

On the Fundamentals of Extended Thermodynamics (ET) of a One-Dimensional Rarefied Gas

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Extended thermodynamics (ET) of degree r for a one-dimensional rarefied gas based, by definition, on a finite set $A^r = \{a^0, a^2, \dots, a^r\}$ of the first $r-1$ ($3 \leq r$) direct internal moments of the one-point distribution function f is carefully investigated. With the aid of the second axiom of thermodynamics, the new representation for f , depending in a local and nonlinear way on A^r , is explicitly derived. It is demonstrated that in ET of degree r an infinite sequence $\{b^{r+1}, b^{r+2}, \dots\}$ of higher order Hermite coefficients, which normally drops out of Grad's proposition for f fashioned by mathematical apparatus such as the Hermite polynomials, cannot be considered negligible in the case when nonlinear constitutive functions are established. Using Ma's kinetic equation corresponding to a one-dimensional rarefied gas as well as the generalized representation for f , collision productions in the nonconservative moment equations are then calculated for a special choice of the rate of collisions between particles.

KEY WORDS: Extended thermodynamics (ET); one-dimensional rarefied gases; Ma's kinetic equation; hierarchy of moment equations; truncation of the hierarchy; Grad's moment procedure and its generalization.

1. INTRODUCTION

Extended thermodynamics (ET) of rarefied gases, which takes as independent state variables the slow (conservative) quantities plus the fast dissipative fluxes, has been a subject of considerable interest.⁽¹⁻⁴⁾ In Grad's pioneering work^(5,6) a variety of problems were considered—kinetic theory with the one-point distribution function f expanded in terms of Hermite polynomials,⁽⁷⁾ hydrodynamics, ET—as well as a discussion of how these

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somewhat different topics complement each other to make up the rudiments of a well-rounded and unified theory.

Nothing can be more illuminating for ET than a reliable relevant example from the kinetic theory of even a highly simplified model. With this remark in mind, our attention will be directed more particularly to the derivation of extended phenomenological theories within the framework of a restricted class of kinetic equations for one-dimensional rarefied gases—Ma's kinetic equation,⁽⁸⁾ for instance.

In the paper we proceed as follows. On the basis of a suitable contraction of the kinetic equation(s), we arrive in Section 2 at the system of balance equations for a macroscopic velocity v and a finite set $A^r = \{a^0, a^2, \dots, a^r\}$ of the first $r - 1$ ($3 \leq r$) direct internal moments of f . It can readily be verified that the above system of balance equations never closes on itself, so that we must supplement it by constitutive relations constructed in full harmony with the principle of entropy growth.⁽⁹⁾

To this end, given the collision productions $P^n(f)$ ($3 \leq n \leq r$) on the rhs of the deduced equations of transfer, their explicit dependence upon the distribution function suggests first of all Grad's expansion^(5,6) of f about a Maxwellian in terms of a complete set of functions, which are taken to be one-dimensional Hermite polynomials B^m ($3 \leq m$).⁽⁷⁾ Elementary inspection shows that f involves time (t) and space (x) through v , the two conserved moments a^0, a^2 in the local Maxwellian, and the Hermite expansion coefficients b^m ($3 \leq m$).^(5,6) For the convenience of the reader, these standard problems^(5,6) are reconsidered in Section 2 as well.

On transforming the coupled hierarchy of equations of transfer for the state variables A^r of ET of degree r into the thermomechanical system of field equations, we provide a means of singling out appropriate constitutive relations for the flux moment a^{r+1} in the r th hierarchy equation and an infinite sequence of Hermite coefficients in P^n . More specifically, the constitutive functions for excessive unknowns are characterized in the most apparent way by their local and generally nonlinear dependence upon the state variables A^r (Sections 3.1 and 3.2).²

In Sections 3 and 4 the proposed theory affords an example of how to reduce the generality of constitutive assumptions to special ones by demanding their consistency with the second axiom of thermodynamics formulated in the Liu–Müller spirit^(2,11) on one hand and with the fixed class of kinetic equations for one-dimensional rarefied gases on the other. A full list of helpful formulas applicable for the investigations of Section 4.2 is summarized, for the sake of simplicity, in an Appendix.

² Due to the local constitutive assumption (LCA), the principle of material frame indifference^(9,10) does not permit v to play the role of a constitutive variable.

Since ET of isotropic systems, when it is reasonable combined with kinetic arguments, imposes sufficiently stringent restrictions upon the variety of constitutive fields so as to determine them explicitly, actual computation of the *higher order* Hermite coefficients $\{b^{r+1}, b^{r+2}, \dots\}$ in terms of A^r leads automatically to a new moment representation for f . It can be compared and contrasted, if required, with the older one,^(5,6) also fashioned by mathematical apparatus such as the Hermite polynomials.⁽⁷⁾ Different but interrelated forms of the generalized representation are written down in Section 5.1 and utilized (Section 5.2) in order to test independently the expression for the entropy production σ previously deduced on the grounds of macroscopic arguments only (Section 3.1).

In this context, one important remark is of interest. Because, regardless of the collision integral in the kinetic equation for a rarefied gas, we shall always end up with the same one-point distribution function *generating* field equations of ET of degree r , the deduced moment representation regarding f can never be interpreted in this work as a solution—exact or approximate—to the kinetic equation.

In the treatment of ET of degree r , the dominant role of $\{b^{r+1}, b^{r+2}, \dots\}$ in constructing, from the kinetic point of view, nonlinear thermodynamic theories is also carefully recognized (Sections 3.2 and 5.1). Consequently, the excessive higher order coefficients $\{b^{r+1}, b^{r+2}, \dots\}$ can be omitted, as originally in Grad's approach,^(5,6) only in the simplest case of linear ET. This fact constitutes the essential result of the work.

Using Ma's kinetic equation⁽⁸⁾ (Section 6.1) and the generalized representation for f , we then calculate the collision productions P^n in the nonconservative moment equations for a special choice of the rate of collisions between particles; for more details on this subject, see Section 6.2.

One of the main advantages to be gained by considering one-dimensional rarefied gases is an immediate simplification of mathematical details without significantly affecting the basic idea. In passing, the fruitfulness of taking ET of arbitrary order results surprisingly in the additional compatibility conditions between ET of degree r and that of degree $r+1$; they are of interest, as Sections 3.3 and 4.2 demonstrate.

All results proposed can be treated as formally exact.

2. AN EQUATION OF MOTION FOR f AND ITS FINITE HIERARCHY OF MOMENT EQUATIONS

Let us consider a one-dimensional rarefied gas for which each molecule of unit mass is subject to an external force K ; K may be a

function of position x and time t , but not of momentum λ . We start with a kinetic description of the gas by an equation of change

$$\partial_t f + \nabla_x \lambda f + \nabla_z K f = J(f) \quad (2.1)$$

for the one-point distribution function (df) $f(\lambda, x, t)$, where $J(f)$ is the collision integral with the following elementary properties:

$$\int d\lambda J(f) \ln[Cf] \leq 0 \quad (2.2)$$

$$\int d\lambda \mathcal{N}(\lambda) J(f) = 0 \quad \text{for } \mathcal{N}(\lambda) = 1, \lambda, \lambda^2 \quad (2.3)$$

Otherwise, no additional information concerning $J(f)$ is required at present.³

Obviously, Eqs. (2.2)–(2.3) lead to the familiar local entropy inequality

$$\partial_t h + \nabla_x (h v + \Phi) = \sigma \geq 0 \quad (2.4)$$

with the standard kinetic expressions

$$h = - \int d\lambda f \ln[Cf], \quad \Phi = - \int d\lambda \tilde{\lambda} f \ln[Cf], \quad \tilde{\lambda} = \lambda - v \quad (2.5)$$

$$\sigma = - \int d\lambda J(f) \ln[Cf], \quad v = \int d\lambda \lambda f / \int d\lambda f \quad (2.6)$$

for the entropy density h , the entropy flux Φ , the entropy production σ , and the macroscopic velocity v .

The best of several starting points^(12–14) in forming the various phenomenological theories framed by the kinetic equation (2.1) is that initiated by defining the direct internal moments of the df ,

$$a^n(x, t) = \int d\lambda \tilde{\lambda}^n f(\lambda, x, t), \quad n \in \mathbb{N}_0 \setminus \{1\}, \quad \mathbb{N}_0 = \{0, 1, \dots\} \quad (2.7)$$

On the basis of (2.7) and (2.1), we easily arrive at the system

$$\partial_t a^n + \nabla_x (a^n v + a^{n+1}) + n a^n \nabla_x v - \frac{n a^{n-1}}{a^0} \nabla_x a^2 = P^n(f) \quad (2.8a)$$

³ C is a certain constant of no importance in our further considerations.

$$\partial_t v + v \nabla_x v + \frac{1}{a^0} \nabla_x a^2 - K = 0 \tag{2.8b}$$

$$a^{-1} = 0, \quad a^1 = 0, \quad n \in \mathbb{N}_0 \setminus \{1\}, \quad n \leq r, \quad 3 \leq r \tag{2.8c}$$

of balance equations for $A^r = \{a^0, a^2, \dots, a^r\}$ and v , where the quantities

$$P^n(f) = \int d\lambda \tilde{\lambda}^n J(f) \tag{2.9}$$

(depending on x and t through the df) represent collision productions in the nonconservative moment equations; due to (2.3), the necessary conditions

$$P^0 = 0, \quad P^2 = 0 \tag{2.10}$$

are automatically fulfilled.

Such balance equations, which may alternatively be termed equations of transfer, are of interest in this work, both because they constitute the leading postulates of ET of degree r , and also because, as will later appear, their specific structure characterizing one-dimensional rarefied gases, if appropriately combined with the principle of entropy growth,⁽⁹⁾ determines the df explicitly.

A guide for eliminating f from the rhs of (2.8a) and allowing a treatment in the finite hierarchy (of the first r equations of transfer) of the fields that depend on space and time only, as traditionally in continuum physics, was first sketched by Grad.^(5,6) His method, which we adopt in this work, is based from the outset upon an expansion

$$f(\lambda, x, t) = f^M(\lambda, x, t) \left[1 + \sum_{n=3}^{\infty} \frac{1}{n!} b^n(x, t) B^n(\hat{\lambda}) \right] \tag{2.11}$$

of the df around a local Maxwellian

$$f^M = (2\pi)^{-1/2} \alpha a^0 \exp(-\frac{1}{2} \hat{\lambda}^2), \quad \alpha = (a^0/a^2)^{1/2}, \quad \hat{\lambda} = \alpha \tilde{\lambda} \tag{2.12}$$

in terms of the orthonormal Hermite polynomials

$$B^n(\lambda) = (\lambda - \nabla_\lambda)^n \circ 1 \tag{2.13}$$

that, according to Eq. (2.11), are multiplied by the so-called Hermite expansion coefficients

$$b^n = \frac{1}{a^0} \int d\lambda f(\lambda, x, t) B^n(\hat{\lambda}), \quad 3 \leq n \tag{2.14}$$

In this context, supplementary [with respect to (2.14)] notation is also introduced,

$$b^0 = a^0, \quad b^1 = 0, \quad b^2 = a^2 \quad (2.15)$$

Substituting (2.11) into $P^n(f)$ in (2.8a), we are justified in doing the useful transformation

$$P^n(f) \Rightarrow P^n(H_{-1}^r | H_r^{2r} | H_{2r}^\infty) \quad (2.16)$$

where, by definition,

$$H_m^n = \{b^{m+1}, b^{m+2}, \dots, b^n\} \quad (2.17)$$

3. THE ENTROPY INEQUALITY IN THE LIU-MÜLLER SPIRIT

3.1. Lagrange Multipliers

In neither case can the system (2.8) of balance equations serve as field equations for v and the internal state variables A^r , because excessive quantities have appeared, namely the flux moment a^{r+1} in the r th hierarchy equation and, as the transformation rule (2.16) indicates, the Hermite coefficients b^m ($m \in \mathbb{N}_0$). Consequently, these unknowns must be considered as constitutive quantities

$$a^{r+1} = a^{r+1}(A^r), \quad b^m = b^m(A^r), \quad m \in \mathbb{N}_0 \quad (3.1)$$

The local constitutive assumption (LCA) that we adopt in (3.1) implies that a^{r+1} and b^m depend at one point and time upon the values of A^r at that point and time, generally in a nonlinear way. In passing, observe that v drops out of (3.1), because of the LCA and the principle of material frame indifference.⁽⁹⁾

Since in rational thermodynamics^(9,15) the entropy density h and the entropy flux Φ are derivable from A^r in a materially dependent manner, the LCA attached to h and Φ suggests immediately the so-called auxiliary constitutive relations

$$h = h(A^r), \quad \Phi = \Phi(A^r) \quad (3.2)$$

The basic and auxiliary constitutive functions (3.1)–(3.2) should be such as to ensure that the entropy inequality (2.4) is satisfied in every admissible thermodynamic process, i.e., every solution to the field equations compatible with constitutive assumptions.

Due to the fact that Eqs. (2.8a) form constraints for A^r , one can get rid of those constraints by the use of Lagrange multipliers Δ_n^r ($0 \leq n \leq r$, $n \neq 1$); they depend on A^r as well,⁴

$$\Delta_n^r = \Delta_n^r(A^r) \tag{3.3}$$

Liu has shown⁽¹⁶⁾ that the new [with respect to (2.4)] inequality

$$\begin{aligned} \partial_t h + \nabla_x(hv + \Phi) - \sum_{n=0}^r \Delta_n^r \left[\partial_t a^n + \nabla_x(a^n v + a^{n+1}) + na^n \nabla_x v \right. \\ \left. - \frac{na^{n-1}}{a^0} \nabla_x a^2 - P^n \right] = \sigma \geq 0, \quad \Delta_1^r = 0 \end{aligned} \tag{3.4}$$

holds for all fields A^r . Now, (3.4) may be written in an essentially different form as

$$\begin{aligned} \left[h - \sum_{k=0}^r (k+1) \Delta_k^r a^k \right] \nabla_x v \\ + \sum_{n=0}^r \left\{ \left[\frac{\partial h}{\partial a^n} - \Delta_n^r \right] \partial_t a^n + \left[v \left(\frac{\partial h}{\partial a^n} - \Delta_n^r \right) \right. \right. \\ \left. \left. + \frac{\partial \Phi}{\partial a^n} - \Delta_{n-1}^r - \Delta_r^r \frac{\partial a^{r+1}}{\partial a^n} + \delta_{n2} \sum_{k=0}^r k \Delta_k^r \frac{a^{k-1}}{a^0} \right] \nabla_x a^n \right. \\ \left. + \Delta_n^r P^n \right\} = \sigma \geq 0, \quad \Delta_{-1}^r = 0 \end{aligned} \tag{3.5}$$

where, by definition, δ_{nm} is the Kronecker delta. According to Liu's theorem,⁽¹⁶⁾ the space-time derivatives $\nabla_x v$, $\partial_t a^n$, and $\nabla_x a^n$ can be chosen *arbitrarily* and *independently* of any other term in (3.5). With this in mind, it follows that the quantities in square brackets [...] vanish,

$$\frac{\partial h}{\partial a^n} - \Delta_n^r = 0, \quad h - \sum_{k=0}^r (k+1) \Delta_k^r a^k = 0 \tag{3.6}$$

$$\frac{\partial \Phi}{\partial a^n} - \Delta_{n-1}^r - \Delta_r^r \frac{\partial a^{r+1}}{\partial a^n} + \delta_{n2} \sum_{k=0}^r k \Delta_k^r \frac{a^{k-1}}{a^0} = 0 \tag{3.7}$$

⁴ In order to avoid burdensome notation, and because it makes no changes in Eqs. (3.6) and (3.7), the Lagrange multiplier associated with Eq. (2.8b) does not appear in this work.

where $0 \leq n \leq r$, $n \neq 1$, and the entropy inequality (3.5) reduces to the residual one

$$\sum_{n=0}^r A_n^r P^n = \sigma \geq 0 \tag{3.8}$$

Although the equalities just obtained have the effect of interrelating the basic and auxiliary constitutive representations for a^{r+1} , h , Φ , and A_n^r , none of them yet furnishes what we really want, namely a reduction in the generality of the basic constitutive functions (3.1). Even more, since valuable information concerning $b^m(A^r)$ is not directly derivable from (3.6)–(3.7)—these Hermite expansion coefficients simply do not occur there, but only indirectly through P^n in the residual inequality (3.8)—the critical problem becomes one of extracting, possibly with the aid of supplementary ingredients in the theory, explicit knowledge of $b^m(A^r)$.

3.2. Constitutive Assumptions in the Second-Order Theory

We now consider the two standard equalities in the theory of one-dimensional Hermite polynomials⁽⁷⁾ as providing a tool for constructing $b^n(A^r) = b^n \in H_{-1}^r$, namely

$$B^n(\lambda) = \sum_{k=0}^n X_k^n \lambda^k \tag{3.9a}$$

$$\lambda^n = \sum_{k=0}^n Y_k^n B^k(\lambda) \tag{3.9b}$$

$$n \in \mathbb{N}_0 \tag{3.9c}$$

$$X_k^n, Y_k^n = \begin{cases} 0, & 0 & \text{for } n - k \in 2\mathbb{N}_0 + 1 \\ \frac{(-1)^{(n-k)/2} n!}{k! (n-k)!}, & \frac{n!}{k! (n-k)!} & \text{for } n - k \in 2\mathbb{N}_0 \end{cases} \tag{3.10}$$

where

$$(2n)!! = 2 \circ 4 \circ \dots \circ 2n \tag{3.11}$$

$$2\mathbb{N}_0 = \{0, 2, \dots\}, \quad 2\mathbb{N}_0 + 1 = \{1, 3, \dots\}$$

Substituting (3.9a) in (2.14) and (3.9b) in (2.7), also using the supplementary notation (2.15), one obtains for $b^n \in H_{-1}^\infty$

$$b^n = \sum_{k=0}^n x_k^n a^k \tag{3.12a}$$

$$a^n = \sum_{k=0}^n y_k^n b^k \tag{3.12b}$$

$$n \in \mathbb{N}_0 \tag{3.12c}$$

where

$$x_k^n, y_k^n = \begin{cases} 1, & 1 & \text{for } (n=0, k=0) \text{ or } (n=2, k=2) \\ 0, & 0 & \text{for } n=1 \text{ or } k=1 \text{ or } (n=2, k=0) \\ \frac{\alpha^k}{a^0} X_k^n, & \frac{a^0}{\alpha^n} Y_k^n & \text{for } 3 \leq n \text{ and } k \neq 1 \end{cases} \tag{3.13}$$

If, however, we have additional information that the first n Hermite coefficients b^m can be transformed into the first n direct moments a^m by a nonsingular linear transformation, the specific choice A^r of the internal state variables loses its absolute importance, since then, roughly speaking, dependences of a^{r+1} , $b^n \in H_r^\infty$, A_n^r ($0 \leq n \leq r$, $n \neq 1$), h , and Φ on $b^n \in H_{r-1}^r$ will interest us as well.

It is, of course, possible to conceive of states of the gas slightly removed from local equilibrium. When this is done, the general constitutive representations (3.1b), (3.3), and (3.2) can be expanded in powers of the coefficients $b^n \in H_2^r$, which, by their very nature, vanish in the state of local equilibrium. The second-order representations can be written down easily and we obtain

$$b^n = \sum_{k=3}^r b_k^{r|n} b^k + \sum_{k=3}^r \sum_{m=3}^r b_{km}^{r|n} b^k b^m, \quad r < n \tag{3.14}$$

$$A_n^r = A_0^{r|n} + \sum_{k=3}^r A_k^{r|n} b^k + \sum_{k=3}^r \sum_{m=3}^r A_{km}^{r|n} b^k b^m \tag{3.15}$$

$0 \leq n \leq r, \quad n \neq 1$

where we shall think of the coefficients $b_k^{r|n}$ through $A_{km}^{r|n}$ as parameters depending in general both on $b^0 = a^0$ and $b^2 = a^2$. Obviously, as a result of (3.12a) and (3.14) for $n=r+1$, the constitutive function for the flux moment a^{r+1} can be explicitly formulated, so that we obtain

$$a^{r+1} = -\frac{1}{x_{r+1}^{r+1}} \sum_{k=0}^r x_k^{r+1} a^k + \frac{1}{x_{r+1}^{r+1}} b^{r+1} \tag{3.16}$$

In order to make (3.14)–(3.15) internally consistent with Eqs. (3.6)–(3.7), one must consider h and Φ , which contain also the third-order terms in $b^n \in H_2^r$,

$$\begin{aligned}
 h &= h_0^r + \sum_{k=3}^r h_k^r b^k + \sum_{k=3}^r \sum_{m=3}^r h_{km}^r b^k b^m \\
 &+ \sum_{k=3}^r \sum_{m=3}^r \sum_{p=3}^r h_{kmp}^r b^k b^m b^p \tag{3.17}
 \end{aligned}$$

$$\begin{aligned}
 \Phi &= \sum_{k=3}^r \phi_k^r b^k + \sum_{k=3}^r \sum_{m=3}^r \phi_{km}^r b^k b^m \\
 &+ \sum_{k=3}^r \sum_{m=3}^r \sum_{p=3}^r \phi_{kmp}^r b^k b^m b^p \tag{3.18}
 \end{aligned}$$

At first sight, it would be stimulating to take full account of such a situation for which at the outset the coefficients $b_k^{r|n}$ in (3.14) are not equal to zero, but it has to be recognized that, in doing so, apparent discrepancies, which we want to avoid, with assumptions equivalent to those on which Grad’s theory^(5,6) is founded could not be eliminated. Indeed, in Grad’s truncation procedure^(5,6) $b^n \in H_r^\infty$ are considered to be negligible. It is then no surprise that in the remainder of the work we seek $b_{km}^{r|n}$ in front of $b^k b^m$ [see Eq. (3.14)] under the natural assumption

$$b_k^{r|n} = 0 \tag{3.19}$$

which puts the proposed theory in harmony with the older one.^(5,6)

3.3. Compatibility Conditions

In ET of degree $n - 1$ ($r + 1 \leq n$), the Hermite coefficient b^n can be thought of as being the “first” excessive unknown

$$\begin{aligned}
 b^n &= \sum_{k=3}^{n-1} \sum_{m=3}^{n-1} \underline{b_{km}^{n-1|n} b^k b^m} = \sum_{k=3}^r \sum_{m=3}^r b_{km}^{n-1|n} b^k b^m \\
 &+ 2 \sum_{k=3}^r \sum_{m=r+1}^{n-1} \underline{b_{km}^{n-1|n} b^k b^m} + \sum_{k=r+1}^{n-1} \sum_{m=r+1}^{n-1} \underline{b_{km}^{n-1|n} b^k b^m} \tag{3.20}
 \end{aligned}$$

where the underlined expressions (UE) on the rhs of Eq. (3.20) will only be important for $r + 1 < n$, eventually giving rise to what we have previously called ET of degree r .⁵ Consistent with this observation, we attempt to

⁵ In obtaining the first underlined expression, we assume with no loss of generality that $b_{km}^{n-1|n} = b_{mk}^{n-1|n}$.

arrive at (3.14) supplemented by (3.19) once more by regarding in the second step b^{n-1} as a constitutive quantity rather than an independent state variable,

$$b^{n-1} = \sum_{k=3}^{n-2} \sum_{m=3}^{n-2} b_{km}^{n-2|n-1} b^k b^m \tag{3.21}$$

according to the tenets of ET of degree $n - 2$. Obviously, we do this on the understanding that Eq. (3.21)—when substituted into (3.20)—does not contribute to

$$b^n = \sum_{k=3}^{n-2} \sum_{m=3}^{n-2} b_{km}^{n-2|n} b^k b^m \tag{3.22}$$

because potentially important terms appearing then in the UE are of third (fourth) order with respect to $b^m \in H_2^{n-2}$. In the last $n - r$ step, we write

$$b^{r+1} = \sum_{k=3}^r \sum_{m=3}^r b_{km}^{r|r+1} b^k b^m \tag{3.23}$$

but this equality, due to arguments that in essence are exactly the same as those just formulated, does not contribute to

$$b^n = \sum_{k=3}^r \sum_{m=3}^r b_{km}^{r|n} b^k b^m \tag{3.24}$$

as well. Finally, comparing (3.24) with the first expression on the rhs of (3.20), we obtain the important compatibility conditions

$$b_{km}^{r|n} = b_{km}^{n-1|n}, \quad 3 \leq k \leq r, \quad 3 \leq m \leq r, \quad r < n \tag{3.25}$$

between ET of degree r and that of degree $n - 1$.

If a similar contraction of the level of thermodynamic description based on $b^m \in H_{-1}^{r+1}$ is carried out for h and Φ , by projecting the results of ET of degree $r + 1$ into the space of the state variables $b^m \in H_{-1}^r$, the constitutive functions (3.17)–(3.18) are recovered, with the additional advantages as follows:

$$h_0^{r+1} = h_0^r \tag{3.26}$$

$$h_k^{r+1} = h_k^r, \quad 3 \leq k \leq r \tag{3.27}$$

$$\phi_k^{r+1} = \phi_k^r,$$

$$h_{r+1}^{r+1} b_{km}^{r|r+1} + h_{km}^{r+1} = h_{km}^r, \quad \left\{ \begin{array}{l} 3 \leq k \leq r \\ 3 \leq m \leq r \end{array} \right. \tag{3.28a}$$

$$\phi_{r+1}^{r+1} b_{km}^{r|r+1} + \phi_{km}^{r+1} = \phi_{km}^r, \quad \left\{ \begin{array}{l} 3 \leq k \leq r \\ 3 \leq m \leq r \end{array} \right. \tag{3.28b}$$

$$2h_{r+1(k)}^{r+1} b_{mp}^{r|^{r+1}} + h_{kmp}^{r+1} = h_{kmp}^r, \quad \begin{cases} 3 \leq k \leq r \\ 3 \leq m \leq r \\ 3 \leq p \leq r \end{cases} \quad (3.29a)$$

$$2\phi_{r+1(k)}^{r+1} b_{mp}^{r|^{r+1}} + \phi_{kmp}^{r+1} = \phi_{kmp}^r, \quad \begin{cases} 3 \leq k \leq r \\ 3 \leq m \leq r \\ 3 \leq p \leq r \end{cases} \quad (3.29b)$$

where round brackets $A_{(km \dots p)}$ enclosing a set of n indices represent symmetrization of these indices, i.e., the sum of all permutations of the indices divided by $n!$ (irrespective of whether or not they are distinct).

Although the statements (3.14)–(3.18) and (3.25)–(3.29) remove, as tedious inspection shows, at least part of the difficulty in successfully analyzing the direct thermodynamic consequences (3.6)–(3.7), still one more fact (Section 4.1) is desired in order to get a manageable result. On the contrary, far from seeking to introduce and combine with Eqs. (3.6)–(3.7) compatibility conditions—as well as extra information like that in Section 4.1—the Liu–Müller ET of degree 13 for actual (three-dimensional) rarefied gases makes use of macroscopic axioms alone.⁽²⁾

4. CONSTITUTIVE COEFFICIENTS IN EXPLICIT FORM

4.1. Solutions for h and Φ

Note that Eq. (2.11) can also be written as

$$f = f^M [1 + (\varepsilon_1^r + \varepsilon_2^r)] \quad (4.1)$$

$$\varepsilon_1^r = \sum_{n=3}^r \frac{1}{n!} b^n B^n, \quad \varepsilon_2^r = \sum_{n=r+1}^{\infty} \frac{1}{n!} b^n B^n \quad (4.2)$$

where the coefficients b^n ($r < n$) are now given by (3.14) and (3.19). This form of (2.11) is particularly useful in calculating the characteristic element

$$\hat{\lambda}^p [1 + (\varepsilon_1^r + \varepsilon_2^r)] \ln [1 + (\varepsilon_1^r + \varepsilon_2^r)], \quad p = 0, 1 \quad (4.3)$$

which one extracts easily from Eqs. (2.5).

As far as the auxiliary constitutive functions (3.17)–(3.18) are concerned, in the neighborhood of local equilibrium, a valid approximation to (4.3) may be obtained by using in (2.5) the first three terms of the expansion of the logarithm. A rather lengthy resulting expression simplifies considerably when it is realized that either certain integrals on the rhs of the molecular formulas (2.5) for h and Φ vanish altogether due to the orthogonality properties of Hermite polynomials or, what is equally impor-

tant, they simply lose their further applicability due to an “unsuitable” occurrence of the higher order factors

$$\underbrace{b^k b^m \dots b^p}_n, \quad 3 < n$$

All this justifies the following sequence of transformations:

$$\begin{aligned} & \hat{\lambda}^p [1 + (\varepsilon_1^r + \varepsilon_2^r)] \ln [1 + (\varepsilon_1^r + \varepsilon_2^r)] \\ & \Rightarrow \hat{\lambda}^p [1 + (\varepsilon_1^r + \varepsilon_2^r)] [(\varepsilon_1^r + \varepsilon_2^r) \\ & \quad - \frac{1}{2}(\varepsilon_1^r + \varepsilon_2^r)^2 + \frac{1}{3}(\varepsilon_1^r + \varepsilon_2^r)^3] \\ & \Rightarrow \hat{\lambda}^p [(\varepsilon_1^r + \varepsilon_2^r) + \frac{1}{2}(\varepsilon_1^r + \varepsilon_2^r)^2 - \frac{1}{6}(\varepsilon_1^r + \varepsilon_2^r)^3] \\ & \Rightarrow \frac{1}{2} \hat{\lambda}^p [(\varepsilon_1^r \varepsilon_1^r + 2\varepsilon_1^r \varepsilon_2^r) - \frac{1}{3} \varepsilon_1^r \varepsilon_1^r \varepsilon_1^r] \end{aligned} \tag{4.4}$$

in order to arrive, after a direct calculus, at

$$h_0^r = \frac{1}{2} a^0 - a^0 \ln [(2\pi)^{-1/2} \alpha a^0 \mathbb{C}], \quad h_k^r = 0 \tag{4.5}$$

$$h_{km}^r = -\frac{a^0}{2k! m!} \langle B^k B^m \rangle, \quad h_{kmp}^r = \frac{a^0}{6k! m! p!} \langle B^k B^m B^p \rangle \tag{4.6}$$

and

$$\phi_k^r = \frac{a^0}{2\alpha} \delta_{k3} \tag{4.7}$$

$$\phi_{km}^r = -\frac{a^0}{2\alpha k! m!} [\langle B^{k+1} B^m \rangle + k \langle B^{k-1} B^m \rangle]$$

$$\begin{aligned} \phi_{kmp}^r &= \frac{a^0}{6\alpha k! m! p!} [\langle B^{k+1} B^m B^p \rangle + k \langle B^{k-1} B^m B^p \rangle] \\ & \quad - \frac{a^0}{3\alpha} \left[\frac{1}{k!} \delta_{rk} b_{mp}^{r|k+1} + \frac{1}{m!} \delta_{rm} b_{pk}^{r|m+1} + \frac{1}{p!} \delta_{rp} b_{km}^{r|p+1} \right] \end{aligned} \tag{4.8}$$

where, by definition,

$$\langle B^k B^m \dots B^p \rangle = (2\pi)^{-1/2} \int d\lambda \exp(-\frac{1}{2} \lambda^2) B^k(\lambda) B^m(\lambda) \dots B^p(\lambda) \tag{4.9}$$

The remaining task is then, aside from the natural question of how the specific numbers $b_{km}^{r|k+1}$ should be calculated, and whether or not Eqs.

(3.6)–(3.7) impose sufficiently stringent restrictions upon them, to determine the values of $\langle B^k B^m \rangle$ and $\langle B^k B^m B^p \rangle$. It is possible to show that

$$\langle B^k B^m \rangle = k! \delta_{km} \quad (4.10)$$

$$\langle B^k B^m B^p \rangle = \frac{k! m! p!}{[(k+m-p)/2]! [(m+p-k)/2]! [(p+k-m)/2]!} \quad (4.11)$$

for $k+m+p \in 2\mathbb{N}_0$, $k+m-p \geq 0$, $m+p-k \geq 0$, $p+k-m \geq 0$ and

$$\langle B^k B^m B^p \rangle = 0 \quad (4.12)$$

for other choices of the indices.

Upon adopting (4.5)–(4.8), the compatibility conditions (3.26)–(3.29) are found to be satisfied automatically; hence only Eq. (3.25) exhibits its importance, as we shall soon see, in deriving the new moment representation for f .

4.2. Solutions for Δ'_n ($0 \leq n \leq r$, $n \neq 1$) and b^n ($r < n$)

So far, this work has discussed thermodynamic consequences of the local entropy inequality, which, technically speaking, do not require any knowledge of the assumptions of the second-order theory, except for the observation that the basic and auxiliary constitutive quantities (3.1a) and (3.2) are differentiable functions of A' . However, elementary appeal to Eqs. (3.14)–(3.18) and (4.5)–(4.8) and the transformation rules (3.12) shows that the thermodynamic relations (3.6)–(3.7) are not satisfied unless the coefficients of certain polynomials of second order in $b^m \in H_2^6$, which follow from inserting constitutive representations of Sections 3.2 and 4.1 into (3.6)–(3.7), vanish altogether.

The exploitation of Eqs. (3.6)–(3.7) in this spirit is a very laborious process, so that we cannot hope to treat every detail of the problem. Nevertheless, in an Appendix we summarize briefly useful identities of interest in deriving the simple results regarding the Lagrange multipliers:

$$\Delta_0^{r|0} = -1 - \ln[(2\pi)^{-1/2} \alpha a^0 \mathbb{C}], \quad \Delta_0^{r|2} = \frac{1}{2} \alpha^2 \quad (4.13)$$

$$\Delta_0^{r|n} = 0, \quad 3 \leq n \leq r \quad (4.14)$$

⁶ Since Eqs. (3.17)–(3.18) are given to within fourth-order terms, all contributions of higher than second order in $b^m \in H_2^6$ would not be reliable. The reason for not allowing third-order terms in (3.6)–(3.7) is that the reliable order of $\partial h / \partial a^n$ and $\partial \Phi / \partial a^n$ has been lowered to 2 by differentiation with respect to a^n .

$$\Delta_k^{r|n} = -\frac{\alpha^n}{k!} \sum_{p=n}^r X_n^p \delta_{pk}, \quad \left\{ \begin{array}{l} 0 \leq n \leq r, \quad n \neq 1 \\ 3 \leq k \leq r, \quad 3 \leq m \leq r \end{array} \right. \quad (4.15)$$

$$\Delta_{km}^{r|n} = \frac{\alpha^n}{2k! m!} \sum_{p=n}^r \frac{1}{p!} X_n^p \langle B^p B^k B^m \rangle, \quad \left\{ \begin{array}{l} 3 \leq k \leq r, \quad 3 \leq m \leq r \end{array} \right. \quad (4.16)$$

on the one hand and the excessive flux moment ($a^{r+1} \Leftrightarrow b^{r+1}$)

$$b_{km}^{r|r+1} = \frac{1}{2k! m!} \langle B^{r+1} B^k B^m \rangle, \quad 3 \leq k \leq r, \quad 3 \leq m \leq r \quad (4.17)$$

on the other.

From the compatibility requirement (3.25), it is easy to show that

$$b_{km}^{r|n} = \frac{1}{2k! m!} \langle B^n B^k B^m \rangle, \quad r < n, \quad 3 \leq k \leq r, \quad 3 \leq m \leq r \quad (4.18)$$

Hence

$$b_{km}^{r|n} = 0 \quad \text{for } k + m < n \quad (4.19)$$

In this context, see Eqs. (4.11)–(4.12).

5. THE NEW MOMENT REPRESENTATION FOR THE DISTRIBUTION FUNCTION

5.1. The Two Interrelated Expressions for f

With Eqs. (3.14), (3.19), (4.18), and (2.11), one obtains

$$f = f^M \left[1 + \underbrace{\sum_{k=3}^r \frac{1}{k!} b^k B^k(\hat{\lambda})}_{\varepsilon_1} + \underbrace{\frac{1}{2} \sum_{k=3}^r \sum_{m=3}^r \sum_{n=r+1}^{2r} \frac{1}{k! m! n!} \langle B^n B^k B^m \rangle b^k b^m B^n(\hat{\lambda})}_{\varepsilon_2} \right] \quad (5.1)$$

Hence, the quantity ε_2 can be considered negligible, as in Grad's approach,^(5,6) only in the simplest case of linear ET of degree r .

On replacing $\langle B^n B^k B^m \rangle$ by the identities (4.11)–(4.12), we get the explicit result

$$f = f^M \left[1 + \sum_{k=3}^r \frac{1}{k!} b^k B^k + \sum_{n=p_1}^{2r} \sum_{k=p_2}^{[n/2]} \sum_{m=0}^{w_1} \frac{b^k b^{n-k} B^{n-2m}}{m! (k-m)! (n-m-k)!} - \frac{1}{2} \sum_{k=p_3}^r \sum_{m=0}^{w_2} \frac{b^k b^k B^{2k-2m}}{m! (k-m)! (k-m)!} \right] \tag{5.2}$$

where

$$p_1 = \max(6, r + 1), \quad w_1 = [(n - r - 1)/2] \tag{5.3a}$$

$$p_2 = \max(3, n - r), \quad w_2 = [(2k - r - 1)/2] \tag{5.3b}$$

$$p_3 = \max(3, [(r + 2)/2]) \tag{5.3c}$$

By definition, the symbol $[n/2]$ denotes the integral part of $n/2$.

5.2. On the Microscopic Origin of the Residual Inequality

This section is devoted to the evaluation of the local entropy production

$$\sigma = - \int d\lambda J(f) \ln[\mathbb{C}f] \tag{5.4}$$

We start with

$$\begin{aligned} \sigma &= - \int d\lambda J(f) \ln[1 + (\varepsilon_1^r + \varepsilon_2^r)] \\ &\Rightarrow - \int d\lambda J(f) [\varepsilon_1^r + (\varepsilon_2^r - \frac{1}{2} \varepsilon_1^r \varepsilon_1^r)] \end{aligned} \tag{5.5}$$

Now, by (3.9a), $\hat{\lambda} = \alpha \tilde{\lambda}$, (4.15), and (4.16), the quantity ε_1^r is equal to

$$- \sum_{n=0}^r \sum_{k=3}^r A_k^{r|n} b^k \tilde{\lambda}^n \tag{5.6}$$

while

$$\varepsilon_2^r - \frac{1}{2} \varepsilon_1^r \varepsilon_1^r = - \sum_{n=0}^r \sum_{k=3}^r \sum_{m=3}^r A_{km}^{r|n} b^k b^m \tilde{\lambda}^n \tag{5.7}$$

provided that we make use of the identity

$$\sum_{p=n}^{2r} \frac{1}{p!} X_n^p \langle B^p B^k B^m \rangle - \sum_{i+j=n} \sum_{p=i}^r \sum_{q=j}^r X_i^p X_j^q \delta_{pk} \delta_{qm} = 0 \tag{5.8}$$

Adopting (5.6)–(5.7), and remembering that $P^n = \int d\lambda \tilde{\lambda}^n J(f)$, we arrive at the expression

$$\sigma = \sum_{n=3}^r \Delta_n^r P^n \tag{5.9}$$

which is in full harmony with the so-called residual inequality (3.8). Were this not the case, the derived moment representation (5.1), or, alternatively, (5.2) would not be correct.

If the collision integral $J(f)$ is explicitly specified as a functional of the df , then, since (5.2) allows a reliable evaluation of constitutive functions of the second-order theory, one obtains constitutive relations for the collision productions P^n in the following form:

$$P^n = \sum_{k=3}^r P_k^{r|n} b^k + \sum_{k=3}^r \sum_{m=3}^r P_{km}^{r|n} b^k b^m, \quad 3 \leq n \leq r \tag{5.10}$$

Substituting (5.10) and (3.15) in (5.9) and rejecting the resulting terms that are of higher than third order in $b^m \in H_2^r$,⁷ we obtain for Eq. (5.9)

$$\sigma = \sigma_0 + \sigma_1 \tag{5.11}$$

where

$$\sigma_0 = \sum_{n=3}^r \sum_{k=3}^r \sum_{m=3}^r \Delta_k^{r|n} P_m^{r|n} b^k b^m \tag{5.12}$$

$$\sigma_1 = \sum_{n=3}^r \sum_{k=3}^r \sum_{m=3}^r \sum_{p=3}^r (\Delta_{km}^{r|n} P_p^{r|n} + P_{km}^{r|n} \Delta_p^{r|n}) b^k b^m b^p \tag{5.13}$$

The part σ_0 of σ is required to be nonnegative for all possible choices of the values of $b^m \in H_2^r$ (otherwise linear ET of degree r breaks down), but the local entropy inequality $\sigma = \sigma_0 + \sigma_1 \geq 0$ may formally cease to be true when $b^m \in H_2^r$ are suitably chosen. Fortunately, because the one-dimensional gas departs slightly from local equilibrium, as normally in the constitutive theory of second order—and indeed of arbitrary order—the contribution σ_1 to the entropy production σ is small compared with that

⁷In the second-order theory, σ can be evaluated to within the fourth-order terms in $b^m \in H_2^r$.

due to "linear" effects. As a consequence, the inequality $\sigma \geq 0$ does not lose its importance.⁸

Obvious as these facts are, they are sometimes disregarded in formal extensions of the range of validity of ET to far-from-equilibrium situations.

6. EVALUATION OF THE COLLISION PRODUCTIONS

P^n ($3 \leq n \leq r$)

6.1. Ma's Collision Integral $J(f)$

Ma's choice⁽⁸⁾ of the collision integral $J(f)$ can now be reconsidered. He took

$$J(f) = \iiint \iiint d\lambda' d\lambda'' d\omega d\omega' d\omega'' \mathcal{R}(\lambda, \lambda', \lambda'' | \omega, \omega', \omega'') \times [f(\omega) f(\omega') f(\omega'') - f(\lambda) f(\lambda') f(\lambda'')] \quad (6.1)$$

$$\begin{aligned} & \mathcal{R}(\lambda, \lambda', \lambda'' | \omega, \omega', \omega'') \\ &= \Gamma \delta[\lambda + \lambda' + \lambda'' - \omega - \omega' - \omega''] \\ & \quad \times \delta[\tfrac{1}{2}(\lambda^2 + \lambda'^2 + \lambda''^2) - \tfrac{1}{2}(\omega^2 + \omega'^2 + \omega''^2)] \end{aligned} \quad (6.2)$$

In so doing, wherever the df in (6.1) occurs, it must be evaluated at the same space-time point (x, t) . Here \mathcal{R} is the rate of the collision $\lambda + \lambda' + \lambda'' \leftrightarrow \omega + \omega' + \omega''$, which, as (6.2) indicates, satisfies momentum and energy conservation. Generally, Γ depends on $\lambda, \lambda', \lambda'', \omega, \omega',$ and ω'' . The condition of undistinguishability of the particles implies that Γ remains unaltered on all possible permutations of $(\lambda, \lambda', \lambda'')$ and $(\omega, \omega', \omega'')$, respectively, and, in addition, on interchange $(\lambda, \lambda', \lambda'') \leftrightarrow (\omega, \omega', \omega'')$.

In a fictitious three-dimensional space of vectors $(\lambda, \lambda', \lambda'')$, the principle of conservation of momentum

$$\lambda + \lambda' + \lambda'' = \mathcal{P} \quad (6.3)$$

determines a plane and the principle of conservation of energy

$$\lambda^2 + \lambda'^2 + \lambda''^2 = 2\mathcal{E} \quad (6.4)$$

⁸ Even more, the important work by Liu and Müller⁽²⁾ indicates that $b^m \in H_2^s$ must be small anyway, independent of whether or not linear ET is under consideration, due to the Friedrichs-Lax condition of hyperbolicity.⁽¹⁷⁾

defines a spherical surface. The plane and the spherical surface have an intersection, which is a circle of radius

$$\rho = (2\mathcal{E} - \mathcal{P}^2/3)^{1/2} \tag{6.5}$$

$\mathcal{P}/\sqrt{3}$ is the distance from the plane to the origin and ρ can be interpreted as the energy in the center-of-mass frame. The energy-momentum conservation law demands that $(\lambda, \lambda', \lambda'')$ and $(\omega, \omega', \omega'')$ be on the same circle characterized by (6.5). In other words, the two vectors $(\lambda, \lambda', \lambda'')$ and $(\omega, \omega', \omega'')$ will uniquely be specified by (\mathcal{P}, ρ) and the angles φ and ψ , respectively; φ and ψ are measured along the circle. Now, draw a line from the center of the circle to the intersection of the plane and the λ axis. Following Ma,⁽⁸⁾ we choose this line as $\varphi = 0$ ($\psi = 0$). Then, a little algebra gives

$$\lambda = \mathcal{P}/3 + \rho(2/3)^{1/2} \cos \varphi \tag{6.6a}$$

$$\lambda' = \mathcal{P}/3 - \rho(1/\sqrt{6}) \cos \varphi - \rho(1/\sqrt{2}) \sin \varphi \tag{6.6b}$$

$$\lambda'' = \mathcal{P}/3 - \rho(1/\sqrt{6}) \cos \varphi + \rho(1/\sqrt{2}) \sin \varphi \tag{6.6c}$$

Replacing φ by ψ in (6.6), we immediately arrive at the transformation rule for $(\omega, \omega', \omega'')$.

Although, strictly speaking, $\Gamma = \Gamma(\rho, \varphi, \psi)$, we shall make the simplifying assumption that $\Gamma = \Gamma(\rho)$.⁹ Even more, we postulate

$$\Gamma = \frac{\mathbb{B}c^4}{4\pi^2(6\pi)^{1/2}} \exp[\frac{1}{2}(1-c)\alpha^2\rho^2], \quad 0 < c \leq 1, \quad 0 < \mathbb{B} \tag{6.7}$$

where \mathbb{B} and c are certain unspecified constants. Since the kinetic equation for a one-dimensional rarefied gas should serve some pedagogical purpose, as originally in the work by Ma,⁽⁸⁾ we do not inquire as to whether there exists an interaction potential between particles producing (corresponding to) (6.7).

6.2. The Generating Function

On using Ma's collision integral (6.1)–(6.2) with Γ calculated from (6.7) and the definition (2.9) regarding the collision production P^n , as well as the series representation (2.11) for the df supplemented by Eqs. (3.14),

⁹ In the work by Ma,⁽⁸⁾ Γ is a constant independent of ρ .

(3.19), and the result (4.18), we find for the coefficients $P_k^{r|n}$ and $P_{km}^{r|n}$ in (5.10)

$$P_k^{r|n} = \frac{1}{3} \mathbb{B} v^3 \alpha^{3-n} \sum_{p=3}^n Y_p^n R_k^p \tag{6.8}$$

$$P_{km}^{r|n} = \frac{1}{3} \mathbb{B} v^3 \alpha^{3-n} \sum_{p=3}^n Y_p^n \left[R_{km}^p + \sum_{q=r+1}^{2r} R_q^p b_{km}^{r|q} \right] \tag{6.9}$$

where

$$v = a^0 / \alpha (2\pi)^{1/2} \tag{6.10}$$

and the dimensionless numbers R_k^p and R_{km}^p are given by

$$\begin{aligned} R_k^p &= \frac{c^4}{4\pi^2 (6\pi)^{1/2} k!} \int d\mathcal{P} \, d\rho \, d\varphi \, d\psi \\ &\quad \times \rho \exp \left[-\frac{1}{2} \left(c\rho^2 + \frac{\mathcal{P}^2}{3} \right) \right] B^p(\lambda) \\ &\quad \times [3B^k(\omega) - B^k(\lambda) - 2B^k(\lambda')] \end{aligned} \tag{6.11}$$

$$\begin{aligned} R_{km}^p &= \frac{c^4}{4\pi^2 (6\pi)^{1/2} k! m!} \int d\mathcal{P} \, d\rho \, d\varphi \, d\psi \\ &\quad \times \rho \exp \left[-\frac{1}{2} \left(c\rho^2 + \frac{\mathcal{P}^2}{3} \right) \right] B^p(\lambda) \\ &\quad \times [3B^k(\omega) B^m(\omega') - B^k(\lambda') B^m(\lambda'') \\ &\quad - B^k(\lambda) B^m(\lambda') - B^k(\lambda') B^m(\lambda)] \end{aligned} \tag{6.12}$$

For the convenience of the reader, the abbreviated integral

$$\int d\mathcal{P} \, d\rho \, d\varphi \, d\psi \, \mathcal{N}(\mathcal{P}, \rho, \varphi, \psi)$$

is understood to be the multiple integral

$$\int_{-\infty}^{+\infty} \int_0^{+\infty} \int_0^{2\pi} \int_0^{2\pi} d\mathcal{P} \, d\rho \, d\varphi \, d\psi \, \mathcal{N}(\mathcal{P}, \rho, \varphi, \psi)$$

The procedure for obtaining (6.11)–(6.12) is compounded of two structurally different parts, one of which arises from transforming to $(\mathcal{P}, \rho, \varphi, \psi)$ in place of $(\lambda, \lambda', \lambda'', \omega, \omega', \omega'')$ as variables of integration,¹⁰

¹⁰ This change of variables of integration is described by Ma.⁽⁸⁾

and the second from replacing in the resulting integral ρ by $(1/\alpha)\rho$, $\mathcal{P} - v$ by $(1/\alpha)\mathcal{P}$, λ by $(1/\alpha)\lambda$, etc. Making the above scale transformation, we find that the dependence of the presently dimensionless velocities $(\lambda, \lambda', \lambda'')$, which occur in (6.11)–(6.12) through the Hermite polynomials B^m , upon $(\mathcal{P}, \rho, \varphi)$ is identical with that in Eq. (6.6), except that the variables \mathcal{P} and ρ are now dimensionless quantities. When the angle measured along the circle is chosen to be ψ , an analogous argument obviously applies to the velocities $(\omega, \omega', \omega'')$.

For many applications, the Hermite polynomials are derived by means of their generating function⁽¹⁸⁾

$$\sum_{p=0}^{\infty} \frac{\tau^p}{p!} B^p(\lambda) = \exp(\lambda\tau - \frac{1}{2}\tau^2) = g(\lambda|\tau) \tag{6.13}$$

Equation (6.13) implies that R_k^p divided by $p!$ and R_{km}^p divided by $p!$ are the coefficients of $\tau^p\tau'^k$ and $\tau^p\tau'^k\tau''^m$, respectively, in the power series representations of

$$\begin{aligned} R(\tau, \tau') &= \frac{c^4}{4\pi^2(6\pi)^{1/2}} \int d\mathcal{P} d\rho d\varphi d\psi \\ &\times \rho \exp\left[-\frac{1}{2}\left(c\rho^2 + \frac{\mathcal{P}^2}{3}\right)\right] g(\lambda|\tau) \\ &\times [3g(\omega|\tau') - 2g(\lambda'|\tau') - g(\lambda|\tau')] \end{aligned} \tag{6.14}$$

and

$$\begin{aligned} R(\tau, \tau', \tau'') &= \frac{c^4}{4\pi^2(6\pi)^{1/2}} \int d\mathcal{P} d\rho d\varphi d\psi \\ &\times \rho \exp\left[-\frac{1}{2}\left(c\rho^2 + \frac{\mathcal{P}^2}{3}\right)\right] g(\lambda|\tau) \\ &\times [3g(\omega|\tau') g(\omega'|\tau'') - g(\lambda'|\tau') g(\lambda''|\tau'') \\ &- g(\lambda|\tau') g(\lambda'|\tau'') - g(\lambda'|\tau') g(\lambda|\tau'')] \end{aligned} \tag{6.15}$$

The direct method of performing the integrations over $d\mathcal{P}$, $d\rho$, $d\varphi$, and $d\psi$ in (6.14)–(6.15) rests essentially upon the following values of the definite integrals⁽¹⁹⁾:

$$\int_{-\infty}^{+\infty} d\xi \exp(-p\xi^2 - q\xi) = (\pi/p)^{1/2} \exp \frac{q^2}{4p} \tag{6.16}$$

$$\int_0^{+\infty} d\xi \xi \exp(-p\xi^2) I_0(\delta\xi) = \frac{1}{2p} \exp \frac{\delta^2}{4p} \tag{6.17}$$

$$\int_0^{+\infty} d\xi \xi \exp(-p\xi^2) I_0(\delta\xi) I_0(g\xi) = \frac{1}{2p} \exp\left(\frac{\delta^2 + g^2}{4p}\right) I_0\left(\frac{\delta g}{2p}\right) \quad (6.18)$$

$$\int_0^{2\pi} d\xi \exp(x_1 \cos \xi + x_2 \sin \xi) = 2\pi I_0[(x_1^2 + x_2^2)^{1/2}] \quad (6.19)$$

where $p > 0$, $x_1^2 + x_2^2 \geq 0$, and $I_0(\xi)$ is the modified Bessel function of order zero. From Eqs. (6.16)–(6.19), we have the results for $R(\tau, \tau')$ and $R(\tau, \tau', \tau'')$:

$$\begin{aligned} R(\tau, \tau') &= c^3 \exp\left[\frac{1}{3}\Omega(\tau^2 + \tau'^2)\right] \\ &\times \left\{ 3 \exp\left(\frac{1}{3}\tau\tau'\right) I_0\left(\frac{2}{3c}\tau\tau'\right) \right. \\ &\left. - \exp\left[\left(1 + \frac{2}{3}\Omega\right)\tau\tau'\right] - 2 \exp\left(-\frac{1}{3}\Omega\tau\tau'\right) \right\} \quad (6.20) \end{aligned}$$

$$\begin{aligned} R(\tau, \tau', \tau'') &= c^3 \exp\left[\frac{1}{3}\Omega(\tau^2 + \tau'^2 + \tau''^2)\right] \\ &\times \left\{ 3 \exp\left[\frac{1}{3}(\tau\tau' + \tau\tau'' - \Omega\tau'\tau'')\right] \right. \\ &\times I_0\left[\frac{2}{3c}\tau(\tau'^2 + \tau''^2 - \tau'\tau'')^{1/2}\right] \\ &- \exp\left[-\frac{1}{3}\Omega(\tau\tau' + \tau\tau'' + \tau'\tau'')\right] \\ &- \exp\left[\tau\tau' - \frac{1}{3}\Omega(\tau\tau'' + \tau'\tau'' - 2\tau\tau')\right] \\ &\left. - \exp\left[\tau\tau'' - \frac{1}{3}\Omega(\tau\tau' + \tau'\tau'' - 2\tau\tau'')\right] \right\} \quad (6.21) \end{aligned}$$

where

$$\Omega = (1 - c)/c \quad (6.22)$$

The simplest possible assumption which suggests itself may be expressed by the statement that Γ in (6.7) does not depend on ρ ,¹¹ i.e.,

$$c = 1 \quad (\Rightarrow \Omega = 0) \quad (6.23)$$

¹¹ Ma⁽⁸⁾ makes extensive use of (6.23).

Since then $R(\tau, \tau')$ is a function of $\tau\tau'$, all terms in the power series representation of (6.20) have equal power in τ and τ' and a matrix of the coefficients in front of $\tau^p\tau'^k$ must be diagonal. We can also deduce from (6.21) that, for $c = 1$, $R_{km}^p = 0$ unless $p = k + m$. Consequently, in ET of degree $r = 3, 4, 5$, the quantities $P_{km}^{r|n}$ ($3 \leq n \leq r, 3 \leq k \leq r, 3 \leq m \leq r$) vanish altogether and, in spite of the basic result (5.2)–(5.3), potentially giving rise to nonlinear effects, the nonlinear terms in the constitutive representation (5.10) for P^n are of no importance. Thus, the gain in simplicity of mathematical consequences of the assumption (6.23) is offset by the possibility that the various constitutive coefficients derived may be inadequate.

This will not, however, be the case with “actual” molecules. In a slightly more general situation corresponding to

$$0 < c \leq 1 \tag{6.24}$$

we obtain by means of

$$I_0(\xi) = \sum_{k=0}^{\infty} \frac{1}{k! k!} \left(\frac{\xi}{2}\right)^{2k} \tag{6.25}$$

that the first few coefficients R_k^p and R_k^p are

$$\begin{bmatrix} R_3^3 & R_4^3 & R_5^3 \\ R_6^3 & R_7^3 & R_8^3 \\ R_3^4 & R_4^4 & R_5^4 \\ R_6^4 & R_7^4 & R_8^4 \end{bmatrix} = -\frac{2}{27} \begin{bmatrix} 3 & 0 & \Omega \\ 0 & \frac{1}{6}\Omega^2 & 0 \\ 0 & 4 & 0 \\ \frac{4}{3}\Omega & 0 & \frac{2}{9}\Omega^2 \end{bmatrix} \tag{6.26}$$

$$\begin{bmatrix} R_{33}^3 & R_{33}^4 \\ R_{34}^3 & R_{34}^4 \\ R_{43}^3 & R_{43}^4 \\ R_{44}^3 & R_{44}^4 \end{bmatrix} = \frac{5}{81} \begin{bmatrix} 0 & -\frac{16}{3}\Omega \\ \frac{1}{2}\Omega^2 & 0 \\ \frac{1}{2}\Omega^2 & 0 \\ 0 & \frac{4}{3}\Omega^2 \end{bmatrix} \tag{6.27}$$

As elementary inspection shows, Eqs. (6.26)–(6.27) throw light on the values of $P_k^{4|n}$ and $P_{km}^{4|n}$ ($3 \leq n \leq 4, 3 \leq k \leq 4, 3 \leq m \leq 4$), but by themselves

they do not give unambiguous information as to the constitutive representation (5.10) for P^n in ET of degree $r = 5, 6, \dots$. However, the complicated nature of the formulas (6.20)–(6.21) makes it difficult to predict from them the precise law of the c dependence of $P_k^{r|n}$ and $P_{km}^{r|n}$: only for sufficiently small values of r can definite predictions be made.

We are now in a position to test independently the appropriateness of an intuitive observation of Section 5.2 concerning the sign of σ_0 in (5.12) and, accordingly, that of σ in (5.11). In order to evaluate the rhs of (5.12), we return to Eqs. (4.15) and (6.8). It follows immediately that

$$\sum_{n=3}^r \Delta_k^{r|n} P_m^{r|n} = -\frac{1}{3} \frac{\mathbb{B} v^3 \alpha^3}{k!} R_m^k \quad (6.28)$$

Within the framework of the simplifying assumption (6.23), the part σ_0 of the entropy production σ is then essentially positive, provided that the coefficients R_m^k for $k = m$ are negative numbers.¹² Insofar as an Ω factor much smaller than 1 is concerned, σ_0 may also be expected to be essentially positive, because of the continuous Ω dependence of the coefficients R_m^k .

7. FINAL REMARKS

A further complication of the theory arises when three-dimensional simple gases are taken into account. Of course, results of similar form on actual such rarefied gases are familiar,⁽¹⁵⁾ but in the older view they referred only to the particular systems of equations of transfer, possibly in various combinations. It seems to have been possible to construct ET of three-dimensional rarefied gases that avoids them.

Still, a *reliable* formulation of extended theories is required for dense gases and fluids. Since in this more general case the advent of a finite size of molecules affects encounters considerably, it is doubtful whether a discussion of constitutive functions that depend locally upon the state variables, such as was made in Section 3.2, is adequate in the present connection. A treatment of ET of fluids (gases), inspired by the so-called revised Enskog equation, has been attempted; this work,⁽²⁰⁾ however, is outside the scope of these investigations.

¹² In this context, see the matrix (6.26) with $\Omega = 0$.

APPENDIX

In this Appendix we summarize, for the convenience of the reader, useful identities concerning

$$z_m^k = \begin{cases} \frac{1}{2} \sum_{p=m}^k p x_p^k y_m^p & \text{for } m \leq k \\ 0 & \text{for } m > k \end{cases} \tag{A.1}$$

which are of great importance in deriving (4.13)–(4.19) from Eqs. (3.6)–(3.7). Taking (A.1), we readily find that

$$\begin{aligned} m! z_m^k + k! z_k^m &= mm! \delta_{\cdot m}^k + \frac{1}{2}m! \delta_{\cdot m-2}^k + \frac{1}{2}k! \delta_{\cdot m+2}^k \\ &= \frac{1}{2} \langle B^2 B^k B^m \rangle \end{aligned} \tag{A.2}$$

$$\begin{aligned} m! z_m^{k+1} + k! z_k^{m+1} + mk! z_k^{m-1} + km! z_m^{k-1} \\ &= \frac{1}{2}m! \delta_{\cdot m}^{k+3} + \frac{3}{2}m! (k+1) \delta_{\cdot m}^{k+1} + \frac{3}{2}k! (m+1) \delta_{\cdot m}^{k-1} + \frac{1}{2}k! \delta_{\cdot m}^{k-3} \\ &= \frac{1}{2} \langle B^3 B^k B^m \rangle + \frac{3}{2} \langle B^1 B^k B^m \rangle \end{aligned} \tag{A.3}$$

for $k \geq 3, m \geq 3$, and that

$$z_2^k + \alpha^2 z_0^k = 0 \tag{A.4}$$

$$z_k^{k+2m} = \frac{1}{2} [k \delta_{m0} + (k+1)(k+2) \delta_{m1}] \tag{A.5}$$

for $k \geq 3, m = 0, 1, \dots$; in Eqs. (A.2)–(A.3), the symbol $\delta_{\cdot m}^k$ denotes the Kronecker delta.

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