \tag{4.101d}$$

$$\frac{\partial \overline{Q}_e}{\partial \overline{\omega}} = \left[\left(\frac{\rho_\alpha}{\rho}\right)^2 \frac{e^{-\overline{M}^2}}{\Pi^{1/2}\overline{M}^5}\right] \frac{\overline{\omega}}{16} \overline{N}'''(\overline{\omega}) \tag{4.101e}$$

where subscript e denotes a local equilibrium value. Equations (4.101) can be integrated with respect to $\overline{\omega}$ (with use of eqs. (4.75) where needed) to obtain, in regions of translational equilibrium in one-dimensional flow:

$$\overline{\rho}_e(\vec{\zeta},\omega,\varepsilon) = \left[\left(\frac{\rho}{\rho_\alpha}\right) \frac{e^{-\overline{M}^2}}{\Pi^{1/2}\overline{M}}\right] [\overline{\omega}\, B(\overline{\omega}) + \overline{M}\, B(-\overline{M})] \tag{4.102a}$$

$$\overline{J}_e(\vec{\zeta},\omega,\varepsilon) = \frac{1}{2}\left[\frac{e^{-\overline{M}^2}}{\Pi^{1/2}\overline{M}^3}\right] [\overline{\omega}\, \overline{N}(\overline{\omega}) + \overline{M}\, \overline{N}(-\overline{M}) - \overline{\omega}\, B(\overline{\omega}) - \overline{M}\, B(-\overline{M})] \tag{4.102b}$$

$$\overline{P}_e(\vec{\zeta},\omega,\varepsilon) = \frac{1}{2}\left[\left(\frac{\rho_\alpha}{\rho}\right) \frac{e^{-\overline{M}^2}}{\Pi^{1/2}\overline{M}^5}\right] [\overline{\omega}^3\, \overline{N}(\overline{\omega}) + \overline{M}^3\, \overline{N}(-\overline{M})] \tag{4.102c}$$

$$\overline{E}_e(\vec{\zeta},\omega,\varepsilon) = \frac{1}{8}\left[\left(\frac{\rho_\alpha}{\rho}\right) \frac{e^{-\overline{M}^2}}{\Pi^{1/2}\overline{M}^3}\right] [\overline{N}'(\overline{\omega}) - \overline{N}'(-\overline{M})] \tag{4.102d}$$

$$\overline{Q}_e(\vec{\zeta},\omega,\varepsilon) = \frac{1}{32}\left[\left(\frac{\rho_\alpha}{\rho}\right)^2 \frac{e^{-\overline{M}^2}}{\Pi^{1/2}\overline{M}^5}\right] [\overline{N}'''(\overline{\omega}) - \overline{N}'''(-\overline{M}) - 10\, \overline{N}'(\overline{\omega}) + 10\, \overline{N}'(-\overline{M})] \tag{4.102e}$$

Equations (4.102) have been made to satisfy the following conditions (which are consistent with conditions (4.91) and (4.92) and the definitions in (4.93)):

at $\omega = -1$, all $\vec{\zeta}$:

$$\overline{\rho}_e = \overline{J}_e = \overline{P}_e = \overline{E}_e = \overline{Q}_e = 0 \tag{4.103}$$

and

at $\omega = +1$, all $\vec{\zeta}$:

$$\overline{\rho}_e(\vec{\zeta},1,\varepsilon) = \overline{\rho}(\vec{\zeta},1,\varepsilon) = \rho/\rho_\alpha \tag{4.104a}$$

$$\overline{J}_e(\vec{\zeta},1,\varepsilon) = \overline{J}(\vec{\zeta},1,\varepsilon) = \rho u/\rho_\alpha u_\alpha \tag{4.104b}$$

$$\overline{P}_e(\vec{\zeta},1,\varepsilon) = \frac{p+\rho u^2}{\rho_\alpha u_\alpha^2} = \frac{\rho u^2}{\rho_\alpha u_\alpha^2}\left(1 + \frac{1/2}{\overline{M}^2}\right) \tag{4.104c}$$

$$2\overline{E}_e(\vec{\zeta},1,\varepsilon) = 2\overline{E}(\vec{\zeta},1,\varepsilon) = \frac{\rho u^2}{\rho_\alpha u_\alpha^2}\left(1 + \frac{3/2}{\overline{M}^2}\right) \tag{4.104d}$$

$$2\overline{Q}_e(\vec{\zeta},1,\varepsilon) = \frac{2\,\rho u(h + \frac{1}{2}u^2)}{\rho_\alpha u_\alpha^3} = \frac{\rho u^3}{\rho_\alpha u_\alpha^3}\left(1 + \frac{5/2}{\overline{M}^2}\right) \tag{4.104e}$$

Therefore the quantities ρ/ρ_α and $\overline{M}$ in the local equilibrium expressions (eqs. (4.100) to (4.102)) are, from (4.104a), (4.104b), and (4.104d):

$$\rho/\rho_\alpha = \overline{\rho}(\vec{\zeta},1,\varepsilon) \tag{4.105a}$$

$$\overline{M} \equiv \sqrt{5/6}\ M = \left\{ \frac{3/2}{\left[\frac{2\overline{E}(\vec{\zeta},1,\varepsilon)}{\overline{\rho}(\vec{\zeta},1,\varepsilon)}\right]\left[\frac{\overline{\rho}(\vec{\zeta},1,\varepsilon)}{\overline{J}(\vec{\zeta},1,\varepsilon)}\right]^2 - 1} \right\}^{1/2} \tag{4.105b}$$

which may be evaluated in a nonequilibrium solution of the equations. These expressions are useful later.

4.4.5 Reduction of directional-average collision models for one-dimensional flow

The quantities in equations (4.97) that are denoted by $(\ )'$ are functions of ω evaluated at ω', where, for one-dimensional flow, with $\vec{V}/V \equiv \vec{e} = \vec{e}_1$,

$$\omega \equiv \cos \varphi = \vec{e} \cdot \vec{e}_{\theta\varphi}$$
$$\omega' \equiv \cos \varphi' = \vec{e} \cdot \vec{e}_{\theta'\varphi'} \tag{4.106a}$$

and where, in general,

$$\omega' = \omega'(\vec{\zeta}, \omega, \varepsilon) \tag{4.106b}$$

However, for collision model I, $\omega' = 1$ and ${}^{(\ell)}\overline{Z} = 1$, so equations (4.97) are simply written without the $\overline{Z}$ factors and without the "primes" on the gain terms.

For collision model II, with equations (4.12), equations (4.97) become:

$$\varepsilon \left(\frac{\partial^2 \overline{\rho}}{\partial \zeta_4 \, \partial \omega} + \frac{\partial^2 \overline{J}}{\partial \zeta_1 \, \partial \omega} \right) = \tilde{H}_e \left(\frac{\partial \tilde{\overline{\rho}}_e}{\partial \omega} \right) - H \left(\frac{\partial \overline{\rho}}{\partial \omega} \right) \tag{4.107a}$$

$$\varepsilon \left(\frac{\partial^2 \overline{J}}{\partial \zeta_4 \, \partial \omega} + \frac{\partial^2 \overline{P}}{\partial \zeta_1 \, \partial \omega} \right) = \tilde{H}_e \left(\frac{\partial \tilde{\overline{J}}_e}{\partial \omega} \right) - H \left(\frac{\partial \overline{J}}{\partial \omega} \right) \tag{4.107b}$$

$$\varepsilon \left(\frac{\partial^2 \overline{E}}{\partial \zeta_4 \, \partial \omega} + \frac{\partial^2 \overline{Q}}{\partial \zeta_1 \, \partial \omega} \right) = \tilde{H}_e \left(\frac{\partial \tilde{\overline{E}}_e}{\partial \omega} \right) - H \left(\frac{\partial \overline{E}}{\partial \omega} \right) \tag{4.107c}$$

$$\frac{\partial \overline{E}}{\partial \omega} = \frac{1}{2\omega^2} \frac{\partial \overline{P}}{\partial \omega} \tag{4.107d}$$

where $\partial \overline{\rho}_e / \partial \omega$, $\partial \overline{J}_e / \partial \omega$, and $\partial \overline{E}_e / \partial \omega$ are given by equations (4.100) and (4.101), with ρ / ρ_α and $\overline{M}$ given by (4.105).

For collision model IIIa (from eqs. (4.18b), (4.22), (4.23), (4.24), and definitions in (4.90) and (4.92)):

$$\omega' = \omega'(\vec{\zeta},\omega,\varepsilon) = \frac{\omega\tilde{v}_{\varphi} - (\tilde{u}-u)}{[(\tilde{u}-u)^2 + \tilde{v}_{\varphi}^2 - 2\omega\,\tilde{v}_{\varphi}(\tilde{u}-u)]^{1/2}}$$

$$= \frac{\omega}{|\omega|}\,[1-A(\vec{\zeta},\omega,\varepsilon)]\left\{[1-A(\vec{\zeta},\omega,\varepsilon)]^2 + \frac{1-\omega^2}{\omega^2}\right\}^{-\frac{1}{2}} \qquad (4.108)$$

and

$$^{(\ell)}Z_{IIIa}(\vec{\zeta},\omega,\varepsilon) = \left[\left(\frac{\tilde{u}-u}{\tilde{v}_{\varphi}}\right)^2 + 1 - 2\omega\left(\frac{\tilde{u}-u}{\tilde{v}_{\varphi}}\right)\right]^{-\frac{1}{2}} \left|1 - \omega\left(\frac{\tilde{u}-u}{\tilde{v}_{\varphi}}\right)\right|^{-1}$$

$$= |\omega|^{-3}\left\{[1-A(\vec{\zeta},\omega,\varepsilon)]^2 + \frac{1-\omega^2}{\omega^2}\right\}^{-\frac{1}{2}} \left|1-A(\vec{\zeta},\omega,\varepsilon) + \frac{1-\omega^2}{\omega^2}\right|^{-1} \qquad (4.109)$$

where

$$A(\vec{\zeta},\omega,\varepsilon) \equiv \frac{\tilde{u}-u}{\omega\tilde{v}_{\varphi}} = \frac{\left[\frac{\partial\overline{\rho}(\vec{z},\omega,\varepsilon)}{\partial\omega}\right]}{\left[\frac{\partial\overline{J}(\vec{z},\omega,\varepsilon)}{\partial\omega}\right]}\left[\frac{\overline{J}(\vec{z},1,\varepsilon)}{\overline{\rho}(\vec{z},1,\varepsilon)} - \frac{\overline{J}(\vec{\zeta},1,\varepsilon)}{\overline{\rho}(\vec{\zeta},1,\varepsilon)}\right] \qquad (4.110)$$

The use of the equations given in this section (§ 4.4) is illustrated below in Chapter VII in steady-flow shock-wave structure. The equations can first be appreciably simplified by a suitable approximation scheme, developed in Chapter V, with its application in the present method indicated in Chapter VI.

CHAPTER V

VECTOR GENERALIZATIONS OF LAGRANGE'S EXPANSION, AND A PERTURBATION-EXPANSION SCHEME

5.1 Introductory Remarks

Lagrange's expansion is a generalization (first derived by Lagrange in 1770) of Taylor's expansion in which the independent variable is defined by an implicit equation. Recently Sack (1965a) has reviewed a number of approaches to, and applications of, Lagrange's expansion and has discussed generalizations of certain forms of the expansion to several variables (see also Sack, 1965b, 1966; Sturrock, 1960; and Good, 1960).

In addition to the forms that have been given, an especially simple, direct, and useful generalization to N variables of the standard form of Lagrange's expansion can also be found, and is derived here. It can be written completely in vector form, which is useful in application to vector formulations of physical problems, especially where transformations to different coordinate systems are to be considered.

Two simple derivations of Lagrange's expansion with one independent variable are first outlined (§ 5.2), and the development of a perturbation-expansion scheme shown (§ 5.3). It is then shown (§ 5.4.1) how each step in the first derivation of the standard form of Lagrange's expansion in § 5.2.1 can be simply generalized to two independent variables; and the analogous steps in the generalization to arbitrary N dimensions then become clear, as shown in § 5.4.2. An alternate derivation which is a generalization, to N independent variables, of the alternate derivation outlined in § 5.2.2, is then given in § 5.4.3. It is advantageous to consider both these derivations because: (a) the first derivation results in the more concise final form for one independent variable (although the expanded forms are termwise identical), (b) the alternate derivation results in the more concise final form in arbitrary N dimensions (although the expanded forms are termwise identical, and (c) the two derivations are

independent and are believed to be both new. The development of the perturbation-expansion scheme for arbitrary - N independent variables follows in § 5.5 by analogy with the one-dimensional development in § 5.3.

5.2 Lagrange's Expansion in One Variable

If an independent variable z is defined implicitly by the equation

$$z = z(\zeta,\varepsilon) \equiv \zeta + \varepsilon\mu(z) \tag{5.1a}$$

where $\varepsilon\mu(z)$ is sufficiently small, the standard form of Lagrange's expansion (cf.Whittaker and Watson, 1927, or Sack, 1965a) for any function $f(z)$ is

$$f(z) = f(\zeta) + \sum_{n=1}^{\infty} \frac{\varepsilon^n}{n!} \frac{d^{n-1}}{d\zeta^{n-1}} \left[\mu^n(\zeta) \frac{df(\zeta)}{d\zeta} \right] \tag{5.1b}$$

5.2.1 First derivation

A simple derivation of equation (5.1b) is given here (for convenience of comparing the steps in the later generalizations).

Differentiation of (5.1a) gives

$$dz = d\zeta + \varepsilon\mu'(z)\, dz + \mu(z)\, d\varepsilon$$

from which

$$dz = \frac{1}{1 - \varepsilon\mu'(z)}\, d\zeta + \frac{\mu(z)}{1 - \varepsilon\mu'(z)}\, d\varepsilon \tag{5.2a}$$

Also

$$dz = z_\zeta\, d\zeta + z_\varepsilon\, d\varepsilon \tag{5.2b}$$

(where $z_\zeta \equiv \partial z/\partial\zeta$ and $z_\varepsilon \equiv \partial z/\partial\varepsilon$) so that, by comparison of (5.2a) with (5.2b); or, equivalently, by combining (5.2a) with (5.2b) to obtain

$$\{[1 - \varepsilon\mu'(z)]z_\zeta - 1\}d\zeta + \{[1 - \varepsilon\mu'(z)]z_\varepsilon - \mu(z)\}d\varepsilon = 0 \qquad (5.2c)$$

and by equating the coefficients of $d\zeta$ and of $d\varepsilon$ in (5.2c) to zero (because the differentials $d\zeta$ and $d\varepsilon$ are <u>arbitrary</u>, so that equation (5.2c) must apply for <u>any</u> $d\zeta$ and <u>any</u> $d\varepsilon$ independently, the coefficients of $d\zeta$ and of $d\varepsilon$ must vanish); one obtains

$$z_\zeta = \frac{1}{1 - \varepsilon\mu'(z)} \; ; \qquad z_\varepsilon = \frac{\mu(z)}{1 - \varepsilon\mu'(z)} \qquad (5.3)$$

For any function of z: $F(z) = F[z(\zeta,\varepsilon)]$, one may write

$$\frac{\partial F[z(\zeta,\varepsilon)]}{\partial\varepsilon} = z_\varepsilon \frac{dF}{dz} \qquad (5.4a)$$

and

$$\frac{\partial F(z)}{\partial\zeta} = z_\zeta \frac{dF}{dz} \qquad (5.4b)$$

so that, with use of (5.3), equations (5.4) give

$$\frac{\partial F(z)}{\partial\varepsilon} = \frac{z_\varepsilon}{z_\zeta} \frac{\partial F(z)}{\partial\zeta} = \mu(z) \frac{\partial F(z)}{\partial\zeta} \qquad (5.5)$$

From (5.5),

$$\frac{\partial^2 F}{\partial\varepsilon^2} = \frac{\partial\mu(z)}{\partial\varepsilon} \frac{\partial F(z)}{\partial\zeta} + \mu(z) \frac{\partial}{\partial\zeta} \left[\frac{\partial F(z)}{\partial\varepsilon}\right]$$

$$= \left[\mu(z) \frac{\partial\mu(z)}{\partial\zeta}\right] \frac{\partial F(z)}{\partial\zeta} + \mu(z) \frac{\partial}{\partial\zeta} \left[\mu(z) \frac{\partial F(z)}{\partial\zeta}\right]$$

$$= \frac{\partial}{\partial\zeta} \left[\mu^2(z) \frac{\partial F(z)}{\partial\zeta}\right] \qquad (5.6)$$

$$\frac{\partial^3 F}{\partial \varepsilon^3} = \frac{\partial}{\partial \zeta}\left\{ \mu^2(z) \frac{\partial}{\partial \zeta}\left[\frac{\partial F(z)}{\partial \varepsilon}\right] + \frac{\partial F(z)}{\partial \zeta} \frac{\partial \mu^2(z)}{\partial \varepsilon} \right\}$$

$$= \frac{\partial}{\partial \zeta}\left\{ \mu^2(z) \frac{\partial}{\partial \zeta}\left[\mu(z) \frac{\partial F(z)}{\partial \zeta}\right] + \frac{\partial F(z)}{\partial \zeta} \mu(z) \frac{\partial \mu^2(z)}{\partial \zeta} \right\}$$

$$= \frac{\partial^2}{\partial \zeta^2}\left[\mu^3(z) \frac{\partial F(z)}{\partial \zeta}\right] \tag{5.7}$$

Further, by induction, one finds

$$\frac{\partial^n F(z)}{\partial \varepsilon^n} = \frac{\partial^{n-1}}{\partial \zeta^{n-1}}\left[\mu^n(z) \frac{\partial F(z)}{\partial \zeta} \right] \tag{5.8}$$

A direct derivation of equation (5.1b) that uses (5.5) through (5.8) is now the following: From Taylor's expansion about $\varepsilon = 0$, one writes:

$$f(z) \equiv f[z(\zeta,\varepsilon)] = f[z(\zeta,0)] + \sum_{n=1}^{\infty} \frac{\varepsilon^n}{n!}\left[\frac{\partial^n f[z(\zeta,\varepsilon)]}{\partial \varepsilon^n}\right]_{\varepsilon=0} \tag{5.9}$$

Since at $\varepsilon=0$, $z=\zeta$, use of (5.8) in (5.9) gives directly

$$f(z) = f(\zeta) + \sum_{n=1}^{\infty} \frac{\varepsilon^n}{n!} \frac{\partial^{n-1}}{\partial \zeta^{n-1}}\left[\mu^n(\zeta) \frac{\partial f(\zeta)}{\partial \zeta} \right] \tag{5.10}$$

which is equivalent to the result sought, (5.1b).

The steps in this derivation from equations (5.1a) to (5.5) and from (5.8) to (5.10) are equivalent to the corresponding steps in Laplace's derivation in 1780 (e.g., as outlined by Sack, 1965a). However, the steps from (5.5) to (5.8) do not employ one additional identity that was used by Laplace, but are carried out quite naturally without the additional identity, and in a manner that will be seen to provide a simplification in an analogous procedure in the generalization to N dimensions, considered in later sections.

5.2.2 An alternate derivation for one independent variable

An independent, alternate derivation of Lagrange's expansion in a form that is termwise identical to (5.1b) is the following: With (5.1a), one may write Taylor's expansion as

$$f(z) = f(\zeta) + \sum_{n=1}^{\infty} \frac{(z-\zeta)^n}{n!} \frac{d^n f(\zeta)}{d\zeta^n}$$

$$= f(\zeta) + \sum_{n=1}^{\infty} \frac{\varepsilon^n}{n!} [\mu(z)]^n \frac{d^n f(\zeta)}{d\zeta^n} \qquad (5.11a)$$

Therefore also

$$\mu(z) = \mu(\zeta) + \sum_{m=1}^{\infty} \frac{\varepsilon^m}{m!} [\mu(z)]^m \frac{d^m \mu(\zeta)}{d\zeta^m} \qquad (5.11b)$$

Although not as concisely expressed as equation (5.1b), equations (5.11) give the same result as equation (5.1b) to any desired order. For example, to order ε^2, (5.11a) gives

$$f(z) = f(\zeta) + \varepsilon\mu(z) \frac{df(\zeta)}{d\zeta} + \frac{\varepsilon^2}{2} [\mu(z)]^2 \frac{d^2 f(\zeta)}{d\zeta^2} + O(\varepsilon^3) \qquad (5.12a)$$

where, from (5.11b)

$$\mu(z) = \mu(\zeta) + \varepsilon\mu(z) \frac{d\mu(\zeta)}{d\zeta} + \frac{\varepsilon^2}{2} [\mu(z)]^2 \frac{d^2\mu(\zeta)}{d\zeta^2} + O(\varepsilon^3)$$

$$= \mu(\zeta) + \varepsilon[\mu(\zeta) + \varepsilon\mu(z) \frac{d\mu(\zeta)}{d\zeta} + O(\varepsilon^2)] \frac{d\mu(\zeta)}{d\zeta}$$

$$+ \frac{\varepsilon^2}{2} \{[\mu(\zeta)]^2 + O(\varepsilon)\} \frac{d^2\mu(\zeta)}{d\zeta^2} + O(\varepsilon^3)$$

$$= \mu(\zeta) + \varepsilon\mu(\zeta) \frac{d\mu(\zeta)}{d\zeta} + \varepsilon^2 \left\{ \mu(\zeta) \left[\frac{d\mu(\zeta)}{d\zeta} \right]^2 \right.$$

$$\left. + \frac{1}{2} [\mu(\zeta)]^2 \frac{d^2\mu(\zeta)}{d\zeta^2} \right\} + O(\varepsilon^3) \qquad (5.12b)$$

thus (5.12a) becomes

$$f(z) = f(\zeta) + \varepsilon\mu(\zeta)\frac{df(\zeta)}{d\zeta} + \varepsilon^2\left\{\mu(\zeta)\frac{d\mu(\zeta)}{d\zeta}\frac{df(\zeta)}{d\zeta} + \frac{1}{2}[\mu(\zeta)]^2\frac{d^2f(\zeta)}{d\zeta}\right\} + O(\varepsilon^3) \tag{5.12c}$$

which is equivalent to (5.1b) to order ε^2 .

Obviously, the form of equations (5.11) is not as convenient as the concise form (5.1b), but this derivation has been given because its generalization to N independent variables (§ 5.4.3 below) provides a more concise final form than does the generalization of the first derivation.

5.3 Lagrange's Expansion in One Variable with Additional Parameters, and Development of Perturbation-Expansion Scheme

In a development exactly analogous to that in § 5.2, it is easily shown that equations (5.1a) and (5.1b) may be generalized to include an arbitrary number of parameters; thus, if

$$z = z(\zeta,\varepsilon,\alpha,\beta,\gamma,\ldots) \equiv \zeta + \varepsilon\mu(z,\alpha,\beta,\gamma,\ldots) \tag{5.13a}$$

then

(5.13b)

$$f(z,\alpha,\beta,\gamma,\ldots) = f(\zeta,\alpha,\beta,\gamma,\ldots) + \sum_{n=1}^{\infty}\frac{\varepsilon^n}{n!}\frac{\partial^{n-1}}{\partial\zeta^{n-1}}\left[\mu^n(\zeta,\alpha,\beta,\gamma,\ldots)\frac{\partial f(\zeta,\alpha,\ldots)}{\partial\zeta}\right]$$

Equation (5.13a) has the expansion

$$z = \zeta + \sum_{n=1}^{\infty}\frac{\varepsilon^n}{n!}\frac{\partial^{n-1}}{\partial\zeta^{n-1}}[\mu^n(\zeta,\alpha,\beta,\gamma,\ldots)] \tag{5.13c}$$

Consider now the special case of equations (5.13) in which only one parameter, α, is included, and suppose $f(z,\alpha)$ and $\mu(z,\alpha)$ can be

expanded in power series in α :

$$f(z,\alpha) = \sum_{k=1}^{\infty} \alpha^{k-1} f_k(z) \tag{5.14a}$$

$$\mu(z,\alpha) = \sum_{k=1}^{\infty} \alpha^{k-1} \mu_k(z) \tag{5.14b}$$

Then equations (5.13b) and (5.13c) become

$$f(z,\alpha) = \sum_{n=1}^{\infty} \alpha^{n-1} f_n(\zeta) + \sum_{n=1}^{\infty} \frac{\varepsilon^n}{n!} \frac{\partial^{n-1}}{\partial \zeta^{n-1}} \left\{ \left[\sum_{k=1}^{\infty} \alpha^{k-1} \mu_k(\zeta) \right]^n \left[\sum_{k=1}^{\infty} \alpha^{k-1} f_k'(\zeta) \right] \right\} \tag{5.15a}$$

where

$$z = \zeta + \sum_{n=1}^{\infty} \frac{\varepsilon^n}{n!} \frac{\partial^{n-1}}{\partial \zeta^{n-1}} \left\{ \left[\sum_{k=1}^{\infty} \alpha^{k-1} \mu_k(\zeta) \right]^n \right\} \tag{5.15b}$$

These equations may be further specialized to the case where $\alpha = \varepsilon$, for which the terms of equations (5.15) to order ε^3 are:

$$\begin{aligned} f(z,\varepsilon) = {} & f_1(\zeta) + \varepsilon[f_2(\zeta)+\mu_1(\zeta)f_1'(\zeta)] + \varepsilon^2\{f_3(\zeta)+\mu_1(\zeta)f_2'(\zeta) \\ & + \mu_2(\zeta)f_1'(\zeta)+(1/2)(d/d\zeta)[\mu_1^2(\zeta)f_1'(\zeta)]\} + \varepsilon^3\{f_4(\zeta) \\ & + \mu_1(\zeta)f_3'(\zeta)+\mu_2(\zeta)f_2'(\zeta) + \mu_3(\zeta)f_1'(\zeta) \\ & + (1/2)(d/d\zeta)[\mu_1^2(\zeta)f_2'(\zeta) + 2\,\mu_1(\zeta)\mu_2(\zeta)f_1'(\zeta)] \\ & + (1/6)(d^2/d\zeta^2)[\mu_1^3(\zeta)f_1'(\zeta)]\} + O(\varepsilon^4) \end{aligned} \tag{5.16a}$$

$$\begin{aligned} z = {} & \zeta + \varepsilon\mu_1(\zeta) + \varepsilon^2[\mu_2(\zeta)+\mu_1(\zeta)\mu_1'(\zeta)] + \varepsilon^3\{\mu_3(\zeta) \\ & + \mu_1(\zeta)\mu_2'(\zeta)+\mu_2(\zeta)\mu_1'(\zeta)+(1/2)(d/d\zeta)[\mu_1^2(\zeta)\mu_1'(\zeta)]\} + O(\varepsilon^4) \end{aligned} \tag{5.16b}$$

(Equations (5.16) have been found to be useful in applying Lighthill's uniformization technique; see Martin, 1967a.)

5.4 Generalizations of Lagrange's Expansion to N Variables

The standard form of Lagrange's expansion (eq.(5.1b) with (5.1a)) can be generalized to N dimensions in vector form. The independent variable $\vec{z}$ (cf. eq. (5.1a)) is defined implicitly by

$$\vec{z} = \vec{z}(\vec{\zeta},\varepsilon) \equiv \vec{\zeta} + \varepsilon\vec{\mu}(\vec{z}) \tag{5.17}$$

where $\vec{z}$, $\vec{\zeta}$, and $\vec{\mu}$ are vectors each having N independent components, and thus are considered to be vectors in the N -dimensional space having orthogonal unit base vectors $\vec{e}_k$ (k=1,2,...,N), in the directions of the respective z_k coordinates (e.g., refer to Karamcheti, 1967). The vectors may therefore be written as

$$\vec{z} \equiv \sum_{k=1}^{N} \vec{e}_k \, z_k \, (\zeta_1,\zeta_2,\ldots,\zeta_N,\varepsilon) \tag{5.18a}$$

$$\vec{\zeta} \equiv \sum_{k=1}^{N} \vec{e}_k \, \zeta_k \tag{5.18b}$$

$$\vec{\mu} \equiv \sum_{k=1}^{N} \vec{e}_k \, \mu_k \, (z_1,z_2,\ldots,z_N) \tag{5.18c}$$

where the unit vectors satisfy the orthogonality condition (which also defines the "dot product"):

$$\left.\begin{aligned} \vec{e}_i \cdot \vec{e}_j = \delta_{ij} &= 1 \quad \text{for } i = j \\ &= 0 \quad \text{for } i \neq j \end{aligned}\right\} \tag{5.19}$$

in which i and j may have values from 1 to N.

Then, for any function $f(\vec{z}) \equiv f(z_1, z_2, \ldots, z_N)$, (which itself may be a scalar, vector, or higher order tensor), the result (to be derived below) for the extension of the standard form of Lagrange's expansion to N dimensions, in vector form, is

$$
\begin{aligned}
f(\vec{z}) \;=\; & f(\vec{\zeta}) + \varepsilon\{\vec{\mu}(\vec{\zeta}) \cdot \nabla_\zeta f(\vec{\zeta})\} \\
& + (\varepsilon^2/2!)\{\vec{\mu} \cdot \nabla_\zeta(\vec{\mu}\cdot\nabla_\zeta f) + (\vec{\mu}\cdot\nabla_\zeta\vec{\mu}) \cdot \nabla_\zeta f\} \\
& + (\varepsilon^3/3!)\{\vec{\mu} \cdot\nabla_\zeta[\vec{\mu}\cdot\nabla_\zeta(\vec{\mu}\cdot\nabla_\zeta f) + (\vec{\mu}\cdot\nabla_\zeta\vec{\mu}) \cdot \nabla_\zeta f] \\
& + 2(\vec{\mu}\cdot\nabla_\zeta\vec{\mu}) \cdot \nabla_\zeta(\vec{\mu}\cdot\nabla_\zeta f) + [\vec{\mu}\cdot\nabla_\zeta(\vec{\mu}\cdot\nabla_\zeta\vec{\mu}) \\
& + (\vec{\mu}\cdot\nabla_\zeta\vec{\mu}) \cdot \nabla_\zeta\vec{\mu}] \cdot \nabla_\zeta f\} + O(\varepsilon^4)
\end{aligned}
\tag{5.20}
$$

where $\vec{z}$ is defined implicitly by equation (5.15); where the argument of each function of the right side of (5.20) is $\vec{\zeta}$; and where

$$
\nabla_\zeta \equiv \sum_{k=1}^{N} \vec{e}_k \frac{\partial}{\partial \zeta_k} \tag{5.21}
$$

Formulas for the higher order terms will be given below.

It is to be noted that if $\vec{\mu}$ is a constant vector, then equations (5.17) and (5.20) reduce to the vector form of Taylor's expansion in N dimensions (cf. Korn and Korn, 1961). If, on the other hand, N=1, so that f and μ are functions of only one variable, z, equation (5.20) reduces directly to the standard form of Lagrange's expansion in one variable, equation (5.1b).

To derive equation (5.20) (to any order in ε), one can proceed in a manner directly analogous to that in either § 5.2.1 or § 5.2.2, as demonstrated in the following.

5.4.1 The two-dimensional case, N = 2; first derivation

The generalization for N=2 is carried out most simply, which will be outlined here. The extension to arbitrary N then follows directly. All major steps in this section are analogous to those in § 5.2.1.

From equation (5.17), for N=2,

$$\left.\begin{aligned} z_1 &= z_1(\zeta_1,\zeta_2,\varepsilon) \equiv \zeta_1 + \varepsilon\mu_1(z_1,z_2) \\ z_2 &= z_2(\zeta_1,\zeta_2,\varepsilon) \equiv \zeta_2 + \varepsilon\mu_2(z_1,z_2) \end{aligned}\right\} \quad (5.22)$$

Then

$$\begin{aligned} dz_1 &= d\zeta_1 + \varepsilon \frac{\partial\mu_1}{\partial z_1} dz_1 + \varepsilon \frac{\partial\mu_1}{\partial z_2} dz_2 + \mu_1\, d\varepsilon \\ dz_2 &= d\zeta_2 + \varepsilon \frac{\partial\mu_2}{\partial z_1} dz_1 + \varepsilon \frac{\partial\mu_2}{\partial z_2} dz_2 + \mu_2\, d\varepsilon \end{aligned}$$

from which

$$\left.\begin{aligned} \left(1 - \varepsilon \frac{\partial\mu_1}{\partial z_1}\right) dz_1 - \varepsilon \frac{\partial\mu_1}{\partial z_2} dz_2 &= d\zeta_1 + \mu_1\, d\varepsilon \\ -\varepsilon \frac{\partial\mu_2}{\partial z_1} dz_1 + \left(1 - \varepsilon \frac{\partial\mu_2}{\partial z_2}\right) dz_2 &= d\zeta_2 + \mu_2\, d\varepsilon \end{aligned}\right\} \quad (5.23)$$

Also:

$$\left.\begin{aligned} dz_1 &= \frac{\partial z_1}{\partial \zeta_1} d\zeta_1 + \frac{\partial z_1}{\partial \zeta_2} d\zeta_2 + \frac{\partial z_1}{\partial \varepsilon} d\varepsilon \\ dz_2 &= \frac{\partial z_2}{\partial \zeta_1} d\zeta_1 + \frac{\partial z_2}{\partial \zeta_2} d\zeta_2 + \frac{\partial z_2}{\partial \varepsilon} d\varepsilon \end{aligned}\right\} \quad (5.24)$$

which may be substituted into equations (5.23) to obtain:

$$\left[\left(1 - \varepsilon \frac{\partial \mu_1}{\partial z_1}\right) \frac{\partial z_1}{\partial \zeta_1} - \varepsilon \frac{\partial \mu_1}{\partial z_2} \frac{\partial z_2}{\partial \zeta_2} - 1\right] d\zeta_1$$

$$+ \left[\left(1 - \varepsilon \frac{\partial \mu_1}{\partial z_1}\right) \frac{\partial z_1}{\partial \zeta_2} - \varepsilon \frac{\partial \mu_1}{\partial z_2} \frac{\partial z_2}{\partial \zeta_2}\right] d\zeta_2$$

$$+ \left[\left(1 - \varepsilon \frac{\partial \mu_1}{\partial z_1}\right) \frac{\partial z_1}{\partial \varepsilon} - \varepsilon \frac{\partial \mu_1}{\partial z_2} \frac{\partial z_2}{\partial \varepsilon} - \mu_1\right] d\varepsilon = 0 \qquad (5.25a)$$

and

$$\left[-\varepsilon \frac{\partial \mu_2}{\partial z_1} \frac{\partial z_1}{\partial \zeta_1} + \left(1 - \varepsilon \frac{\partial \mu_2}{\partial z_2}\right) \frac{\partial z_2}{\partial \zeta_2}\right] d\zeta_1$$

$$+ \left[-\varepsilon \frac{\partial \mu_2}{\partial z_1} \frac{\partial z_1}{\partial \zeta_2} + \left(1 - \varepsilon \frac{\partial \mu_2}{\partial z_2}\right) \frac{\partial z_2}{\partial \zeta_2} - 1\right] d\zeta_2$$

$$+ \left[-\varepsilon \frac{\partial \mu_2}{\partial z_1} \frac{\partial z_1}{\partial \varepsilon} + \left(1 - \varepsilon \frac{\partial \mu_2}{\partial z_2}\right) \frac{\partial z_2}{\partial \varepsilon} - \mu_2\right] d\varepsilon = 0 \qquad (5.25b)$$

The factors multiplying $d\zeta_1$, $d\zeta_2$, and $d\varepsilon$ in equations (5.25a) and (5.25b) must vanish (as in eq. (5.2c); see discussion of eqs. (5.2) above), so the six equations for the six unknowns, $\partial z_1/\partial \zeta_1$, $\partial z_1/\partial \zeta_2$, $\partial z_1/\partial \varepsilon$, $\partial z_2/\partial \zeta_1$, $\partial z_2/\partial \zeta_2$, $\partial z_2/\partial \varepsilon$, yield, with

$$D \equiv \begin{vmatrix} 1 - \varepsilon \frac{\partial \mu_1}{\partial z_1} & -\varepsilon \frac{\partial \mu_1}{\partial z_2} \\ -\varepsilon \frac{\partial \mu_2}{\partial z_1} & 1 - \varepsilon \frac{\partial \mu_2}{\partial z_2} \end{vmatrix} \qquad (5.26)$$

$$= \left(1 - \varepsilon \frac{\partial \mu_1}{\partial z_1}\right)\left(1 - \varepsilon \frac{\partial \mu_2}{\partial z_2}\right) - \varepsilon^2 \frac{\partial \mu_1}{\partial z_2} \frac{\partial \mu_2}{\partial z_1}$$

the following:

$$\left.\begin{aligned}
&\frac{\partial z_1}{\partial \zeta_1} = \frac{1}{D}\left(1 - \varepsilon \frac{\partial \mu_2}{\partial z_2}\right) ; \quad \frac{\partial z_1}{\partial \zeta_2} = \frac{1}{D} \varepsilon \frac{\partial \mu_1}{\partial z_2} ; \\
&\frac{\partial z_1}{\partial \varepsilon} = \frac{1}{D}\left[\left(1 - \varepsilon \frac{\partial \mu_2}{\partial z_2}\right)\mu_1 + \varepsilon \frac{\partial \mu_1}{\partial z_2} \mu_2\right] ; \quad \frac{\partial z_2}{\partial \zeta_1} = \frac{1}{D} \varepsilon \frac{\partial \mu_2}{\partial z_1} ; \\
&\frac{\partial z_2}{\partial \zeta_2} = \frac{1}{D}\left(1 - \varepsilon \frac{\partial \mu_1}{\partial z_1}\right) ; \quad \frac{\partial z_2}{\partial \varepsilon} = \frac{1}{D}\left[\left(1 - \varepsilon \frac{\partial \mu_1}{\partial z_1}\right)\mu_2 + \varepsilon \frac{\partial \mu_2}{\partial z_1} \mu_1\right]
\end{aligned}\right\} \quad (5.27)$$

For any function of $\vec{z}$ only,

$$F(\vec{z}) = F[\vec{z}(\vec{\zeta},\varepsilon)] \equiv F[z_1(\zeta_1,\zeta_2,\varepsilon) , z_2(\zeta_1,\zeta_2,\varepsilon)]$$

we have

$$\left.\begin{aligned}
\frac{\partial F(\vec{z})}{\partial \varepsilon} &= \frac{\partial z_1}{\partial \varepsilon} \frac{\partial F}{\partial z_1} + \frac{\partial z_2}{\partial \varepsilon} \frac{\partial F}{\partial z_2} \\
\frac{\partial F(\vec{z})}{\partial \zeta_1} &= \frac{\partial z_1}{\partial \zeta_1} \frac{\partial F}{\partial z_1} + \frac{\partial z_2}{\partial \zeta_1} \frac{\partial F}{\partial z_2} \\
\frac{\partial F(\vec{z})}{\partial \zeta_2} &= \frac{\partial z_1}{\partial \zeta_2} \frac{\partial F}{\partial z_1} + \frac{\partial z_2}{\partial \zeta_2} \frac{\partial F}{\partial z_2}
\end{aligned}\right\} \quad (5.28)$$

from which, with use of equations (5.27), it is readily found that

$$\frac{\partial F(\vec{z})}{\partial \varepsilon} \equiv \frac{\partial F(z_1,z_2)}{\partial \varepsilon} = \mu_1(z_1,z_2) \frac{\partial F(z_1,z_2)}{\partial \zeta_1} + \mu_2(z_1,z_2) \frac{\partial F(z_1,z_2)}{\partial \zeta_2}$$

or

$$\frac{\partial F(\vec{z})}{\partial \varepsilon} = \vec{\mu}(\vec{z}) \cdot \nabla_\zeta F(\vec{z}) \quad (5.29)$$

Equation (5.29) may be differentiated as follows:

$$\frac{\partial^2 F(\vec{z})}{\partial \varepsilon^2} = \vec{\mu}(\vec{z}) \cdot \nabla_\zeta \left[\frac{\partial F(\vec{z})}{\partial \varepsilon}\right] + \left[\frac{\partial \vec{\mu}(\vec{z})}{\partial \varepsilon}\right] \cdot \nabla_\zeta [F(\vec{z})]$$

$$\frac{\partial^3 F(\vec{z})}{\partial \varepsilon^3} = \vec{\mu}(\vec{z}) \cdot \nabla_\zeta \left[\frac{\partial^2 F(\vec{z})}{\partial \varepsilon^2}\right] + 2\left[\frac{\partial \vec{\mu}(\vec{z})}{\partial \varepsilon}\right] \cdot \nabla_\zeta \left[\frac{\partial F(\vec{z})}{\partial \varepsilon}\right]$$

$$+ \left[\frac{\partial^2 \vec{\mu}(\vec{z})}{\partial \varepsilon^2}\right] \cdot \nabla_\zeta F(\vec{z})$$

and by induction one finds

$$\frac{\partial^i F(\vec{z})}{\partial \varepsilon^i} = \sum_{j=0}^{i-1} \binom{i-1}{j} \frac{\partial^j \vec{\mu}(\vec{z})}{\partial \varepsilon^j} \cdot \nabla_\zeta \left[\frac{\partial^{i-j-1} F(\vec{z})}{\partial \varepsilon^{i-j-1}}\right] \tag{5.30}$$

where the Binomial coefficient is defined by

$$\binom{a}{b} \equiv \frac{a!}{(a-b)!\, b!} \tag{5.31}$$

Equation (5.30) is then used as follows:

Taylor's expansion about $\varepsilon=0$ for $f[\vec{z}(\vec{\zeta},\varepsilon)]$ is

$$f(\vec{z}) \equiv f[\vec{z}(\vec{\zeta},\varepsilon)] = f[\vec{z}(\vec{\zeta},0)] + \sum_{n=1}^{\infty} \frac{\varepsilon^n}{n!} \left[\frac{\partial^n f[\vec{z}(\vec{\zeta},\varepsilon)]}{\partial \varepsilon^n}\right]_{\varepsilon=0} \tag{5.32}$$

Since at $\varepsilon=0$, $\vec{z}=\vec{\zeta}$, this is also

$$f(\vec{z}) = f(\vec{\zeta}) + \sum_{n=1}^{\infty} \frac{\varepsilon^n}{n!} \left[\frac{\partial^n f[\vec{z}(\vec{\zeta},\varepsilon)]}{\partial \varepsilon^n}\right]_{\varepsilon=0} \tag{5.33a}$$

where the terms in the summation are found (using 5.30)) from:

$$\frac{\partial^i f[\vec{z}(\vec{\zeta},\varepsilon)]}{\partial \varepsilon^i} = \sum_{j=0}^{i-1} \binom{i-1}{j} \left[\frac{\partial^j \vec{\mu}[\vec{z}(\vec{\zeta},\varepsilon)]}{\partial \varepsilon^j}\right] \cdot \nabla_\zeta \left[\frac{\partial^{i-j-1} f[\vec{z}(\vec{\zeta},\varepsilon)]}{\partial \varepsilon^{i-j-1}}\right] \qquad (5.33b)$$

and also

$$\frac{\partial^i \vec{\mu}[\vec{z}(\vec{\zeta},\varepsilon)]}{\partial \varepsilon^i} = \sum_{j=0}^{i-1} \binom{i-1}{j} \left[\frac{\partial^j \vec{\mu}[\vec{z}(\vec{\zeta},\varepsilon)]}{\partial \varepsilon^j}\right] \cdot \nabla_\zeta \left[\frac{\partial^{i-j-1} \vec{\mu}[\vec{z}(\vec{\zeta},\varepsilon)]}{\partial \varepsilon^{i-j-1}}\right] \qquad (5.33c)$$

and where

$$\vec{z} = \vec{z}(\vec{\zeta},\varepsilon) \equiv \vec{\zeta} + \varepsilon \vec{\mu}(\vec{z}) \qquad (5.34)$$

Each of the terms on the right side of equations (5.33b) and (5.33c) can be found using equations (5.33b) and (5.33c) for a smaller order i. Thus, to any order, the terms of equation (5.33a) must be found successively from equations (5.33b) and (5.33c). The procedure is illustrated as follows:

(a) First take i=1 to find, from equations (5.33b) and (5.33c):

$$\frac{\partial f(\vec{z})}{\partial \varepsilon} = \vec{\mu}(\vec{z}) \cdot \nabla_\zeta f(\vec{z}) \qquad (5.35a)$$

$$\frac{\partial \vec{\mu}(\vec{z})}{\partial \varepsilon} = \vec{\mu}(\vec{z}) \cdot \nabla_\zeta \vec{\mu}(\vec{z}) \qquad (5.35b)$$

Since $\vec{z}=\vec{\zeta}$ at $\varepsilon=0$, we have from (5.35a) for use in (5.33a):

$$\left[\frac{\partial f(\vec{z})}{\partial \varepsilon}\right]_{\varepsilon=0} = \vec{\mu}(\vec{\zeta}) \cdot \nabla_\zeta f(\vec{\zeta}) \qquad (5.35c)$$

(b) Next take i=2 in equations (5.33b) and (5.33c) to obtain

$$\frac{\partial^2 f}{\partial \varepsilon^2} = \vec{\mu}(\vec{z}) \cdot \nabla_\zeta \left[\frac{\partial f(\vec{z})}{\partial \varepsilon}\right] + \left[\frac{\partial \vec{\mu}(\vec{z})}{\partial \varepsilon}\right] \cdot \nabla_\zeta f(\vec{z})$$

and, with use of equations (5.35a) and (5.35b),

$$\frac{\partial^2 f(\vec{z})}{\partial \varepsilon^2} = \vec{\mu}(\vec{z}) \cdot \nabla_\zeta [\vec{\mu}(\vec{z}) \cdot \nabla_\zeta f(\vec{z})] + [\vec{\mu}(\vec{z}) \cdot \nabla_\zeta \vec{\mu}(\vec{z})] \cdot \nabla_\zeta f(\vec{z}) \qquad (5.35d)$$

Similarly,

$$\frac{\partial^2 \vec{\mu}(\vec{z})}{\partial \varepsilon^2} = \vec{\mu}(\vec{z}) \cdot \nabla_\zeta [\vec{\mu}(\vec{z}) \cdot \nabla_\zeta \vec{\mu}(\vec{z})] + [\vec{\mu}(\vec{z}) \cdot \nabla_\zeta \vec{\mu}(\vec{z})] \cdot \nabla_\zeta \vec{\mu}(\vec{z}) \qquad (5.35e)$$

Since $\vec{z}=\vec{\zeta}$ at $\varepsilon=0$, we have from (5.35d) for use in equation (5.33a):

$$\left[\frac{\partial^2 f(\vec{z})}{\partial \varepsilon^2}\right]_{\varepsilon=0} = \vec{\mu}(\vec{\zeta}) \cdot \nabla_\zeta [\vec{\mu}(\vec{\zeta}) \cdot \nabla_\zeta f(\vec{\zeta})] + [\vec{\mu}(\vec{\zeta}) \cdot \nabla_\zeta \vec{\mu}(\vec{\zeta})] \cdot \nabla_\zeta f(\vec{\zeta}) \qquad (5.35f)$$

(c) Higher order terms follow similarly. Thus, for $N=2$, the "standard form" of Lagrange's expansion in vector form has been derived, the first few terms of which are given by equation (5.20).

5.4.2 Arbitrary-N dimensions; first derivation

For arbitrary N the major steps in the derivation are directly analogous to those above (§ 5.4.1) for $N=2$. Differentiation of equation (5.17):

$$\vec{z} = \vec{z}(\vec{\zeta},\varepsilon) \equiv \vec{\zeta} + \varepsilon\vec{\mu}(\vec{z}) \qquad (5.17)$$

(with arbitrary N in equations (5.18)) gives

$$d\vec{z} = d\vec{\zeta} + \varepsilon\, d\vec{z} \cdot \nabla_z \vec{\mu} + \vec{\mu}\, d\varepsilon \qquad (5.36a)$$

from which

$$d\vec{z} \cdot [\, \mathbf{I} - \varepsilon \nabla_z \vec{\mu}(\vec{z})] = d\vec{\zeta} + \vec{\mu}\, d\varepsilon \qquad (5.36b)$$

where

$$\nabla_z \equiv \sum_{k=1}^{N} \vec{e}_k \frac{\partial}{\partial z_k} \tag{5.37a}$$

and where $\mathbf{I}$ is the <u>idemtensor</u> (unit tensor):

$$\mathbf{I} = \sum_{i=1}^{N} \sum_{j=1}^{N} \vec{e}_i \vec{e}_j \delta_{ij} = \sum_{i=1}^{N} \vec{e}_i \vec{e}_i \tag{5.37b}$$

(cf. eq. (5.19)). Also, since $\vec{z} = \vec{z}(\vec{\zeta},\varepsilon)$, one may write

$$d\vec{z} = d\vec{\zeta} \cdot \nabla_\zeta \vec{z} + \frac{\partial \vec{z}}{\partial \varepsilon} d\varepsilon \tag{5.38}$$

Substitution of equation (5.38) into (5.36) gives

$$d\vec{\zeta} \cdot \{(\nabla_\zeta \vec{z}) \cdot [\mathbf{I} - \varepsilon \nabla_z \vec{\mu}(\vec{z})] - \mathbf{I}\}$$

$$+ d\varepsilon \{ \frac{\partial \vec{z}}{\partial \varepsilon} \cdot [\mathbf{I} - \varepsilon \nabla_z \vec{\mu}(\vec{z})] - \vec{\mu}\} = 0 \tag{5.39a}$$

Equation (5.39a) is a vector equation with N components. In each of the N equations for the components, the coefficients of $d\varepsilon$ and of each $d\zeta_k$ must vanish (as in eqs. (5.25) and (5.2c)). One therefore obtains $N(N+1)$ equations to evaluate the $N(N+1)$ unknowns, $\partial z_i/\partial \zeta_j$ and $\partial z_i/\partial \varepsilon$ $(i,j = 1, 2, \ldots, N)$, as follows:

From (5.39a):

$$d\vec{\zeta} \cdot (\nabla_\zeta \vec{z}) \cdot [\mathbf{I} - \varepsilon \nabla_z \vec{\mu}] = d\vec{\zeta} \tag{5.39b}$$

and

$$\frac{\partial \vec{z}}{\partial \varepsilon} \cdot [\mathbf{I} - \varepsilon \nabla_z \vec{\mu}] = \vec{\mu} \tag{5.39c}$$

From (5.39b)

$$\left[d\zeta_1 \frac{\partial \vec{z}}{\partial \zeta_1} + d\zeta_2 \frac{\partial \vec{z}}{\partial \zeta_2} + \cdots + d\zeta_N \frac{\partial \vec{z}}{\partial \zeta_N} \right] \cdot [\mathbf{I} - \varepsilon \nabla_z \vec{\mu}] = d\vec{\zeta}$$

By expanding this equation into its components and setting the coefficients of each $d\zeta_k$ equal to zero, one obtains finally a set of N^2 equations for the N^2 quantities $\partial z_i/\partial \zeta_j$, $(i,j = 1, 2, \ldots, N)$, that may be written in the form:

$$\sum_{k=1}^{N} \left(\delta_{ik} - \varepsilon \frac{\partial \mu_i}{\partial z_k} \right) \frac{\partial z_k}{\partial \zeta_j} = \delta_{ij} \quad , \quad (i,j = 1, 2, \ldots, N) \tag{5.40a}$$

Similarly, from (5.39c), one obtains N equations for the N quantities $\partial z_j/\partial \varepsilon$ $(j = 1, 2, \ldots, N)$ that may be written in the form

$$\sum_{k=1}^{N} \left(\delta_{ik} - \varepsilon \frac{\partial \mu_i}{\partial z_k} \right) \frac{\partial z_k}{\partial \varepsilon} = \mu_i \quad , \quad (i = 1, 2, \ldots, N) \tag{5.40b}$$

Equations (5.40a) and (5.40b) now represent $N(N+1)$ equations, consisting of $N+1$ sets of N equations each. The $N(N+1)$ unknowns $\partial z_k/\partial \zeta_j$ and $\partial z_k/\partial \varepsilon$ can be found by Cramer's Rule (see, e.g., Hildebrand, 1952) from these $N+1$ sets of N equations each. Define

$$a_{ik} \equiv \delta_{ik} - \varepsilon \, \partial \mu_i/\partial z_k \tag{5.41}$$

and define the <u>minor</u> of a_{ij} as M_{ij} and the <u>cofactor</u> of a_{ij} by

$$A_{ij} = (-1)^{i+j} M_{ij} \tag{5.42}$$

Denote the <u>determinant</u> of the matrix a_{ij} by $|\underline{a}|$. Then

$$|\underline{a}| = \sum_{k=1}^{N} a_{ik} A_{ik}$$

and

$$|\underline{a}| = \sum_{k=1}^{N} a_{kj} A_{kj} \qquad (5.43)$$

and also

$$\sum_{k=1}^{N} a_{rk} A_{ik} = 0 \quad \text{for} \quad r \neq i$$

and

$$\sum_{k=1}^{N} a_{ks} A_{kj} = 0 \quad \text{for} \quad s \neq j \qquad (5.44)$$

Then Cramer's Rule gives the solutions of equations (5.40b) and (5.40a) for each j as

$$\frac{\partial z_r}{\partial \zeta_j} = \frac{1}{|\underline{a}|} \sum_{i=1}^{N} A_{ir} \delta_{ij} = \frac{1}{|\underline{a}|} A_{jr} \qquad (r,j=1,2,\ldots,N) \qquad (5.45a)$$

and

$$\frac{\partial z_r}{\partial \varepsilon} = \frac{1}{|\underline{a}|} \sum_{i=1}^{N} A_{ir} \mu_i \qquad (r=1,2,\ldots,N) \qquad (5.45b)$$

Now, since for any function

$$F(\vec{z}) = F[\vec{z}(\vec{\zeta},\varepsilon)] = F[z_1(\zeta_1,\zeta_2,\ldots,\zeta_N,\varepsilon),\ z_2(\zeta_1,\ldots,\zeta_N,\varepsilon),\ldots,z_N]$$

one may write

$$\left.\begin{aligned} \frac{\partial F}{\partial \zeta_j} &= \sum_{r=1}^{N} \frac{\partial z_r}{\partial \zeta_j} \frac{\partial F}{\partial z_r} \qquad (j = 1, 2, \ldots, N) \\ \text{and} \\ \frac{\partial F}{\partial \varepsilon} &= \sum_{r=1}^{N} \frac{\partial z_r}{\partial \varepsilon} \frac{\partial F}{\partial z_r} \end{aligned}\right\} \tag{5.46}$$

substitution of equations (5.45) into (5.46) gives

$$\frac{\partial F}{\partial \zeta_j} = \frac{1}{|\underline{a}|} \sum_{r=1}^{N} A_{jr} \frac{\partial F}{\partial z_r} \qquad (j = 1, 2, \ldots, N) \tag{5.47a}$$

$$\frac{\partial F}{\partial \varepsilon} = \frac{1}{|\underline{a}|} \sum_{r=1}^{N} \sum_{i=1}^{N} A_{ir} \mu_i \frac{\partial F}{\partial z_r} \tag{5.47b}$$

Upon multiplying equation (5.47a) by μ_j and summing over j from 1 to N, one finds

$$\frac{\partial F(\vec{z})}{\partial \varepsilon} = \sum_{j=1}^{N} \mu_j(\vec{z}) \frac{\partial F(\vec{z})}{\partial \zeta_j} \tag{5.48a}$$

This result may also be written in the form

$$\frac{\partial F(\vec{z})}{\partial \varepsilon} = \vec{\mu}(\vec{z}) \cdot \nabla_{\zeta} F(\vec{z}) \tag{5.48b}$$

The remainder of the development for arbitrary N is identical to that from equations (5.29) to (5.35). Thus, an extension of the "standard form" of Lagrange's expansion has been derived for arbitrary N dimensions, with the first few terms given by (5.20).

It should be noted that in equation (5.17) and the result (5.20) the appearance of ε is extraneous (since it appears only in the product $\varepsilon\vec{\mu}$), and so ε could be taken to be unity. The nature of the <u>convergence</u> of (5.20) then depends on each of the components μ_i being sufficiently

small (rather than each $\varepsilon\mu_i$). Each μ_i could then be replaced in (5.17) and (5.20) by $\varepsilon_i\bar{\mu}_i$, and since the μ_i's are independent, the ε_i's could be considered as representing different orders of magnitude (such as $\varepsilon_1 = \varepsilon$, $\varepsilon_2 = \varepsilon^2 \log \varepsilon$, $\varepsilon_3 = \varepsilon^2$, $\varepsilon_4 = \varepsilon$, etc.) (Actually the same results had originally been found by carrying out the entire derivation starting with arbitrary different ε_i's, rather than the simpler derivation in terms of one ε given above. Since the results are equivalent, the simpler derivation that uses only one ε has been given here.)

5.4.3 An alternate derivation for N independent variables

A generalization, to N independent variables, of the derivation given above in § 5.2.2 is described here. The final result is somewhat more concise than that given in §§ 5.4.1 and 5.4.2 above. The expanded terms are identical.

It is convenient to first introduce some additional vector and tensor notation not previously used. Consider the vectors $\vec{z}$, $\vec{\zeta}$, $\vec{\mu}$, and the Cartesian base vectors $\vec{e}_k$ defined as in equations (5.17) to (5.19), and the vector operators ∇_ζ and ∇_z defined as in (5.21) and (5.37a). For arbitrary N-dimensional vectors

$$\vec{A} \equiv \sum_{k=1}^{N} \vec{e}_k A_k \quad , \quad \vec{B} \equiv \sum_{k=1}^{N} \vec{e}_k B_k \tag{5.49}$$

define the nth order tensors

$$\vec{A}^{(n)} \equiv \underbrace{\vec{A}\vec{A}\vec{A}\ldots\vec{A}}_{n \text{ times}} \quad , \quad \vec{B}^{(n)} \equiv \underbrace{\vec{B}\vec{B}\vec{B}\ldots\vec{B}}_{n \text{ times}} \tag{5.50}$$

(We might call $\vec{A}^{(n)}$ and $\vec{B}^{(n)}$ "polyadics," since the special cases for n = 2, 3, and 4 are known respectively as dyadics, triadics, and tetradics; cf. Morse and Feshbach, 1953.) Further, define the scalar products (which follow from (5.19)):

$$\vec{A}\cdot\vec{B} \equiv \sum_{i=1}^{N} A_i B_i \tag{5.51a}$$

$$\vec{\vec{A}}:\vec{\vec{B}} \equiv \vec{A}\cdot(\vec{A}\cdot\vec{\vec{B}}) = \sum_{i=1}^{N}\sum_{j=1}^{N} A_i A_j B_j B_i \tag{5.51b}$$

$$\vec{\vec{\vec{A}}}:\vec{\vec{\vec{B}}} \equiv \vec{A}\cdot[\vec{A}\cdot(\vec{A}\cdot\vec{\vec{\vec{B}}})] = \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N} A_i A_j A_k B_k B_j B_i \tag{5.51c}$$

and, in general, define the following notation for the nth scalar product:

$$\vec{A}^{(n)} \overset{n}{(\cdot)} \vec{B}^{(n)} \equiv \sum_{i_1=1}^{N}\sum_{i_2=1}^{N}\cdots\sum_{i_n=1}^{N} A_{i_1} A_{i_2}\cdots A_{i_n} B_{i_n} B_{i_{n-1}}\cdots B_{i_1} \tag{5.51d}$$

Then, in particular,

$$[\vec{\mu}(\vec{\zeta})]^{(n)} \equiv \underbrace{\vec{\mu}(\vec{\zeta})\vec{\mu}(\vec{\zeta})\ldots\vec{\mu}(\vec{\zeta})}_{n \text{ times}} = \sum_{i_1=1}^{N}\sum_{i_2=1}^{N}\cdots\sum_{i_n=1}^{N} \vec{e}_{i_1}\ldots\vec{e}_{i_n}\,\mu_{i_1}(\vec{\zeta})\ldots\mu_{i_n}(\vec{\zeta}) \tag{5.52a}$$

and

$$\nabla_{\zeta}^{(n)} \equiv \underbrace{\nabla_{\zeta}\nabla_{\zeta}\ldots\nabla_{\zeta}}_{n \text{ times}} = \sum_{i_1=1}^{N}\sum_{i_2=1}^{N}\cdots\sum_{i_n=1}^{N} \vec{e}_{i_1}\ldots\vec{e}_{i_n}\,\frac{\partial^n}{\partial\zeta_{i_1}\partial\zeta_{i_2}\ldots\partial\zeta_{i_n}} \tag{5.52b}$$

and with equation (5.17) the N-dimensional Taylor's expansion is

$$f(z_1,z_2,\ldots,z_N) = f(\zeta_1,\zeta_2,\ldots,\zeta_N) + \sum_{i=1}^{N}(z_i-\zeta_i)\,\frac{\partial f(\zeta_1,\zeta_2,\ldots,\zeta_N)}{\partial\zeta_i}$$

$$+ \frac{1}{2!}\sum_{i=1}^{N}\sum_{j=1}^{N}(z_i-\zeta_i)(z_j-\zeta_j)\,\frac{\partial^2 f(\zeta_1,\zeta_2,\ldots,\zeta_N)}{\partial\zeta_i\,\partial\zeta_j} + \cdots \tag{5.53}$$

which, in the above-defined notation, is equivalent to:

$$f(\vec{z}) = f(\vec{\zeta}) + \sum_{n=1}^{\infty} \frac{\varepsilon^n}{n!} [\vec{\mu}(\vec{z})]^{(n)}(\overset{n}{\cdot}) \nabla_\zeta^{(n)} f(\vec{\zeta}) \tag{5.54a}$$

(compare with eq. (5.11a)). Then also

$$\vec{\mu}(\vec{z}) = \vec{\mu}(\vec{\zeta}) + \sum_{n=1}^{\infty} \frac{\varepsilon^n}{n!} [\vec{\mu}(\vec{z})]^{(n)}(\overset{n}{\cdot}) \nabla_\zeta^{(n)} \vec{\mu}(\vec{\zeta}) \tag{5.54b}$$

(cf. eq. (5.11b)), and these latter two equations determine the N -dimensional Lagrange's expansion to any desired order. For example, to order ε^2 ,

$$f(\vec{z}) = f(\vec{\zeta}) + \varepsilon\vec{\mu}(\vec{z}) \cdot \nabla_\zeta f(\vec{\zeta}) + \frac{1}{2} \varepsilon^2 [\vec{\mu}(\vec{z})\vec{\mu}(\vec{z})] : \nabla_\zeta \nabla_\zeta f(\vec{\zeta}) + O(\varepsilon^3) \tag{5.55a}$$

where

$$\vec{\mu}(\vec{z}) = \vec{\mu}(\vec{\zeta}) + \varepsilon\vec{\mu}(\vec{z}) \cdot \nabla_\zeta \vec{\mu}(\vec{\zeta}) + O(\varepsilon^2) = \vec{\mu}(\vec{\zeta}) + \varepsilon\vec{\mu}(\vec{\zeta}) \cdot \nabla_\zeta \vec{\mu}(\vec{\zeta}) + O(\varepsilon^2) \tag{5.55b}$$

Thus (5.55a) becomes

$$f(\vec{z}) = f(\vec{\zeta}) + \varepsilon\vec{\mu}(\vec{\zeta}) \cdot \nabla_\zeta f(\vec{\zeta}) + \varepsilon^2 \{ [\vec{\mu}(\vec{\zeta}) \cdot \nabla_\zeta \vec{\mu}(\vec{\zeta})] \cdot \nabla_\zeta f(\vec{\zeta}) + \frac{1}{2} [\vec{\mu}(\vec{\zeta})\vec{\mu}(\vec{\zeta})] : \nabla_\zeta \nabla_\zeta f(\vec{\zeta}) \} + O(\varepsilon^3) \tag{5.55c}$$

Since it is easily verified that

$$\vec{\mu}(\vec{\zeta})\vec{\mu}(\vec{\zeta}) : \nabla_\zeta \nabla_\zeta f(\vec{\zeta}) \equiv \vec{\mu}(\vec{\zeta}) \cdot \nabla_\zeta [\vec{\mu}(\vec{\zeta}) \cdot \nabla_\zeta f(\vec{\zeta})] - [\vec{\mu}(\vec{\zeta}) \cdot \nabla_\zeta \vec{\mu}(\vec{\zeta})] \cdot \nabla_\zeta f(\vec{\zeta}) \tag{5.56}$$

equation (5.55c) is seen to be equivalent to equation (5.20) to order ε^2.

5.5 Inclusion of Additional Parameters in the N-Dimensional Lagrange Expansion, and Development of Perturbation-Expansion Scheme

As in § 5.3 one may also include additional parameters as arguments of f, $\vec{\mu}$, and $\vec{z}$ in equations (5.17) through (5.20) or in equations (5.33) and (5.34).

Thus, equations (5.33) and (5.34) may be generalized to:

If

$$\vec{z} = \vec{z}(\vec{\zeta},\varepsilon,\alpha,\beta,\ldots) \equiv \vec{\zeta} + \varepsilon\vec{\mu}(\vec{z},\alpha,\beta,\ldots) \tag{5.57}$$

then

$$f(\vec{z},\alpha,\beta,\ldots) = f(\vec{\zeta},\alpha,\beta,\ldots) + \sum_{n=1}^{\infty} \frac{\varepsilon^n}{n!} \left[\frac{\partial^n f[\vec{z}(\vec{\zeta},\varepsilon,\alpha,\beta,\ldots),\ \alpha,\beta,\ldots]}{\partial\varepsilon^n} \right]_{\varepsilon=0} \tag{5.58a}$$

where

$$\frac{\partial^i f[\vec{z}(\vec{\zeta},\varepsilon,\alpha,\beta,\ldots),\ \alpha,\beta,\ldots]}{\partial\varepsilon^i} = \sum_{j=0}^{i-1} \binom{i-1}{j} \left[\frac{\partial^j \vec{\mu}(\vec{z},\alpha,\beta,\ldots)}{\partial\varepsilon^j} \right] \cdot \nabla_\zeta \left[\frac{\partial^{i-j-1} f(\vec{z},\alpha,\beta,\ldots)}{\partial\varepsilon^{i-j-1}} \right] \tag{5.58b}$$

and $\partial^i\vec{\mu}(\vec{z},\alpha,\beta,\ldots)/\partial\varepsilon^i$

$$= \sum_{j=0}^{i-1} \binom{i-1}{j} \left[\frac{\partial^j \vec{\mu}(\vec{z},\alpha,\beta,\ldots)}{\partial\varepsilon^j} \right] \cdot \nabla_\zeta \left[\frac{\partial^{i-j-1}\vec{\mu}(\vec{z},\alpha,\beta,\ldots)}{\partial\varepsilon^{i-j-1}} \right] \tag{5.58c}$$

The expansion of (5.57) may also be found from (5.58a) by taking $f = \vec{\mu}(\vec{z},\alpha,\beta,\ldots)$. In more explicit form for the first few terms, the corresponding generalization of equations (5.17) and (5.20) is:

If

$$\vec{z} = \vec{z}(\vec{\zeta},\varepsilon,\alpha,\beta,\ldots) \equiv \vec{\zeta} + \varepsilon\vec{\mu}(\vec{z},\alpha,\beta,\ldots) \tag{5.59a}$$

then

$$f(\vec{z},\alpha,\beta,\ldots) = f(\vec{\zeta},\alpha,\beta,\ldots) + \varepsilon\{\vec{\mu}(\vec{\zeta},\alpha,\beta,\ldots)\cdot\nabla_{\zeta} f(\vec{\zeta},\alpha,\beta,\ldots)\}$$

$$+ [\text{terms same as in eq. (5.20), but with } f \text{ and } \vec{\mu} \text{ having arguments } (\vec{\zeta},\alpha,\beta,\ldots)] \tag{5.59b}$$

and

$$\vec{\mu}(\vec{z},\alpha,\beta,\ldots) = \vec{\mu}(\vec{\zeta},\alpha,\beta,\ldots) + \varepsilon\{\vec{\mu}(\vec{\zeta},\alpha,\beta,\ldots)\cdot\nabla_{\zeta}\vec{\mu}(\vec{\zeta},\alpha,\beta,\ldots)\} + \cdots \tag{5.59c}$$

Consider the special case of only one parameter α (as in eqs. (5.14)); that is,

$$f(\vec{z},\alpha) = \sum_{k=1}^{\infty} \alpha^{k-1} f_k(\vec{z}) \tag{5.60a}$$

$$\vec{\mu}(\vec{z},\alpha) = \sum_{k=1}^{\infty} \alpha^{k-1} \vec{\mu}_k(\vec{z}) \tag{5.60b}$$

Then equations (5.59) become

$$f(\vec{z},\alpha) = \sum_{k=1}^{\infty} \alpha^{k-1} f_k(\vec{\zeta})$$

$$+ \varepsilon\{[\sum_{k=1}^{\infty} \alpha^{k-1} \vec{\mu}_k\cdot\nabla_{\zeta}][\sum_{k=1}^{\infty} \alpha^{k-1} f_k(\vec{\zeta})]\} + O(\varepsilon^2) \tag{5.61a}$$

where

$$\vec{z} = \vec{\zeta} + \varepsilon\{\sum_{k=1}^{\infty} \alpha^{k-1} \vec{\mu}_k(\vec{\zeta})\} + O(\varepsilon^2) \tag{5.61b}$$

In particular, for $\alpha = \varepsilon$,

$$\left.\begin{aligned} f(\vec{z},\alpha) &= f(\vec{z},\varepsilon) = f_1(\vec{z}) + \varepsilon\, f_2(\vec{z}) + \varepsilon^2 f_3(\vec{z}) + \cdots \\ \vec{\mu}(\vec{z},\alpha) &= \vec{\mu}(\vec{z},\varepsilon) = \vec{\mu}_1(\vec{z}) + \varepsilon\, \vec{\mu}_2(\vec{z}) + \varepsilon^2 \vec{\mu}_3(\vec{z}) + \cdots \end{aligned}\right\} \quad (5.62)$$

and equations (5.59) become (cf. eq. (5.20)):

$$\begin{aligned} f(\vec{z},\varepsilon) &= f_1(\vec{\zeta}) + \varepsilon\, f_2(\vec{\zeta}) + \varepsilon^2 f_3(\vec{\zeta}) + O(\varepsilon^3) \\ &\quad + \varepsilon\{[\vec{\mu}_1(\vec{\zeta})\cdot\nabla_\zeta + \varepsilon\, \vec{\mu}_2(\vec{\zeta})\cdot\nabla_\zeta + \cdots][f_1(\vec{\zeta}) + \varepsilon\, f_2(\vec{\zeta}) + \cdots] \\ &\quad + (1/2!)\,\varepsilon^2\{[\vec{\mu}_1(\vec{\zeta})\cdot\nabla_\zeta + O(\varepsilon)][\vec{\mu}_1(\vec{\zeta})\cdot\nabla_\zeta f_1(\vec{\zeta}) + O(\varepsilon)] \\ &\quad + [\vec{\mu}_1(\vec{\zeta})\cdot\nabla_\zeta \vec{\mu}_1(\vec{\zeta})]\cdot\nabla_\zeta f_1(\vec{\zeta})\} + O(\varepsilon^3) \end{aligned}$$

where

$$\begin{aligned} \vec{z} &= \vec{\zeta} + \varepsilon\{\vec{\mu}_1(\vec{\zeta}) + \varepsilon\, \vec{\mu}_2(\vec{\zeta}) + O(\varepsilon^2)\} \\ &\quad + \varepsilon^2\{\vec{\mu}_1(\vec{\zeta})\cdot\nabla_\zeta \vec{\mu}_1(\vec{\zeta}) + O(\varepsilon)\} + O(\varepsilon^3) \end{aligned}$$

or

$$\begin{aligned} f(\vec{z},\varepsilon) &= f_1(\vec{\zeta}) + \varepsilon\{f_2(\vec{\zeta}) + \vec{\mu}_1(\vec{\zeta})\cdot\nabla_\zeta f_1(\vec{\zeta})\} \\ &\quad + \varepsilon^2\{f_3(\vec{\zeta}) + \vec{\mu}_1(\vec{\zeta})\cdot\nabla_\zeta f_2(\vec{\zeta}) + \vec{\mu}_2(\vec{\zeta})\cdot\nabla_\zeta f_1(\vec{\zeta}) \\ &\quad + (1/2)\,\vec{\mu}_1(\vec{\zeta})\cdot\nabla_\zeta [\vec{\mu}_1(\vec{\zeta})\cdot\nabla_\zeta f_1(\vec{\zeta})] + (1/2)[\vec{\mu}_1(\vec{\zeta})\cdot\nabla_\zeta \vec{\mu}_1(\vec{\zeta})]\cdot\nabla_\zeta f_1(\vec{\zeta})\} \\ &\quad + O(\varepsilon^3) \end{aligned} \quad (5.63a)$$

where

$$\vec{z} = \vec{\zeta} + \varepsilon \vec{\mu}_1(\vec{\zeta}) + \varepsilon^2\{\vec{\mu}_2(\vec{\zeta}) + \vec{\mu}_1(\vec{\zeta})\cdot\nabla_\zeta \vec{\mu}_1(\vec{\zeta})\} + O(\varepsilon^3) \qquad (5.63b)$$

This result (eqs. (5.63)) has been derived for use in the method of Chapter IV, to be shown in Chapter VI.

CHAPTER VI

APPLICATION OF LAGRANGE-EXPANSION PERTURBATION SCHEME IN THE DIRECTIONAL-MEAN-FREE-PATH METHOD

6.1 Introductory Remarks

The Lagrange-expansion perturbation scheme can be applied, purely formally, directly to the gain term in each of the directional equations of change (i.e., to the first term on the right side of each of eqs. (4.43a,b,c), or of eqs. (4.97a,b,c) in the special case of one-dimensional flow).

For validity of the scheme (sufficient convergence or asymptotic convergence), it is not necessary that ε be small. In fact, ε can be taken to be unity (so that $L = u_\alpha/\theta_\alpha$), since the "arbitrary length," L, has not previously been defined. Lagrange's expansion is often written without a small parameter (cf. Whittaker and Watson, 1927), which is equivalent to taking $\varepsilon = 1$ in the forms given in Chapter V. It is only necessary that the product $\varepsilon\vec{\mu}$ be "sufficiently small" in equation (4.41) or in equation (4.95), that is, that $\vec{z}-\vec{\zeta}$ be sufficiently small. However, the parameter ε can still be left in the equations for convenience in "ordering" of the terms, discussed further in § 6.3 below. (See also related discussion of "artificial parameters" by Chang (1961), pp. 816, 820-825.)

Each of the vector and scalar functions of $\vec{z}$ (denoted by $(\tilde{\ })$) in the right side of equations (4.43a,b,c) for general three-dimensional flow can be expanded by use of equations (5.63), and subsequently treated by the scheme discussed below in § 6.3.

It may be instructive at this point to recall that the relation (cf. eq. (4.41))

$$\vec{z} = \vec{\zeta} + \varepsilon\vec{\mu}(\vec{z},\theta,\varphi,\varepsilon) \tag{6.1}$$

is a dimensionless vector equation with four components (cf. eqs. (4.2), (4.3), (4.28), (4.34), and (4.40)) representing

$$\left.\begin{aligned}
\tilde{x}_1 &= x_1 - (\cos\varphi)\,\lambda^*_{\theta\varphi}(\tilde{x}_1,\tilde{x}_2,\tilde{x}_3,\theta,\varphi,\tilde{t}) \\
\tilde{x}_2 &= x_2 - (\sin\varphi\,\cos\theta)\lambda^*_{\theta\varphi}(\tilde{x}_1,\tilde{x}_2,\tilde{x}_3,\theta,\varphi,\tilde{t}) \\
\tilde{x}_3 &= x_3 - (\sin\varphi\,\sin\theta)\,\lambda^*_{\theta\varphi}(\tilde{x}_1,\tilde{x}_2,\tilde{x}_3,\theta,\varphi,\tilde{t}) \\
\tilde{t} &= t - \frac{\lambda^*_{\theta\varphi}(\tilde{x}_1,\tilde{x}_2,\tilde{x}_3,\theta,\varphi,\tilde{t})}{v^{(1)}_{\theta\varphi}(\tilde{x}_1,\tilde{x}_2,\tilde{x}_3,\theta,\varphi,\tilde{t})}
\end{aligned}\right\} \quad (6.2)$$

Since the procedure in three configuration-space dimensions (with time as the fourth dimension) is directly analogous to that in the simplified one-dimensional-flow case, for simplicity and economy of space only the latter is treated in detail in §§ 6.2 and 6.3 below. In one-dimensional flow, only the components ζ_1 and ζ_4 of $\vec{\zeta}$ are of significance, and $\vec{\mu}$ is therefore a function only of ζ_1, ζ_4, ω, and ε (but is independent of ζ_4 in steady flow).

6.2 Expansions for One-Dimensional Flow

In the equations for one-dimensional flow (§ 4.4), assume that each function of $\vec{\zeta}$ and ε, or of $\vec{\zeta}$, ω, and ε, can be expanded in a power series* in ε:

$$\left.\begin{aligned}
F(\zeta,\vec{\varepsilon}) &= F_1(\vec{\zeta}) + \varepsilon\,F_2(\vec{\zeta}) + \varepsilon^2\,F_3(\vec{\zeta}) + O(\varepsilon^3) \\
F(\vec{\zeta},\omega,\varepsilon) &= F_1(\vec{\zeta},\omega) + \varepsilon\,F_2(\vec{\zeta},\omega) + \varepsilon^2\,F_3(\vec{\zeta},\omega) + O(\varepsilon^3)
\end{aligned}\right\} \quad (6.3)$$

---

* These expansions may be only asymptotically valid as $\varepsilon \to 0$, and not "analytic" in ε, but this does not preclude use of the "=" symbol because the order symbol (e.g., $O(\varepsilon^3)$ as $\varepsilon \to 0$) is used (see, e.g., Erdélyi, 1956, or Martin, 1967b).

and each function of $\vec{z}$, ω, and ε has the expansion

$$F(\vec{z},\omega,\varepsilon) = F_1(\vec{z},\omega) + \varepsilon F_2(\vec{z},\omega) + \varepsilon^2 F_3(\vec{z},\omega) + O(\varepsilon^3) \tag{6.4}$$

Thus:

$$\left.\begin{aligned}
\overline{\rho}(\vec{\zeta},\omega,\varepsilon) &= \overline{\rho}_1(\vec{\zeta},\omega) + \varepsilon\, \overline{\rho}_2(\vec{\zeta},\omega) + O(\varepsilon^2) \\
\overline{J}(\vec{\zeta},\omega,\varepsilon) &= \overline{J}_1(\vec{\zeta},\omega) + \varepsilon\, \overline{J}_2(\vec{\zeta},\omega) + O(\varepsilon^2) \\
\overline{P}(\vec{\zeta},\omega,\varepsilon) &= \overline{P}_1(\vec{\zeta},\omega) + \varepsilon\, \overline{P}_2(\vec{\zeta},\omega) + O(\varepsilon^2) \\
\overline{E}(\vec{\zeta},\omega,\varepsilon) &= \overline{E}_1(\vec{\zeta},\omega) + \varepsilon\, \overline{E}_2(\vec{\zeta},\omega) + O(\varepsilon^2) \\
\overline{Q}(\vec{\zeta},\omega,\varepsilon) &= \overline{Q}_1(\vec{\zeta},\omega) + \varepsilon\, \overline{Q}_2(\vec{\zeta},\omega) + O(\varepsilon^2)
\end{aligned}\right\} \tag{6.5a}$$

and

$$\left.\begin{aligned}
H(\vec{\zeta},\omega,\varepsilon) &= H_1(\vec{\zeta},\omega) + \varepsilon\, H_2(\vec{\zeta},\omega) + O(\varepsilon^2) \\
\overline{Z}(\vec{\zeta},\omega,\varepsilon) &= \overline{Z}_1(\vec{\zeta},\omega) + \varepsilon\, \overline{Z}_2(\vec{\zeta},\omega) + O(\varepsilon^2) \\
\vec{\mu}(\vec{\zeta},\omega,\varepsilon) &= \vec{\mu}_1(\vec{\zeta},\omega) + \varepsilon\, \vec{\mu}_2(\vec{\zeta},\omega) + O(\varepsilon^2) \\
M(\vec{\zeta},\varepsilon) &= M_1(\vec{\zeta}) + \varepsilon\, M_2(\vec{\zeta}) + O(\varepsilon^2)
\end{aligned}\right\} \tag{6.5b}$$

Since for one-dimensional flow the functions vary with only two components of $\vec{\zeta}$ (or $\vec{z}$), as well as with ω, the Lagrange expansion perturbation scheme for

$$\vec{z} = \vec{\zeta} + \varepsilon\vec{\mu}(\vec{z},\omega,\varepsilon) \tag{6.6}$$

and for any function such as (6.4), takes the form (cf. eqs. (5.63)):

$$\tilde{F} = F(\vec{z},\omega,\varepsilon) = F_1(\vec{\zeta},\omega) + \varepsilon[F_2(\vec{\zeta},\omega) + \vec{\mu}_1(\vec{\zeta},\omega)\cdot\nabla_{\zeta} F_1(\vec{\zeta},\omega)]$$

$$+ O(\varepsilon^2)$$

$$= F_1(\vec{\zeta},\omega) + \varepsilon[F_2(\vec{\zeta},\omega) + (\mu_1)_1(\vec{\zeta},\omega)\frac{\partial}{\partial\zeta_1} F(\vec{\zeta},\omega)$$

$$+ (\mu_4)_1(\zeta,\omega)\frac{\partial}{\partial\zeta_4} F_1(\vec{\zeta},\omega)] + O(\varepsilon^2) \qquad (6.7)$$

where (see eq. (4.69)):

$$\vec{e}_1\cdot\vec{\mu}(\vec{\zeta},\omega,\varepsilon) = \frac{-\partial\bar{J}/\partial\omega}{H\,\partial\bar{\rho}/\partial\omega} = \frac{\partial\bar{J}_1/\partial\omega + \varepsilon\,\partial\bar{J}_2/\partial\omega + O(\varepsilon^2)}{[H_1 + \varepsilon H_2 + O(\varepsilon^2)][\partial\bar{\rho}_1/\partial\omega + \varepsilon\,\partial\bar{\rho}_2/\partial\omega + O(\varepsilon^2)]} \qquad (6.8a)$$

$$= \frac{-\partial\bar{J}_1/\partial\omega}{H_1\,\partial\bar{\rho}_1/\partial\omega} - \varepsilon\left[\frac{\partial\bar{J}_2/\partial\omega}{H_1\,\partial\bar{\rho}_1/\partial\omega} - \left(\frac{\partial\bar{J}_1/\partial\omega}{H_1\,\partial\bar{\rho}_1/\partial\omega}\right)\left(\frac{H_2}{H_1} + \frac{\partial\bar{\rho}_2/\partial\omega}{\partial\bar{\rho}_1/\partial\omega}\right)\right] + O(\varepsilon^2)$$

$$= (\mu_1)_1(\vec{\zeta},\omega) + \varepsilon(\mu_1)_2(\vec{\zeta},\omega) + O(\varepsilon^2) \qquad (6.8b)$$

and

$$\vec{e}_4\cdot\vec{\mu}(\vec{\zeta},\omega,\varepsilon) = -\frac{1}{H} = \frac{-1}{H_1(\vec{\zeta},\omega)} + \varepsilon\frac{H_2(\vec{\zeta},\omega)}{H_1^2(\vec{\zeta},\omega)} + O(\varepsilon^2) \qquad (6.9a)$$

$$= (\mu_4)_1(\vec{\zeta},\omega) + \varepsilon(\mu_4)_2(\vec{\zeta},\omega) + O(\varepsilon^2) \qquad (6.9b)$$

Thus, in the expansion form of equation (6.7), for any function $F(\vec{z},\omega,\varepsilon)$:

$$(\mu_1)_1(\vec{\zeta},\omega) = -\frac{\partial\bar{J}_1(\vec{\zeta},\omega)}{\partial\omega} \Big/ H_1(\vec{\zeta},\omega)\frac{\partial\bar{\rho}_1(\vec{\zeta},\omega)}{\partial\omega} \qquad (6.10a)$$

and

$$(\mu_4)_1(\vec{\zeta},\omega) = -1/H_1(\vec{\zeta},\omega) \qquad (6.10b)$$

For equations that use collision model II, only the expansion forms (6.3) and (6.7) with (6.10) are needed. Thus the directional equations of change for that case (eqs. (4.107)) become:

$$\varepsilon\left(\frac{\partial^2\overline{\rho}_1}{\partial\zeta_4\partial\omega}+\frac{\partial^2\overline{J}_1}{\partial\zeta_1\partial\omega}\right)+\varepsilon^2\left(\frac{\partial^2\overline{\rho}_2}{\partial\zeta_4\partial\omega}+\frac{\partial^2\overline{J}_2}{\partial\zeta_1\partial\omega}\right)+O(\varepsilon^3)$$

$$=H_{1e}\frac{\partial\overline{\rho}_{1e}}{\partial\omega}-H_1\frac{\partial\overline{\rho}_1}{\partial\omega}+\varepsilon\left\{H_{1e}\left[\frac{\partial\overline{\rho}_{2e}}{\partial\omega}+(\mu_1)_1\frac{\partial}{\partial\zeta_1}\left(\frac{\partial\overline{\rho}_{1e}}{\partial\omega}\right)+(\mu_4)_1\frac{\partial}{\partial\zeta_4}\left(\frac{\partial\overline{\rho}_{1e}}{\partial\omega}\right)\right]\right.$$

$$\left.+\frac{\partial\overline{\rho}_{1e}}{\partial\omega}\left[H_{2e}+(\mu_1)_1\frac{\partial H_{1e}}{\partial\zeta_1}+(\mu_4)_1\frac{\partial H_{1e}}{\partial\zeta_4}\right]-H_1\frac{\partial\overline{\rho}_2}{\partial\omega}-H_2\frac{\partial\overline{\rho}_1}{\partial\omega}\right\}$$

$$+O(\varepsilon^2) \qquad (6.11a)$$

$$\varepsilon\left(\frac{\partial^2\overline{J}_1}{\partial\zeta_4\partial\omega}+\frac{\partial^2\overline{P}_1}{\partial\zeta_1\partial\omega}\right)+\varepsilon^2\left(\frac{\partial^2\overline{J}_2}{\partial\zeta_4\partial\omega}+\frac{\partial^2\overline{P}_2}{\partial\zeta_4\partial\omega}\right)+O(\varepsilon^3)$$

$$=H_{1e}\frac{\partial\overline{J}_{1e}}{\partial\omega}-H_1\frac{\partial\overline{J}_1}{\partial\omega}+\varepsilon\left\{H_{1e}\left[\frac{\partial\overline{J}_{2e}}{\partial\omega}+(\mu_1)_1\frac{\partial}{\partial\zeta_1}\left(\frac{\partial\overline{J}_{1e}}{\partial\omega}\right)+(\mu_4)_1\frac{\partial}{\partial\zeta_4}\left(\frac{\partial\overline{J}_{1e}}{\partial\omega}\right)\right]\right.$$

$$\left.+\frac{\partial\overline{J}_{1e}}{\partial\omega}\left[H_{2e}+(\mu_1)_1\frac{\partial H_{1e}}{\partial\zeta_1}+(\mu_4)_1\frac{\partial H_{1e}}{\partial\zeta_4}\right]-H_1\frac{\partial\overline{J}_2}{\partial\omega}-H_2\frac{\partial\overline{J}_1}{\partial\omega}\right\}$$

$$+O(\varepsilon^2) \qquad (6.11b)$$

$$\varepsilon\left(\frac{\partial^2\overline{E}_1}{\partial\zeta_4\partial\omega}+\frac{\partial^2\overline{Q}_1}{\partial\zeta_1\partial\omega}\right)+\varepsilon^2\left(\frac{\partial^2\overline{E}_2}{\partial\zeta_4\partial\omega}+\frac{\partial^2\overline{Q}_2}{\partial\zeta_1\partial\omega}\right)+O(\varepsilon^3)$$

$$=H_{1e}\frac{\partial\overline{E}_{1e}}{\partial\omega}-H_1\frac{\partial\overline{E}_1}{\partial\omega}+\varepsilon\left\{H_{1e}\left[\frac{\partial\overline{E}_{2e}}{\partial\omega}+(\mu_1)_1\frac{\partial}{\partial\zeta_1}\left(\frac{\partial\overline{E}_{1e}}{\partial\omega}\right)+(\mu_4)_1\frac{\partial}{\partial\zeta_4}\left(\frac{\partial\overline{E}_{1e}}{\partial\omega}\right)\right]\right.$$

$$\left.+\frac{\partial\overline{E}_{1e}}{\partial\omega}\left[H_{2e}+(\mu_1)_1\frac{\partial H_{1e}}{\partial\zeta_1}+(\mu_4)_1\frac{\partial H_{1e}}{\partial\zeta_4}\right]-H_1\frac{\partial\overline{E}_2}{\partial\omega}-H_2\frac{\partial\overline{E}_1}{\partial\omega}\right\}+O(\varepsilon^2) \qquad (6.11c)$$

and

$$\frac{\partial \bar{E}_1}{\partial \omega} + \varepsilon \frac{\partial \bar{E}_2}{\partial \omega} + O(\varepsilon^2) = \frac{1}{2\omega^2} \frac{\partial \bar{P}_1}{\partial \omega} + \varepsilon \frac{1}{2\omega^2} \frac{\partial \bar{P}_2}{\partial \omega} + O(\varepsilon^2) \tag{6.11d}$$

For other collision models, evaluation of functions of $\vec{z}$ and ω' in equations (4.97) is required. Since ω' is given in general by (4.106b), it is convenient to write the expansion

$$\omega'(\vec{\zeta},\omega,\varepsilon) = \omega_1'(\vec{\zeta},\omega) + \varepsilon\, \omega_2'(\vec{\zeta},\omega) + O(\varepsilon^2) \tag{6.12}$$

and then to write (cf. eqs. (6.3) and (6.7)):

$$F(\vec{\zeta},\omega,\varepsilon) = F_1(\vec{\zeta},\omega) + \varepsilon\, F_2(\vec{\zeta},\omega) + O(\varepsilon^2) \tag{6.13a}$$

$$\tilde{F}' \equiv F(\vec{z},\omega',\varepsilon) = F_1(\vec{\zeta},\omega') + \varepsilon[F_2(\vec{\zeta},\omega') + (\mu_1)_1(\vec{\zeta},\omega) \frac{\partial}{\partial \zeta_1} F_1(\vec{\zeta},\omega')$$

$$+ (\mu_4)_1(\vec{\zeta},\omega) \frac{\partial}{\partial \zeta_4} F_1(\vec{\zeta},\omega')] + O(\varepsilon^2) \tag{6.13b}$$

and, writing each $F_j(\vec{\zeta},\omega')$ in terms of a Taylor's series about $\omega' = \omega_1'(\vec{\zeta},\omega)$:

$$F_j(\vec{\zeta},\omega') = F_j(\vec{\zeta},\omega_1') + (\omega'-\omega_1') \frac{\partial F_j(\vec{\zeta},\omega_1')}{\partial \omega_1'}$$

$$+ \frac{(\omega'-\omega_1')^2}{2!} \frac{\partial^2 F_j(\vec{\zeta},\omega_1')}{\partial \omega_1'^2} + \cdots$$

one obtains (6.13b) in the form (with use of (6.12)):

$$\tilde{F}' \equiv F(\vec{z},\omega',\varepsilon) = F_1(\vec{\zeta},\omega_1') + \varepsilon[\omega_2'(\vec{\zeta},\omega) \frac{\partial F_1(\vec{\zeta},\omega_1')}{\partial \omega_1'} + F_2(\vec{\zeta},\omega_1')$$

$$+ (\mu_1)_1(\vec{\zeta},\omega) \frac{\partial}{\partial \zeta_1} F_1(\vec{\zeta},\omega_1') + (\mu_4)_1(\vec{\zeta},\omega) \frac{\partial}{\partial \zeta_4} F_1(\vec{\zeta},\omega_1')] + O(\varepsilon^2) \tag{6.13c}$$

As a corollary of (6.13c) one may also write

$$\left(\frac{\widetilde{\partial F}}{\partial \omega}\right)' \equiv \frac{\partial F(\vec{z},\omega',\varepsilon)}{\partial \omega'} = \frac{\partial F_1(\vec{\zeta},\omega_1')}{\partial \omega_1'} + \varepsilon \left[\frac{\partial F_2(\vec{\zeta},\omega_1')}{\partial \omega_1'} + \omega_2'(\vec{\zeta},\omega) \frac{\partial^2 F_1(\vec{\zeta},\omega_1')}{\partial \omega_1'^2}\right. \tag{6.13d}$$

$$\left. + (\mu_1)_1(\vec{\zeta},\omega) \frac{\partial}{\partial \zeta_1}\left(\frac{\partial F_1(\vec{\zeta},\omega_1')}{\partial \omega_1'}\right) + (\mu_4)_1(\vec{\zeta},\omega) \frac{\partial}{\partial \zeta_4}\left(\frac{\partial F_1(\vec{\zeta},\omega_1')}{\partial \omega_1'}\right)\right] + O(\varepsilon^2)$$

Note that, for any function $G(\vec{\zeta},\omega_1')$ in these expressions, one may write

$$\frac{\partial G(\vec{\zeta},\omega_1')}{\partial \omega_1'} = \frac{\left(\frac{\partial G[\vec{\zeta},\omega_1'(\vec{\zeta},\omega)]}{\partial \omega}\right)}{\left(\frac{\partial \omega_1'(\vec{\zeta},\omega)}{\partial \omega}\right)} \tag{6.14}$$

For collision model IIIa, the terms in (6.12), from (4.108), are

$$\omega_1'(\vec{\zeta},\omega) = \frac{\omega}{|\omega|}[1-A_1(\vec{\zeta},\omega)]\left\{[1-A_1(\vec{\zeta},\omega)]^2 + \frac{1-\omega^2}{\omega^2}\right\}^{-\frac{1}{2}} \tag{6.15a}$$

$$\omega_2'(\vec{\zeta},\omega) = \frac{\omega_1'(\vec{\zeta},\omega)A_2(\vec{\zeta},\omega)}{1-A_1(\vec{\zeta},\omega)}\left\{\left[(1-A_1^2) + \frac{1-\omega^2}{\omega^2}\right]^{-1} - 1\right\} \tag{6.15b}$$

where the expansion

$$A(\vec{\zeta},\omega,\varepsilon) = A_1(\vec{\zeta},\omega) + \varepsilon A_2(\vec{\zeta},\omega) + O(\varepsilon^2) \tag{6.16}$$

has been used. The expression for $\overline{Z}_{IIIa}$ from (4.109), combined with (4.108), is

$$\overline{Z}_{IIIa}(\vec{\zeta},\omega,\varepsilon) = \frac{\omega'(\vec{\zeta},\omega,\varepsilon)}{\omega[1-A(\vec{\zeta},\omega,\varepsilon)]\left|1-\omega^2 A(\vec{\zeta},\omega,\varepsilon)\right|} \tag{6.17}$$

With the expansion of (6.17) given in (6.5b), one finds

$$\bar{Z}_1(\vec{\zeta},\omega) = \frac{\omega_1'(\vec{\zeta},\omega)}{\omega[1-A_1(\vec{\zeta},\omega)]\left|1-\omega^2 A_1(\vec{\zeta},\omega)\right|} \tag{6.18a}$$

$$\bar{Z}_2(\vec{\zeta},\omega) = \bar{Z}_1(\vec{\zeta},\omega)\left[\frac{\omega_2'(\vec{\zeta},\omega)}{\omega_1'(\vec{\zeta},\omega)} + \frac{A_2(\vec{\zeta},\omega)}{1-A_1(\vec{\zeta},\omega)} + \frac{\omega^2 A_2(\vec{\zeta},\omega)}{1-\omega^2 A_1(\vec{\zeta},\omega)}\right]$$

or, with use of (6.15),

$$\bar{Z}_2(\vec{\zeta},\omega) = \frac{\bar{Z}_1(\vec{\zeta},\omega)A_2(\vec{\zeta},\omega)}{1-A_1(\vec{\zeta},\omega)}\left[\frac{\omega^2}{\omega^2(1-A_1)^2+1-\omega^2} + \frac{\omega^2(1-A_1)}{1-\omega^2 A_1}\right] \tag{6.18b}$$

From the definition in (4.110) one finds, upon using the appropriate expansions,

$$A(\vec{\zeta},\omega,\varepsilon) = 0 + \varepsilon\left[\frac{\partial\bar{\rho}_1(\vec{\zeta},\omega)/\partial\omega}{\partial\bar{J}_1(\vec{\zeta},\omega)/\partial\omega}\right]\left[\frac{\bar{J}_1(\vec{\zeta},1)}{\bar{\rho}_1(\vec{\zeta},1)}\right]\left[\frac{(\mu_1)_1(\vec{\zeta},\omega)}{\bar{J}_1(\vec{\zeta},1)}\ \frac{\partial\bar{J}_1(\vec{\zeta},1)}{\partial\zeta_1}\right.$$

$$+ \frac{(\mu_4)_1(\vec{\zeta},\omega)}{\bar{J}_1(\vec{\zeta},1)}\ \frac{\partial\bar{J}_1(\vec{\zeta},1)}{\partial\zeta_1} - \frac{(\mu_1)_1(\vec{\zeta},\omega)}{\bar{\rho}_1(\vec{\zeta},1)}\ \frac{\partial\bar{\rho}_1(\vec{\zeta},1)}{\partial\zeta_1}$$

$$\left. - \frac{(\mu_4)_1(\vec{\zeta},\omega)}{\bar{\rho}_1(\vec{\zeta},1)}\ \frac{\partial\bar{\rho}_1(\vec{\zeta},1)}{\partial\zeta_4}\right] + O(\varepsilon^2) \tag{6.19a}$$

$$= A_1(\vec{\zeta},\omega) + \varepsilon\, A_2(\vec{\zeta},\omega) + O(\varepsilon^2) \tag{6.19b}$$

The vanishing of the first term in (6.19a), its consequences, and a remedy are discussed below in § 6.3.

In the following, denote by superscript ( )" a function of $\vec{\zeta}$ and ω with ω replaced by ω_1' ; that is

$$F'' \equiv F(\vec{\zeta},\omega_1') \tag{6.20}$$

Then, in terms of the above expansion forms ((6.13) with (6.10)), equations (4.97) become:

$$\varepsilon\left(\frac{\partial^2\overline{\rho}_1}{\partial\zeta_4\partial\omega} + \frac{\partial^2\overline{J}_1}{\partial\zeta_1\partial\omega}\right) + \varepsilon^2\left(\frac{\partial^2\overline{\rho}_2}{\partial\zeta_4\partial\omega} + \frac{\partial^2\overline{J}_2}{\partial\zeta_1\partial\omega}\right) + O(\varepsilon^3)$$

$$= {}^{(0)}\overline{Z}_1 H_1'' \frac{\partial\overline{\rho}_1''}{\partial\omega_1'} - H_1\frac{\partial\overline{\rho}_1}{\partial\omega} + \varepsilon\left\{{}^{(0)}\overline{Z}_1 H_1''\left[\frac{\partial\overline{\rho}_2''}{\partial\omega_1'} + \omega_2'\frac{\partial^2\overline{\rho}_1''}{\partial\omega_1'^2}\right.\right.$$

$$\left. + (\mu_1)_1\frac{\partial^2\overline{\rho}_1''}{\partial\zeta_1\partial\omega_1'} + (\mu_4)_1\frac{\partial^2\overline{\rho}_1''}{\partial\zeta_4\partial\omega_1'}\right] + {}^{(0)}\overline{Z}_1\frac{\partial\overline{\rho}_1''}{\partial\omega_1'}\left[H_2'' + \omega_2'\frac{\partial H_1''}{\partial\omega_1'}\right.$$

$$\left. + (\mu_1)_1\frac{\partial H_1''}{\partial\zeta_1} + (\mu_4)_1\frac{\partial H_1''}{\partial\zeta_4}\right] + {}^{(0)}\overline{Z}_2 H_1''\frac{\partial\overline{\rho}_1''}{\partial\omega_1'} - H_1\frac{\partial\overline{\rho}_2}{\partial\omega}$$

$$\left. - H_2\frac{\partial\overline{\rho}_1}{\partial\omega}\right\} + O(\varepsilon^2) \tag{6.21a}$$

$$\varepsilon\left(\frac{\partial^2\overline{J}_1}{\partial\zeta_4\partial\omega} + \frac{\partial^2\overline{P}_1}{\partial\zeta_1\partial\omega}\right) + \varepsilon^2\left(\frac{\partial^2\overline{J}_2}{\partial\zeta_4\partial\omega} + \frac{\partial^2\overline{P}_2}{\partial\zeta_1\partial\omega}\right) + O(\varepsilon^3)$$

$$= {}^{(1)}\overline{Z}_1 H_1''\frac{\partial\overline{J}_1''}{\partial\omega_1'} - H_1\frac{\partial\overline{J}_1}{\partial\omega} + \varepsilon\left\{{}^{(1)}\overline{Z}_1 H_1''\left[\frac{\partial\overline{J}_2''}{\partial\omega_1'} + \omega_2'\frac{\partial^2\overline{J}_1''}{\partial\omega_1'^2}\right.\right.$$

$$\left. + (\mu_1)_1\frac{\partial^2\overline{J}_1''}{\partial\zeta_1\partial\omega_1'} + (\mu_4)_1\frac{\partial^2\overline{J}_1''}{\partial\zeta_1\partial\omega_1'}\right] + {}^{(1)}\overline{Z}_1\frac{\partial\overline{J}_1''}{\partial\omega_1'}\left[H_2'' + \omega_2'\frac{\partial H_1''}{\partial\omega_1'}\right.$$

$$\left. + (\mu_1)_1\frac{\partial H_1''}{\partial\zeta_1} + (\mu_4)_1\frac{\partial H_1''}{\partial\zeta_4}\right] + {}^{(1)}\overline{Z}_2 H_1''\frac{\partial\overline{J}_1''}{\partial\omega_1'} - H_1\frac{\partial\overline{J}_2}{\partial\omega} - H_2\frac{\partial\overline{J}_1}{\partial\omega}\left.\right\} + O(\varepsilon^2) \tag{6.21b}$$

$$\varepsilon\left(\frac{\partial^2\overline{E}_1}{\partial\zeta_4\partial\omega}+\frac{\partial^2\overline{Q}_1}{\partial\zeta_1\partial\omega}\right)+\varepsilon^2\left(\frac{\partial^2\overline{E}_1}{\partial\zeta_4\partial\omega}+\frac{\partial^2\overline{Q}_1}{\partial\zeta_1\partial\omega}\right)+O(\varepsilon^3)$$

$$=\ {}^{(2)}\overline{Z}_1H_1''\frac{\partial\overline{E}_1''}{\partial\omega_1'}-H_1\frac{\partial\overline{E}_1}{\partial\omega}+\varepsilon\Bigg\{{}^{(2)}\overline{Z}_1H_1''\left[\frac{\partial\overline{E}_2''}{\partial\omega_1'}+\omega_2'\frac{\partial^2\overline{E}_1''}{\partial\omega_1'^2}\right.$$

$$\left.+(\mu_1)_1\frac{\partial^2\overline{E}_1''}{\partial\zeta_1\partial\omega_1'}+(\mu_4)_1\frac{\partial^2\overline{E}_1''}{\partial\zeta_4\partial\omega_1'}\right]+{}^{(2)}\overline{Z}_1\frac{\partial\overline{E}_1''}{\partial\omega_1'}\left[H_2''+\omega_2'\frac{\partial H_1''}{\partial\omega_1'}\right.$$

$$\left.+(\mu_1)_1\frac{\partial H_1''}{\partial\zeta_1}+(\mu_4)_1\frac{\partial H_1''}{\partial\zeta_4}\right]+{}^{(2)}\overline{Z}_2H_1''\frac{\partial\overline{E}_1''}{\partial\omega_1'}-H_1\frac{\partial\overline{E}_2}{\partial\omega}$$

$$-H_2\frac{\partial\overline{E}_1}{\partial\omega}\Bigg\}+O(\varepsilon^2) \qquad (6.21c)$$

and

$$\frac{\partial\overline{E}_1}{\partial\omega}+\varepsilon\frac{\partial\overline{E}_2}{\partial\omega}+O(\varepsilon^2)=\frac{1}{2\omega^2}\frac{\partial\overline{P}_1}{\partial\omega}+\varepsilon\frac{1}{2\omega^2}\frac{\partial\overline{P}_2}{\partial\omega}+O(\varepsilon^2) \qquad (6.21d)$$

The macroscopic conservation equations, in the form of equations (4.97) for one-dimensional flow, become:

$$\left[\frac{\partial\overline{\rho}_1(\vec{\zeta},1)}{\partial\zeta_4}+\frac{\partial\overline{J}_1(\vec{\zeta},1)}{\partial\zeta_1}\right]+\varepsilon\left[\frac{\partial\overline{\rho}_2(\vec{\zeta},1)}{\partial\zeta_4}+\frac{\partial\overline{J}_2(\vec{\zeta},1)}{\partial\zeta_1}\right]+O(\varepsilon^2)=0 \qquad (6.22a)$$

$$\left[\frac{\partial\overline{J}_1(\vec{\zeta},1)}{\partial\zeta_4}+\frac{\partial\overline{P}_1(\vec{\zeta},1)}{\partial\zeta_1}\right]+\varepsilon\left[\frac{\partial\overline{J}_2(\vec{\zeta},1)}{\partial\zeta_4}+\frac{\partial\overline{P}_2(\vec{\zeta},1)}{\partial\zeta_1}\right]+O(\varepsilon^2)=0 \qquad (6.22b)$$

$$\left[\frac{\partial\overline{E}_1(\vec{\zeta},1)}{\partial\zeta_4}+\frac{\partial\overline{Q}_1(\vec{\zeta},1)}{\partial\zeta_1}\right]+\varepsilon\left[\frac{\partial\overline{E}_2(\vec{\zeta},1)}{\partial\zeta_4}+\frac{\partial\overline{Q}_2(\vec{\zeta},1)}{\partial\zeta_1}\right]+O(\varepsilon^2)=0 \qquad (6.22c)$$

The expansions of the functions ψ, $\psi^{(2)}$, and $\psi^{(3)}$ defined by equations (4.99) for use in the implicit closure equation (4.70a),

representing equations (4.69), are:

$$\psi^{(2)} = \psi_1^{(2)} + \varepsilon\, \psi_2^{(2)} + O(\varepsilon^2)$$

$$= \frac{(\partial\overline{P}_1/\partial\omega)(\partial\overline{\rho}_1/\partial\omega)}{(\partial\overline{J}_1/\partial\omega)^2} \left\{ 1 + \varepsilon \left[\frac{\partial\overline{P}_2/\partial\omega}{\partial\overline{P}_1/\partial\omega} + \frac{\partial\overline{\rho}_2/\partial\omega}{\partial\overline{\rho}_1/\partial\omega} - 2\,\frac{\partial\overline{J}_2/\partial\omega}{\partial\overline{J}_1/\partial\omega} \right] + O(\varepsilon^2) \right\} \tag{6.23a}$$

$$\psi^{(3)} = \psi_1^{(3)} + \varepsilon\, \psi_2^{(3)} + O(\varepsilon^2)$$

$$= \frac{2\omega^2(\partial\overline{Q}_1/\partial\omega)(\partial\overline{\rho}_1/\partial\omega)^2}{(\partial\overline{J}_1/\partial\omega)^3} \left\{ 1 + \varepsilon \left[\frac{\partial\overline{Q}_2/\partial\omega}{\partial\overline{Q}_1/\partial\omega} + 2\,\frac{\partial\overline{\rho}_2/\partial\omega}{\partial\overline{\rho}_1/\partial\omega} - 3\,\frac{\partial\overline{J}_2/\partial\omega}{\partial\overline{J}_1/\partial\omega} \right] + O(\varepsilon^2) \right\} \tag{6.23b}$$

and

$$\psi = \psi_1 + \varepsilon\, \psi_2 + O(\varepsilon^2)$$

$$= \frac{(\partial\overline{P}_1/\partial\omega)^2}{2\omega^2(\partial\overline{Q}_1/\partial\omega)(\partial\overline{J}_1/\partial\omega)} + O(\varepsilon) \tag{6.23c}$$

6.3 A Truncation Scheme by Introduction of an Additional Artificial Parameter, Illustrated in One-Dimensional Flow

As alluded to briefly in § 6.1, an asymptotic expansion in an "artificial parameter" ε may be used in a scheme of successive

approximations in different ways: (a) In a most conventional manner, one may substitute the expansions into the problem and let $\varepsilon \to 0$ successively to obtain equations and boundary conditions for the respective terms of the expansions; or (b) one may let $\varepsilon = 1$ (thus defining the "arbitrary length" in the definition of ε) and suitably truncate the expansions to obtain the solution at each step of the approximation scheme. (An important illustration of one way of using the latter approach is the Chapman-Enskog procedure of kinetic theory; cf. Chapman and Cowling, 1961, Chap. 7; or Grad, 1958, pp. 253, 259-266.)

To circumvent nonuniformities in the mathematical solution in the first approach, it is often necessary to prevent the system of equations from degenerating (e.g., because of elimination of higher order derivatives) in the limit as $\varepsilon \to 0$ by some means such as introducing suitable transformations of variables (see, e.g., Van Dyke, 1964; or Martin, 1967b). For similar purposes, the "suitable truncation" in the second approach above can be taken to be whatever appropriate means prevents the degeneracy.

The second approach, including the "suitable truncation", can be formalized by: leaving the parameter ε in the equations, to aid in ordering the terms, and by introducing another artificial parameter ε' (which in the final analysis will also have the value unity) at appropriate places in the equations; then letting $\varepsilon \to 0$ to obtain an asymptotic solution and at the same time letting $\varepsilon' \to 0$ such that, for example, $\varepsilon'/\varepsilon = 0(1)$ as $\varepsilon \to 0$. This procedure and its motivation are discussed and illustrated in the following treatment of the equations from § 6.2.

Consider first equations (6.3) to (6.23) in which ε is not yet defined. Suppose we used these equations as they stand and let $\varepsilon \to 0$ to obtain an asymptotic solution (i.e., the first approach mentioned above). If we used either collision model I or collision model IIIa (with $\overline{Z}_1$ and $\overline{Z}_2$ found from eqs. (6.15) to (6.19)) in equations (6.21), we would find (for the steady-flow shock-structure problem of Chapter VII) that the first-order term on the right side of each of equations (6.21a,b,c) would vanish identically; and with the resulting set of equations, in the limit as $\varepsilon \to 0$, it would not be possible to obtain variations of the flow variables with the independent variable x because there would

be no way to determine a length scale in this formulation. (Any scale factor on ζ would cancel out.) The only possible solution that would satisfy both upstream and downstream boundary conditions would be discontinuous in x, and a continuous shock-structure solution could not therefore be obtained.

On the other hand, the limit $\varepsilon \to 0$ in equations (6.11) for collision model II would cause the equations to degenerate to lower-order differential equations. The first approximation would then correspond to local-translational-equilibrium flow (with a local-Maxwellian velocity distribution), goverened by the Euler equations of inviscid flow, as found in the Chapman-Enskog procedure, with only a discontinuous shock solution possible for collision model II (as for I and IIIa).

The nonuniform limits described above can then be prevented for collision models II and IIIa as follows:

For collision model II: Arbitrarily divide the left side of each of equations (6.11a,b,c) by ε' and require $\varepsilon'/\varepsilon = 1$ as $\varepsilon \to 0$. (This step is motivated also by the fact that the left-side and right-side terms of the Boltzmann equation are of the same order very near and within a shock; cf. Grad, 1960, p. 117.) By this procedure we obtain the first-order equations as $\varepsilon \to 0$ with $\varepsilon'/\varepsilon = 1$:

$$\frac{\partial^2 \overline{\rho}_1}{\partial \zeta_4 \partial \omega} + \frac{\partial^2 \overline{J}_1}{\partial \zeta_1 \partial \omega} = H_{1e} \frac{\partial \overline{\rho}_{1e}}{\partial \omega} - H_1 \frac{\partial \overline{\rho}_1}{\partial \omega} \tag{6.24a}$$

$$\frac{\partial^2 \overline{J}_1}{\partial \zeta_4 \partial \omega} + \frac{\partial^2 \overline{P}_1}{\partial \zeta_1 \partial \omega} = H_{1e} \frac{\partial \overline{J}_{1e}}{\partial \omega} - H_1 \frac{\partial \overline{J}_1}{\partial \omega} \tag{6.24b}$$

$$\frac{\partial^2 \overline{E}_1}{\partial \zeta_4 \partial \omega} + \frac{\partial^2 \overline{Q}_1}{\partial \zeta_1 \partial \omega} = H_{1e} \frac{\partial \overline{E}_{1e}}{\partial \omega} - H_1 \frac{\partial \overline{E}_1}{\partial \omega} \tag{6.24c}$$

$$\frac{\partial \overline{E}_1}{\partial \omega} = \frac{1}{2\omega^2} \frac{\partial \overline{P}_1}{\partial \omega} \tag{6.24d}$$

where, from equations (4.100), (4.101), and the expansions (6.5),

$$\overline{\omega}_1 \equiv \overline{M}_1 \omega \equiv \sqrt{5/6}\, M_1 \omega \tag{6.25}$$

and

$$\frac{\partial \overline{\rho}_{1e}}{\partial \omega} = \left[\frac{\overline{\rho}_1(\vec{\zeta},1) e^{-\overline{M}_1^2}}{\Pi^{1/2}} \right] \overline{N}(\overline{\omega}_1) \tag{6.26a}$$

$$\frac{\partial \overline{J}_{1e}}{\partial \omega} = \left[\frac{e^{-\overline{M}_1^2}}{\Pi^{1/2}\overline{M}_1^2} \right] \frac{\overline{\omega}_1}{2} \overline{N}'(\overline{\omega}_1) \tag{6.26b}$$

$$\frac{\partial \overline{E}_{1e}}{\partial \omega} = \left[\frac{e^{-\overline{M}_1^2}}{2\,\overline{\rho}_1(\vec{\zeta},1)\Pi^{1/2}\overline{M}_1^2} \right] \frac{1}{4} \overline{N}''(\overline{\omega}_1) \tag{6.26c}$$

where $\overline{M}_1 = \overline{M}_1(\vec{\zeta})$ is given by (4.105b) with subscript 1 on all functions.

For collision model IIIa: Divide the left side of each of equations (6.21a,b,c) by ε' and at the same time divide the right side of equation (6.19a) by ε' (to prevent degeneracy of the collision term); then require $\varepsilon'/\varepsilon = 1$ as $\varepsilon \to 0$. By this procedure the first order equations as $\varepsilon \to 0$ for collision model IIIa are obtained:

$$\frac{\partial^2 \overline{\rho}_1}{\partial \zeta_4 \partial \omega} + \frac{\partial^2 \overline{J}_1}{\partial \zeta_1 \partial \omega} = \overline{Z}_1 H_1'' \frac{\partial \overline{\rho}_1''}{\partial \omega_1'} - H_1 \frac{\partial \overline{\rho}_1}{\partial \omega} \tag{6.27a}$$

$$\frac{\partial^2 \overline{J}_1}{\partial \zeta_4 \partial \omega} + \frac{\partial^2 \overline{P}_1}{\partial \zeta_1 \partial \omega} = \overline{Z}_1 H_1'' \frac{\partial \overline{J}_1''}{\partial \omega_1'} - H_1 \frac{\partial \overline{J}_1}{\partial \omega} \tag{6.27b}$$

$$\frac{\partial^2 \overline{E}_1}{\partial \zeta_4 \partial \omega} + \frac{\partial^2 \overline{Q}_1}{\partial \zeta_1 \partial \omega} = \overline{Z}_1 H_1'' \frac{\partial \overline{E}_1''}{\partial \omega_1'} - H_1 \frac{\partial \overline{E}_1}{\partial \omega} \tag{6.27c}$$

$$\frac{\partial \overline{E}_1}{\partial \omega} = \frac{1}{2\omega^2} \frac{\partial \overline{P}_1}{\partial \omega} \tag{6.27d}$$

where $\omega' = \omega_1'(\vec{\zeta},\omega)$ is given by (6.15a), $\overline{Z}_1 = \overline{Z}_1(\vec{\zeta},\omega)$ is given by (6.18a), in which A_1, from equations (6.19), becomes

$$A_1(\vec{\zeta},\omega) = \left(\frac{\partial\overline{\rho}_1/\partial\omega}{\partial\overline{J}_1/\partial\omega}\right)\left[\frac{\overline{J}_1(\vec{\zeta},1)}{\overline{\rho}_1(\vec{\zeta},1)}\right]\left[\frac{(\mu_1)_1}{\overline{J}_1(\vec{\zeta},1)}\frac{\partial\overline{J}_1(\vec{\zeta},1)}{\partial\zeta_1} + \frac{(\mu_4)_1}{\overline{J}_1(\vec{\zeta},1)}\frac{\partial\overline{J}_1(\vec{\zeta},1)}{\partial\zeta_4}\right.$$
$$\left. - \frac{(\mu_1)_1}{\overline{\rho}_1(\vec{\zeta},1)}\frac{\partial\overline{\rho}_1(\vec{\zeta},1)}{\partial\zeta_1} - \frac{(\mu_4)_1}{\overline{\rho}_1(\vec{\zeta},1)}\frac{\partial\overline{\rho}_1(\vec{\zeta},1)}{\partial\zeta_4}\right] \qquad (6.28)$$

and where $(\mu_1)_1$ and $(\mu_4)_1$ are given by (6.10).

For either collision model II or collision model IIIa, the systems of equations (6.24) or (6.27) are closed by

$$\psi_1^{(2)} = \Psi(\psi_1) \qquad (6.29a)$$

where

$$\psi_1 \equiv (\psi_1^{(2)})^2/\psi_1^{(3)} \qquad (6.29b)$$

and where ψ_1, $\psi_1^{(2)}$, and $\psi_1^{(3)}$ are the first terms in (6.23). Also imposed are the conditions from macroscopic conservation of mass, momentum, and energy (from (6.22)):

$$\frac{\partial}{\partial\zeta_4}\overline{\rho}_1(\vec{\zeta},1) + \frac{\partial}{\partial\zeta_1}\overline{J}_1(\vec{\zeta},1) = 0 \qquad (6.30a)$$

$$\frac{\partial}{\partial\zeta_4}\overline{J}_1(\vec{\zeta},1) + \frac{\partial}{\partial\zeta_1}\overline{P}_1(\vec{\zeta},1) = 0 \qquad (6.30b)$$

$$\frac{\partial}{\partial\zeta_4}\overline{E}_1(\vec{\zeta},1) + \frac{\partial}{\partial\zeta_1}\overline{Q}_1(\vec{\zeta},1) = 0 \qquad (6.30c)$$

For a given problem in one-dimensional flow, these equations would of course have additional initial and boundary conditions in the $\vec{\zeta}$ domain, as well as the conditions at $\omega = -1$ (cf. § 4.4):

$$\overline{\rho}_1(\vec{\zeta},-1) = \overline{J}_1(\vec{\zeta},-1) = \overline{P}_1(\vec{\zeta},-1) = \overline{E}_1(\vec{\zeta},-1) = \overline{Q}_1(\vec{\zeta},-1) = 0 \qquad (6.31)$$

Recall that $\omega \equiv \cos \varphi$, $\omega' \equiv \cos \varphi'$, and that

$$\zeta_1 \equiv x_1/L \qquad \text{and} \qquad \zeta_4 \equiv u_\alpha t/L$$

where (with $\varepsilon' = \varepsilon = 1$) $L = u_\alpha/\theta_\alpha$. In a given problem, H_1 and θ_α would be suitably determined as discussed in §§ 4.1.2 and 4.3.3. For example if equation (4.85a) is used, then from (4.92a): $H_1 = H_1(\vec{\zeta}) = \bar{\rho}_1(\vec{\zeta},1)$.

Recall also now that the above procedure has simply constituted a formal means for truncating the equations to obtain a nondegenerate first approximation, and that actually $\varepsilon' = \varepsilon = 1$. Just as the initial introduction of the arbitrary length L was a convenient artifice, so also is the introduction of ε', to obtain a first-order system of equations that is nondegenerate. We take it to be significant that the form of the above first-order equations is very similar to the original unexpanded equations in § 4.4.2. The expansion process and the truncation scheme have simplified the first term on the right side of the directional equations of change in the first approximation and have provided a means for obtaining higher approximations. The utility of higher order solutions by this scheme may be limited in a manner similar to that in which the Burnett equations, and higher order equations, are limited in the Chapman-Enskog method (see Grad 1963, p. 149; or Vincenti and Kruger 1965, pp. 416-418). However, in view of the very recent findings by Khosla (1967) that nonuniformities in the Chapman-Enskog expansion are artificial, and are removable by use of Lighthill's technique (1949, 1961) with the extension by Kuo (magnification of the independent variable; see Tsien 1956), the present higher-order solutions may be expected to be valid (see further discussion below).

Although this method is certainly not equivalent to the Chapman-Enskog procedure, there are similarities that can aid understanding of some aspects of this method with sufficient prior understanding of the Chapman-Enskog procedure. (Substantial understanding of the Chapman-Enskog procedure can be gleaned from the discussions by Chapman and Cowling, 1961; Grad, 1958, 1963; or Vincenti and Kruger, 1965; on the respective pages of those works referred to earlier in this section.)

Conversely, because of similarities, understanding of the present method may also contribute to understanding some aspects of the Chapman-Enskog procedure. The most striking similarity between the present method and the Chapman-Enskog procedure is the occurrence of successively higher derivatives in the higher approximations, which are seen to occur here directly by introduction of the Lagrange-expansion perturbation scheme, developed in Chapter V above, into the formulation of the equations of the directional-mean-free-path method. (However, Khosla, 1967, finds that use of the PLK method eliminates the higher derivatives in the Chapman-Enskog expansion. Similarly, in the higher order terms in the present method, the higher derivatives are only those of previously-determined lower-order-approximation functions; so there is no increased number of boundary conditions required.)

The first approximation in the Chapman-Enskog procedure (resulting in the Euler equations of inviscid flow) would correspond to the method described here in the first approximation if we did not introduce $\varepsilon' = \varepsilon$ into the equations, as described above. The second approximation in the Chapman-Enskog procedure (first translational-nonequilibrium correction to the local Maxwellian distribution function, or to the Euler equations) yields the Navier-Stokes equations. The mathematical mechanism by which the higher order approximations in the Chapman-Enskog method eliminate the degeneracy, and hence the discontinuous solutions of the first (Euler) approximation, is described by Grad (1960), p. 119.

In the present procedure, the use of the truncation scheme with $\varepsilon' = \varepsilon$ gives a nondegenerate solution in the first approximation, and so is fundamentally different from the Chapman-Enskog procedure in that respect. The first nonequilibrium approximation here is not a correction to local translational equilibrium. It is suggested therefore that it may be capable of describing the flow approximately, but realistically, for arbitrarily large deviations from local translational equilibrium, which the Navier-Stokes equations can not.

CHAPTER VII

AN ILLUSTRATION:

PROBLEM OF SHOCK-WAVE STRUCTURE

7.1 Introductory Remarks

As an illustration of the method developed above, consider the equations in § 6.3, for the first approximation in the directional-mean-free-path method, applied to one-dimensional steady flow through a normal shock wave in a perfect (sufficiently rarefied) gas composed of neutral spherically-symmetric monatomic molecules.

Since this chapter is not intended as a thorough study of the shock-structure problem, but only as an illustration of the method, the reader is referred to works such as: Lighthill (1956), Hayes (1960), Vincenti and Kruger (1965), Sherman and Talbot (1960), and Talbot (1962) for comprehensive treatments and further references on shock-wave structure.

The conditions at upstream infinity $(x_1 = -\infty)$ are denoted by subscript α, those at downstream infinity $(x_1 = +\infty)$ by subscript β. Since there is only one component of particular interest in one-dimensional steady flow, we drop the subscript 1 corresponding to the direction x_1 and denote the dimensionless coordinate ζ_1 (with $\varepsilon = 1$) as

$$\zeta = (\theta_\alpha / u_\alpha) x \tag{7.1}$$

where u is the macroscopic average velocity in the $+x$ direction, and θ_α is the upstream collision frequency, which could be represented, for example, by equation (2.20b) with (2.23d). Thus

$$\frac{u_\alpha}{\theta_\alpha} = \frac{m}{(8\pi)^{1/2} \sigma^2 \rho_\alpha} \sqrt{\frac{\gamma}{2}} \, M_\alpha \tag{7.2a}$$

for use in equation (7.1) if desired, where m is the mass of a molecule, σ is an "effective molecular diameter" (see § 2.2.2 above), $\gamma(=5/3)$ is the ratio of specific heats, and M_α is the upstream Mach number. It is also convenient, for comparison with other results, to find the results simply in terms of x/λ_α (e.g., see Vincenti and Kruger, 1965, sec. X-9). Thus from (2.21) and (2.23d):

$$u_\alpha/\theta_\alpha = (1/2)\pi^{1/2}\,\lambda_\alpha(\gamma/2)^{1/2}\,M_\alpha \tag{7.2b}$$

where $\gamma = 5/3$, so that (7.1) may be written

$$\frac{x}{\lambda_\alpha} = \frac{\pi^{1/2}}{2}\left(\sqrt{\frac{5}{6}}\,M_\alpha\right)\zeta \,. \tag{7.3}$$

where λ_α is the upstream mean free path relative to the mean mass motion (cf. Chap. II).

In the following sections of this chapter, use is made of equation (4.85b), with (4.92a) and (6.5), to represent the function H_1 as

$$H_1 = H_1(\zeta) = \bar{H}_1(\zeta)\Big/K_1(T) \tag{7.4a}$$

where

$$K_1(T) = \left(\frac{T}{\eta(T)}\,\frac{\eta_\alpha}{T_\alpha}\right)^{-1}; \qquad \bar{H}_1(\zeta) \equiv \bar{\rho}_1(\zeta,1) \tag{7.4b}$$

and where η is a specified temperature-dependent viscosity coefficient. It is also convenient to define

$$\bar{\zeta} \equiv -\int_{\zeta^*}^{\zeta} [1/K_1(T)]\,d\zeta \tag{7.4c}$$

where ζ^* is some value of ζ, to be defined later. Directional-average collision models II and IIIa are considered, and a numerical solution scheme is outlined for collision model II.

7.2 Equations and Boundary Conditions

For simplicity, in the following we denote partial derivatives with respect to ω by subscript ω. Since H_1, as represented by equations (7.4), does not depend on ω, equations (6.24) for collision model II are written for steady flow as:

$$K_1 \frac{\partial}{\partial \zeta}(\bar{J}_{1\omega}) = -\frac{\partial}{\partial \bar{\zeta}}(\bar{J}_{1\omega}) = \bar{H}_1[\bar{\rho}_{1e\omega} - \bar{\rho}_{1\omega}] \tag{7.5a}$$

$$K_1 \frac{\partial}{\partial \zeta}(\bar{P}_{1\omega}) = -\frac{\partial}{\partial \bar{\zeta}}(\bar{P}_{1\omega}) = \bar{H}_1[\bar{J}_{1e\omega} - \bar{J}_{1\omega}] \tag{7.5b}$$

$$K_1 \frac{\partial}{\partial \zeta}(2\bar{Q}_{1\omega}) = -\frac{\partial}{\partial \bar{\zeta}}(2\bar{Q}_{1\omega}) = \bar{H}_1[2\bar{E}_{1e\omega} - 2\bar{E}_{1\omega}] \tag{7.5c}$$

$$2\bar{E}_{1\omega} = \frac{1}{\omega^2}\bar{P}_{1\omega} \tag{7.5d}$$

where $\bar{\rho}_{1e\omega}$, $\bar{J}_{1e\omega}$, and $\bar{E}_{1e\omega}$ are given by equations (6.26) with (6.25). Note now that equations (7.5a,b,c) are directly integrable to obtain

$$K_1 \frac{\partial}{\partial \zeta}(\bar{J}_1) = -\frac{\partial}{\partial \bar{\zeta}}(\bar{J}_1) = \bar{H}_1[\bar{\rho}_{1e} - \bar{\rho}_1] \tag{7.5e}$$

$$K_1 \frac{\partial}{\partial \zeta}(\bar{P}_1) = -\frac{\partial}{\partial \bar{\zeta}}(\bar{P}_1) = \bar{H}_1[\bar{J}_{1e} - \bar{J}_1] \tag{7.5f}$$

$$K_1 \frac{\partial}{\partial \zeta}(2\bar{Q}_1) = -\frac{\partial}{\partial \bar{\zeta}}(2\bar{Q}_1) = \bar{H}_1[2\bar{E}_{1e} - 2\bar{E}_1] \tag{7.5g}$$

where $\bar{\rho}_{1e}$, $\bar{J}_{1e}$, and $\bar{E}_{1e}$ are given by equations (4.102) with ρ/ρ_α replaced by $\bar{H}_1$ and subscript 1 on $\bar{M}$ and $\bar{\omega}$ (cf. eq. (6.26)).

For collision model III equations (6.27) become, for steady flow,

$$K_1 \frac{\partial}{\partial \zeta}(\bar{J}_{1\omega}) = -\frac{\partial}{\partial \bar{\zeta}}(\bar{J}_{1\omega}) = \bar{H}_1[\bar{Z}_1 \bar{\rho}''_{1\omega_1'} - \bar{\rho}_{1\omega}] \tag{7.6a}$$

$$K_1 \frac{\partial}{\partial \zeta} (\overline{P}_{1\omega}) = -\frac{\partial}{\partial \overline{\zeta}} (\overline{P}_{1\omega}) = \overline{H}_1 [\overline{Z}_1 \overline{J}''_{1\omega_1'} - \overline{J}_{1\omega}] \tag{7.6b}$$

$$K_1 \frac{\partial}{\partial \zeta} (2\overline{Q}_{1\omega}) = -\frac{\partial}{\partial \overline{\zeta}} (2\overline{Q}_{1\omega}) = \overline{H}_1 [\overline{Z}_1 2\overline{E}''_{1\omega_1'} - 2\overline{E}_{1\omega}] \tag{7.6c}$$

$$2\overline{E}_{1\omega} = (1/\omega^2)\, \overline{P}_{1\omega} \tag{7.6d}$$

where $\omega_1' = \omega_1'(\zeta,\omega)$ is given by (6.15a) and $\overline{Z}_1 = \overline{Z}_1(\zeta,\omega)$ is given by (6.18a), where A_1 is given by (6.28) (which is considerably simplified by conditions given below).

With equation (7.4), either equations (7.5a) to (7.5d) or equations (7.6) provide four differential equations for the five unknown functions of ζ and ω : $\overline{\rho}_1$, $\overline{J}_1$, $\overline{P}_1$, $\overline{E}_1$, and $\overline{Q}_1$. The needed fifth equation (the "closure equation") is provided by equations (6.29), obtained from equations (4.70) (which represent (4.69)), in the form:

$$\psi_1^{(2)} \equiv \overline{P}_{1\omega}\, \overline{\rho}_{1\omega} \Big/ (\overline{J}_{1\omega})^2 = \Psi(\psi_1) \tag{7.7a}$$

where

$$\psi_1 \equiv (\psi_1^{(2)})^2 \Big/ \psi_1^{(3)} \equiv (P_{1\omega})^2 \Big/ 2\omega^2\, \overline{Q}_{1\omega}\, \overline{J}_{1\omega} \tag{7.7b}$$

A sufficient number of boundary conditions on the dependent variables in ω and ζ must be provided.

<u>At $\omega = -1$ (all ζ)</u>, the functions $\overline{\rho}_1$, $\overline{J}_1$, $\overline{P}_1$, $\overline{E}_1$, and $\overline{Q}_1$ vanish identically (eqs. (6.31)).

<u>At $\omega = +1$ (all ζ)</u>, equations (6.30), with use of equations (4.92) and (4.60), give, in the first approximation

$$\left.\begin{aligned} \overline{J}_1(\zeta,1) &= (1/\rho_\alpha u_\alpha)(\rho u) = \text{constant} \\ &= \overline{J}_1(-\infty,1) = 1 \end{aligned}\right\} \tag{7.8a}$$

$$\left.\begin{aligned} \overline{P}_1(\zeta,1) &= (1/\rho_\alpha u_\alpha^2)(\rho u^2 + p - \tau) = \text{constant} \\ &= \overline{P}_1(-\infty,1) = 1 + 3/5\, M_\alpha^2 \end{aligned}\right\} \quad (7.8b)$$

$$\left.\begin{aligned} 2\overline{Q}_1(\zeta,1) &= (2/\rho_\alpha u_\alpha^3)[\rho u(h + \tfrac{1}{2}u^2) + q - u\tau] = \text{constant} \\ &= 2\overline{Q}_1(-\infty,1) = 1 + 3/M_\alpha^2 \end{aligned}\right\} \quad (7.8c)$$

Note that the usual forms of the exact one-dimensional steady-flow conservation equations are contained in equations (7.8a,b,c) and that their evaluation at $x = \pm\infty$, where q and τ vanish, gives the well-known Rankine-Hugoniot equations:

$$\left.\begin{aligned} \rho_\alpha u_\alpha &= \rho_\beta u_\beta \\ \rho_\alpha u_\alpha^2 + p_\alpha &= \rho_\beta u_\beta^2 + p_\beta \\ h_\alpha + \tfrac{1}{2}u_\alpha^2 &= h_\beta + \tfrac{1}{2}u_\beta^2 \end{aligned}\right\} \quad (7.9)$$

For the perfect monatomic gas, with specific heat ratio of 5/3, one can obtain from equations (7.9) (see, e.g., Liepmann and Roshko, 1957, pp. 56-59):

$$M_\beta^2 = \frac{3+M_\alpha^2}{5\,M_\alpha^2-1} \quad (7.10a)$$

$$\rho_\beta/\rho_\alpha = \frac{4\,M_\alpha^2}{M_\alpha^2+3} = \frac{4}{1 + \dfrac{5/2}{(5/6)M_\alpha^2}} \quad (7.10b)$$

<u>At $\zeta = \pm\infty$ (all ω)</u>, equations (4.102) give the conditions on $\overline{\rho}$, $\overline{J}$, $\overline{P}$, $\overline{E}$, and $\overline{Q}$ in terms of ρ/ρ_α, $\overline{M}$, and $\overline{\omega} = \overline{M}\omega$, where,

$$\left.\begin{aligned} &\text{at} \quad \zeta = -\infty \ : \ M = M_\alpha \\ &\qquad\qquad \rho/\rho_\alpha = 1 \\ &\text{at} \quad \zeta = +\infty \ : \ M = M_\beta \ , \quad \text{given by (7.10a)} \\ &\qquad\qquad \rho/\rho_\alpha = \rho_\beta/\rho_\alpha \ , \quad \text{given by (7.10b)} \end{aligned}\right\} \tag{7.11}$$

With conditions (7.8a) and equation (7.4b) we now note the simplified results from (4.105b) and (6.28):

$$\overline{M}_1 = \sqrt{\frac{5}{6}}\, M_1 = \left[\frac{3/2}{2\overline{E}_1(\zeta,1)\overline{H}_1(\zeta) - 1} \right]^{1/2} \tag{7.12}$$

and

$$A_1 = \frac{1}{\overline{H}_1^3} \frac{d\overline{H}_1}{d\zeta} \tag{7.13}$$

for use, respectively, in (7.5) and (7.6). Equations (4.102) and (7.11) are used in the first approximation simply by putting subscript 1 on $\overline{H}$, $\overline{M}$, and $\overline{\omega}$ (cf. eqs. (6.25) and (6.26)).

7.3 Description of a Solution Procedure for Collision Model II

Since

$$\overline{\rho}_1(\zeta,\omega) = \int_{-1}^{\omega} \overline{\rho}_{1\omega}\, d\omega \tag{7.14a}$$

and

$$\overline{E}_1(\zeta,\omega) = \int_{-1}^{\omega} \overline{E}_{1\omega}\, d\omega \tag{7.14b}$$

we can regard the set of ten equations including: (7.14a,b), (7.5a) to (7.5g), and (7.7a), as a complete set to determine the ten dependent variables:

$$\overline{\rho}_{1\omega} \ , \ \overline{J}_{1\omega} \ , \ \overline{P}_{1\omega} \ , \ \overline{E}_{1\omega} \ , \ \overline{Q}_{1\omega} \ , \ \overline{\rho}_{1} \ , \ \overline{J}_{1} \ , \ \overline{P}_{1} \ , \ \overline{E}_{1} \ , \ \overline{Q}_{1} \qquad (7.15)$$

as functions of ζ and ω (with $\overline{\zeta}(\zeta)$, $\overline{H}_1(\zeta)$, and $\overline{M}_1(\zeta)$ given by (7.4b) and (7.12)). (To avoid, as much as possible, numerical integrations over ω except for equations (7.14), all of equations (7.5) can be treated as independent.) For each value of ω, equations (7.5) can, in fact, then be regarded as a set of seven ordinary differential equations in the ζ direction, with ω as a parameter, and with the needed values of the three quantities $\overline{\rho}_{1\omega}(\zeta,\omega)$, $\overline{\rho}_{1}(\zeta,\omega)$, and $\overline{E}_{1}(\zeta,\omega)$ at each step in ζ calculated respectively from (7.7), (7.14a), and (7.14b) for each ω. Thus, the following numerical solution procedure can be used:

(a) First, for a large number of values of b, compute and store, versus b : $\psi^{(2)}$, $\psi^{(3)}$, and ψ from equations (4.69) through (4.78). The computer program can be designed to interpolate between values in this table to obtain a value of $\psi^{(2)}$ corresponding to any specified value of ψ in the range calculated. This provides the functional relationship (4.70a).

(b) Define $\zeta = 0$ as the location where $\rho = (1/2)(\rho_\alpha + \rho_\beta)$. The numerical integration can be started at a location in ζ where the state of the gas is very nearly that at either upstream infinity ($\zeta = -\infty$) or downstream infinity ($\zeta = +\infty$). The choice appears arbitrary, However, it has previously been found in the Navier-Stokes solution of shock structure that it is easier to integrate from the downstream state to the upstream state rather than vice versa (Gilbarg and Paolucci, 1953), because of a saddle point in the temperature-velocity phase plane. Therefore the integration in the present approach will be started at $\zeta = \zeta^*$ where the state of the gas has a specified arbitrary small deviation from the downstream state. It is presumed that the values of the ten dependent variables in (7.15) can be approximately determined for all ω

from -1 to 1 at $\zeta = \zeta^*$ from the known conditions at downstream infinity (see § 7.3.2 below). The values of $\overline{H}_1$ and $\overline{M}_1$ are then also known from (7.4b) and (7.12), and the local-equilibrium values of all the dependent variables can be computed, for subsequent use in equations (7.5). Then it is convenient to define the new independent variable

$$\overline{\overline{\zeta}} \equiv \zeta^* - \zeta \tag{7.16}$$

so that (cf. eq. (7.4c)):

$$d\overline{\overline{\zeta}}/d\overline{\zeta} = - d\zeta/d\overline{\zeta} = K_1(T) \tag{7.17a}$$

$$\overline{\overline{\zeta}} = \overline{\zeta} = 0 \quad \text{at} \quad \zeta = \zeta^* \qquad \text{(starting point for integration)} \tag{7.17b}$$

and

$$\overline{\overline{\zeta}} = \zeta^* \quad \text{at} \quad \zeta = 0 \qquad \text{(where } \rho = \tfrac{1}{2}(\rho_\alpha + \rho_\beta)\text{)} \tag{7.17c}$$

and the integration proceeds upstream with increasing positive values of $\overline{\zeta}$ (as ζ decreases from ζ^*).

(c) Divide the range $-1 \leq \omega \leq 1$ into an odd number, ℓ, of intervals ($\Delta\omega = 2/\ell$), such that

$$\omega_j = -1 + j\,\Delta\omega = -1 + 2j/\ell\,, \qquad j = 0, 1, 2, \ldots, \ell \tag{7.18}$$

Calculations are to be made at each ω_j, and the specification of ℓ as an odd number insures that no calculations are made at exactly $\omega = 0$ (where there would be numerical difficulties introduced by dividing zero by zero).

(d) Starting at $\overline{\zeta} = 0$ with the known values of the variables in (7.15), increase $\overline{\zeta}$ by $\Delta\overline{\zeta}$. At $\overline{\zeta}_1 = 0 + \Delta\overline{\zeta}$, and at each of the ω_j in (7.18), calculate $\overline{J}_{1\omega}$, $\overline{P}_{1\omega}$, $\overline{Q}_{1\omega}$, $\overline{J}_1$, $\overline{P}_1$, and $\overline{Q}_1$ from equations

(7.5) and from values at $\bar{\zeta} = 0$, using a standard technique for ordinary differential equations. With each value of $\bar{P}_{1\omega}$ calculated, evaluate $\bar{E}_{1\omega}$ from (7.5d). Also, with known $\bar{J}_{1\omega}$, $\bar{P}_{1\omega}$, and $\bar{Q}_{1\omega}$ at each ω, calculate ψ_1 from (7.7b), then find the corresponding $\psi_1^{(2)}$ from the previously-computed relationship between ψ_1 and $\psi_1^{(2)}$ (cf. eq. (7.7a) and step (a) above), and determine $\bar{\rho}_{1\omega}$ from the definition in (7.7a). Finally, determine $\bar{\rho}_1$ and $\bar{E}_1$ at each ω by the integrations indicated in (7.14). Then, again, $\bar{H}_1$ and $\bar{M}_1$ are known from (7.4b) and (7.12), and the local-equilibrium values of all dependent variables are computed for subsequent use in equations (7.5).

(e) At each $\bar{\zeta}$, and at $\omega = 1$, evaluate all flow quantities of interest (to first order) from equations (4.93). Evaluate $\bar{\bar{\zeta}}$ using (7.17a,b).

(f) Increase $\bar{\zeta}$ again by a small increment, and repeat the procedure. Continue the integration until all the quantities no longer vary with increasing $\bar{\zeta}$, so that the upstream equilibrium state has been reached.

(g) Where $\bar{\rho}_1(\zeta,1) = \frac{1}{2}(1 + \rho_\beta/\rho_\alpha)$, evaluate ζ^* (eq. (7.17c)), so that ζ is known versus $\bar{\zeta}$ from (7.16) and x/λ_α is known from (7.3).

The values of the dependent variables at each ω at $\bar{\zeta} = 0$, for starting the numerical integrations, can be evaluated from integrations of the Chapman-Enskog distribution function for a very small deviation from the downstream state. This procedure is simple and straight forward, either in terms of the BGK model or for Maxwell molecules, in combination with the method of Gilbarg and Paolucci (1953) for evaluating flow variables near the downstream state. It is hoped in the future to obtain numerical results for the shock-structure problem by the procedure outlined above.

CHAPTER VIII

CONCLUDING REMARKS

The most important results of this study are considered to be: (a) the development of concepts and equations for the directional level of description; (b) the introduction of the directional-mean-free-path approximation for the collision integrals in the directional equations of change; (c) the development of new forms of vector (higher dimensional) generalizations of Lagrange's expansion, and a perturbation-expansion scheme based on those generalizations; and (d) the outlining of the calculation procedure for shock-wave structure according to the directional-mean-free-path method.

After successful performance of the numerical calculations outlined in Chapter VII for shock-wave structure, it may be desirable in the future to extend this study in the following several directions:

(a) inclusion of the effects of boundaries, in some approximate manner, in the formulation of the general method;

(b) inclusion of body forces in the equations;

(c) calculation of higher order solutions in the shock-structure problem;

(d) attempt to solve the shock-structure problem with collision-model III;

(e) possible extension of the concepts in an approximate manner to polyatomic gases; and

(f) possible extension of the concepts to gas mixtures.

The first extension suggested, (a), probably will be the most important next step in further development of the directional-mean-free-path method. Future application of the method to any problem with boundaries, however simple, will depend on inclusion of the effects of boundaries in the formulation of the directional-mean-free-path approximation. The main

value of the directional-mean-free-path method would therefore be realized only after such an extension of the theory has been made so that it can be applied to problems that may not be tractable by kinetic theory methods.

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