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Mathematical Physics — *Extended thermodynamics of rarefied polyatomic gases and characteristic velocities*, by TAKASHI ARIMA, ANDREA MENTRELLI and TOMMASO RUGGERI, communicated on 11 April 2014.

ABSTRACT. — Extended thermodynamics of rarefied polyatomic gases is characterized by two hierarchies of equations for moments of a suitable distribution function in which the internal degrees of freedom of a particle is taken into account. To obtain the closed set of the field equations for the system with many moments and for an arbitrary entropy functional that includes degenerate gases, the entropy principle and maximum entropy principle are studied and the equivalence of these two methods is shown as in the well-established case of the monatomic gas. In addition the recent results of the present theory are summarized. On the basis of physical considerations, the truncation orders of the two hierarchies are seen to be not independent on each other. The equilibrium characteristic velocities of the emerging hyperbolic system of partial differential equations are analyzed and compared to those of monatomic gases. Inspection shows that the lower bound estimate of the maximum equilibrium characteristic velocity valid for monatomic gases, which increases as the truncation order increases, is valid for any rarefied polyatomic gas.

KEY WORDS: Extended thermodynamics, maximum entropy principle, rarefied polyatomic gas, maximum characteristic velocity, moments equation.

MATHEMATICS SUBJECT CLASSIFICATION: 82C35, 82C40, 76P05, 76N15, 35L60.

1. INTRODUCTION

Extended thermodynamics [16] is a phenomenological theory whose main aim is to bridge the gap between the two classical approaches to the study of nonequilibrium phenomena in which steep gradients and rapid changes occur, namely the *continuum approach* and the *kinetic approach*. One of the main limitations of Extended thermodynamics (ET), inherited from the kinetic theory to which ET is strictly connected, is its range of applicability, restricted to the study of monatomic rarefied gases.

Recently a 14-moments ET theory for dense gases and for rarefied polyatomic ones has recently been developed by Arima, Taniguchi, Ruggeri and Sugiyama [3]. This theory provides two parallel hierarchical structures of equations for the independent fields, one hierarchy consisting of balance equations for mass density, momentum density and momentum flux (momentum-like hierarchy), the other one consisting of balance equations for energy density and energy flux (energy-like hierarchy). These hierarchies cannot be merged, since the existence of the dynamic pressure (non-equilibrium pressure) breaks the equivalence of the energy density and trace-part of momentum flux, in contrast to what is true

in the monatomic gas case. By means of the closure procedure typical of ET theory, in particular of the entropy principle (EP), the constitutive equations are determined explicitly with the thermal and caloric equations of state. This theory has been thoroughly investigated [2, 4, 5, 8, 20] and its validity has been confirmed by comparing its predictions to experimental evidence in several test cases [6, 7, 21]. Moreover, Pavić, Ruggeri and Simić have recently proven [17] that the maximum entropy principle (MEP) [9, 14, 15] with the kinetic model for rarefied polyatomic gases presented by Borgnakke et al. [11] and by Bourgat et al. [12] yields appropriate macroscopic balance laws in agreement with the 14-moment theory presented in [3]. In particular, the *momentum-like* and the *energy-like* hierarchies obtained in the continuum-approach are related, respectively, to the moments of the distribution function f and to the moments of f in which an additional continuous variable representing the internal degrees of freedom of a particle is considered.

The purpose of the present paper is to summarize some recent contributions to the development and understanding of the new ET theory of rarefied polyatomic gases for any number of moments based on the above-mentioned kinetic model. The following points are studied: (i) It is discussed how, on the basis of physical arguments (Galilean invariance and the requirement that the characteristic velocities depend on the degrees of freedom of a particle), the relation between the orders of truncation of the momentum-like and energy-like hierarchies turn out not to be independent; (ii) For the truncated system of moment equations, following the methodology of the case of monatomic gases [9], the two equivalent closures, i.e. EP and MEP, are introduced and the general framework of these closures are studied; (iii) The characteristic velocities in the equilibrium state are analyzed, playing these quantities an important role in several processes, as the propagation of acceleration waves, the determination of the phase velocity of linear waves in the high-frequency limit, and *subshock* formation. With this regard, it will be discussed how the characteristic velocities of the system depend on the degrees of freedom and on the truncation order of the hierarchies, taking also into account the limit cases of monatomic gases and of a gas with infinite internal degrees of freedom; and (iv) It will be discussed how the lower bound estimate for the maximum characteristic velocity established for monatomic gases [9] and recently used by Slemrod in his analysis of the hydrodynamic limit of the Boltzmann equation and Hilbert's 6th problem [19], still holds independently from the degrees of freedom of a particle, leading to the conclusion that also for polyatomic gases the maximum characteristic velocity increases as the order of the hierarchies tends to infinity and is unbounded.

The proofs of the theorems as well as a more thorough analysis of the results presented here are presented and discussed elsewhere [1]. In this paper, different from the paper [1], the equivalence between EP and MEP is given for an arbitrary entropy functional that includes degenerate gases (Bose and Fermi gases).

The paper is organized as follows. In Section 2, the generalization to the case of the truncation order of *momentum-like* moments N and of *energy-like* moments M of the recently developed ET theory of 14-moment for rarefied

polyatomic gases is outlined. First, in order for a system describing a rarefied polyatomic gas to be well-behaved from a physical point of view, the principle of Galilean invariance is used to gain understanding on the relation that must exist between the orders N and M (Section 2.1), then the closures for Galilean invariant system by EP and MEP are introduced and the equivalence of those is discussed (Section 2.2), and to show clearly the procedure to obtain the constitutive equations the distribution function is expanded in the neighborhood of a local equilibrium state (Section 2.3). In Section 2.4, the calculation of the characteristic velocities of the system with many moments for rarefied polyatomic gases is outlined.

In Section 3 a thorough discussion of the features of the equilibrium characteristic velocities for gases with different degrees of freedom of the gas particles is provided.

In Section 4, the dependence of the maximum equilibrium characteristic velocity on the truncation order is considered and the existence of a lower bound valid for any rarefied gas is discussed.

Finally, some concluding remarks are offered in Section 5.

2. The double-hierarchy system for rarefied polyatomic gases

The kinetic theory is based on the assumption that the state of the gas can be described by the velocity distribution function. For rarefied polyatomic gases, a kinetic model in which the velocity distribution function depends not only on time *t*, position **x** and velocity of particles **c** but also on a non-negative parameter *I* which takes into account the influence of particles internal degrees of freedom on energy transfer during collisions, was proposed by Bourgat et al. [12] in the framework of the Borgnakke-Larsen procedure [11], and then applied to chemically reacting mixtures [13]. In this model, the velocity distribution function $f \equiv f(\mathbf{x}, \mathbf{c}, t, I)$ defined by the number density of particles $f(\mathbf{x}, \mathbf{c}, t, I) \, d\mathbf{x} \, d\mathbf{c} \, dI$ at time *t* in a phase space $d\mathbf{x} \, d\mathbf{c} \, dI$ centered in $(\mathbf{x}, \mathbf{c}, I) \in \mathbb{R}^3 \times \mathbb{R}^3 \times [0, \infty)$ obey the Boltzmann equation in the absence of external forces:

(1)
$$\partial_t f + c_i \partial_i f = Q(f),$$

where the symbols ∂_t and ∂_i denote partial derivatives with respect to time *t* and space variables x_i (i = 1, 2, 3), respectively¹, and the collision integral Q(f) represents the rate of change of the distribution function *f* due to collisions including the influence of internal degrees of freedom through collisional cross section.

¹Throughout the paper summation with respect to repeated indices is assumed, where the range of the sum is to be understood from the context: when the index represents a spatial coordinate, the range of the sum is between 1 and 3; in all the other cases the sum is intended over the range of variability of the repeated index.

Focusing on the case of rarefied polyatomic gases characterized by the following thermal and the polytropic caloric equations of state at equilibrium:

(2)
$$p = \frac{k}{m}\rho T, \quad \varepsilon = \frac{D}{2}\frac{k}{m}T,$$

where k, m and D are, respectively, the Boltzmann constant, mass of a particle and the degrees of freedom of a particle. The hydrodynamic variables ρ (mass density), ρv_i (momentum) and $\rho \varepsilon$ (internal energy) are defined in terms of the collision invariants m, mc_i and $mc^2/2 + I$ as follows:

$$\rho = \int_{\mathbb{R}^3} \int_0^\infty mf \varphi(I) \, dI \, d\mathbf{c}, \quad \rho v_i = \int_{\mathbb{R}^3} \int_0^\infty mf c_i \varphi(I) \, dI \, d\mathbf{c},$$
$$\rho \varepsilon + \frac{1}{2} \rho v^2 = \int_{\mathbb{R}^3} \int_0^\infty mf \left(\frac{c^2}{2} + \frac{I}{m}\right) \varphi(I) \, dI \, d\mathbf{c},$$

where the non-negative measure $\varphi(I) dI$ is a property of the model aimed at recovering the classical (polytropic) caloric equation of state for polyatomic gases at equilibrium (2)₂. To this aim, it can be shown that:

$$\varphi(I) = I^{\delta}, \quad \delta = \frac{D-5}{2} \quad (\delta > -1).$$

Introducing for the sake of compactness the following symbol

$$c_A = \begin{cases} 1 & \text{for } A = 0\\ c_{i_1} \dots c_{i_A} & \text{for } 1 \le A \le N \end{cases}$$

where the indices $i_1 \le i_2 \le \cdots \le i_A$ take the values 1, 2, 3, and defining the moments of the distribution function f as the following quantities² [17]:

 2 An equivalent notation for the moments defined in (3) is the following:

$$F_{A} = \begin{cases} F & \text{for } A = 0 \\ F_{i_{1}...i_{A}} & \text{for } 1 \le A \le N \end{cases} \quad G_{l|A'} = \begin{cases} G_{ll} & \text{for } A' = 0 \\ G_{l|l_{1}...i_{A'}} & \text{for } 1 \le A' \le M \end{cases}$$

$$F_{iA} = \begin{cases} F_{i} & \text{for } A = 0 \\ F_{ii_{1}...i_{A}} & \text{for } 1 \le A \le N \end{cases} \quad G_{l|iA'} = \begin{cases} G_{l|i} & \text{for } A' = 0 \\ G_{l|l_{1}...i_{A'}} & \text{for } 1 \le A' \le M \end{cases}$$

$$P_{A} = \begin{cases} 0 & \text{for } A = 0 \\ 0 & \text{for } A = 1 \\ P_{i_{1}...i_{A}} & \text{for } 2 \le A \le N \text{ (with } P_{l|l} = 0) \end{cases}, \quad Q_{l|A'} = \begin{cases} 0 & \text{for } A' = 0 \\ Q_{l|l_{1}...l_{A'}} & \text{for } 1 \le A' \le M \end{cases}$$

In the following, the capital and primed capital indices, respectively, run from 0 to N and 0 to M.

$$F_{A} = \int_{\mathbb{R}^{3}} \int_{0}^{\infty} mfc_{A}I^{\delta} dI d\mathbf{c}, \quad G_{llA'} = \int_{\mathbb{R}^{3}} \int_{0}^{\infty} mf\left(c^{2} + \frac{2I}{m}\right)c_{A'}I^{\delta} dI d\mathbf{c},$$

(3)
$$F_{iA} = \int_{\mathbb{R}^{3}} \int_{0}^{\infty} mfc_{i}c_{A}I^{\delta} dI d\mathbf{c}, \quad G_{lliA'} = \int_{\mathbb{R}^{3}} \int_{0}^{\infty} mf\left(c^{2} + \frac{2I}{m}\right)c_{i}c_{A'}I^{\delta} dI d\mathbf{c},$$

$$P_{A} = \int_{\mathbb{R}^{3}} \int_{0}^{\infty} mQ(f)c_{A}I^{\delta} dI d\mathbf{c}, \quad Q_{llA'} = \int_{\mathbb{R}^{3}} \int_{0}^{\infty} mQ(f)\left(c^{2} + \frac{2I}{m}\right)c_{A'}I^{\delta} dI d\mathbf{c},$$

it is possible to build two hierarchies of moments that, after truncation, read as follows:

(4)
$$\partial_t F_A + \partial_i F_{iA} = P_A, \quad \partial_t G_{llA'} + \partial_i G_{lliA'} = Q_{llA'}, \\ (0 \le A \le N) \qquad (0 \le A' \le M)$$

being N and M the truncation orders of the F-hierarchy (momentum-like hierarchy) and of the G-hierarchy (energy-like hierarchy), respectively. System (4) will be denoted as "(N, M)-system", being N and M a priori independent. It is worth noting that the first two equations of the F-hierarchy represent the conservation of mass and momentum ($P \equiv 0, P_i \equiv 0$), the first equation of the G-hierarchy represents the conservation of energy ($Q_{ll} \equiv 0$), and in each of the two hierarchies the flux in one equation appears as density in the following one—a feature in common with the single hierarchy of monatomic gases [16].

It is noted that the Euler equations (5-moment system) and the 14-moment system [3, 17] are particular cases of (4) obtained, respectively, with N = 1, M = 0, and with N = 2, M = 1.

2.1. Galilean invariance

It is reasonable to wonder whether a restriction exists on how the two hierarchies introduced in the previous section are truncated. In the spirit of ET, the application of the universal principles—in the present case, the Galilean invariance [18]—leads to the conclusion that in order to have a physically acceptable model, the truncation orders N and M cannot be chosen independently. The following theorem, proven in [1], holds:

THEOREM 1. In order for the (N, M)-system (4) to be Galilean invariant, it must be $M \le N - 1$.

2.2. Closure of the system

In the case of rarefied monatomic gases, the system of moment equations are closed by the method of the entropy principle or maximum entropy principle, and the equivalence of these two closures have been proved by Boillat and Ruggeri. Following the methodology outlined in [9], the Galilean invariant system of moment equations (4) is closed by EP or MEP, and the equivalence of EP and MEP is shown. In the following, the general frameworks of EP and MEP are discussed, and then for the usual entropy density the system is closed.

2.2.1. Entropy principle. The closure of the (N, M)-system is achieved by making use of the entropy principle. This consists in requiring that all the solutions of (4) satisfy the entropy inequality:

(5)
$$\partial_t h + \partial_i h_i = \Sigma \ge 0,$$

where the entropy density h, entropy flux h_i and entropy production Σ are the constitutive functions:

(6)
$$h \equiv h(F_A, G_{A'}), \quad h_i \equiv h_i(F_A, G_{A'}), \quad \Sigma \equiv \Sigma(F_A, G_{A'}).$$

The results of EP are summarized as follows:

THEOREM 2. The necessary and sufficient condition for all solutions of balance equations of (N, M)-system (4) to satisfy the entropy inequality (5) is that the distribution function $f_{(N,M)}$ depends only on the scalar variable

$$\chi_{(N,M)} = u'_A c_A + \left(c^2 + \frac{2I}{m}\right) v'_{A'} c_{A'},$$

where u'_A and $v'_{A'}$ are the so-called main fields defined in [10]. In this case,

(7)

$$h = \int_{\mathbb{R}^{3}} \int_{0}^{\infty} m(\chi_{(N,M)}H' - H)I^{\delta} dI d\mathbf{c},$$

$$h_{i} = \int_{\mathbb{R}^{3}} \int_{0}^{\infty} m(\chi_{(N,M)}H' - H)c_{i}I^{\delta} dI d\mathbf{c},$$

$$\Sigma = \int_{\mathbb{R}^{3}} \int_{0}^{\infty} mQ(f)\chi_{(N,M)}I^{\delta} dI d\mathbf{c},$$

where $H = H(\chi_{(N,M)})$ is a function which satisfies

(8)
$$H' = \frac{dH}{d\chi_{(N,M)}} = f_{(N,M)}(\chi_{(N,M)}).$$

Moreover, with the condition that H'' < 0, the system is rewritten into the symmetric hyperbolic form by adopting the main field as independent fields.

PROOF. The requirement that all solutions of (4) satisfy (5) can be expressed, by introducing the main fields u'_A and $v'_{A'}$, as

$$\partial_t h + \partial_i h_i - u'_A (\partial_t F_A + \partial_i F_{iA} - P_A) - v'_{A'} (\partial_t G_{llA'} + \partial_i G_{lliA'} - Q_{llA'}) \ge 0.$$

Since *h* and h_i are the constitutive function as (6),

(9)
$$dh = u'_A dF_A + v'_{A'} dG_{A'}, \quad dh_i = u'_A dF_{iA} + v'_{A'} dG_{iA'},$$

and

(10)
$$\Sigma = u'_A P_A + v'_{A'} Q_{A'} \ge 0,$$

From (9) the expressions of the main fields are obtained:

$$u'_A = \frac{\partial h}{\partial F_A}, \quad v'_{A'} = \frac{\partial h}{\partial G_{A'}}.$$

In order to transform the independent variables from F_A and $G_{A'}$ to u'_A and $v'_{A'}$, the following new variables are introduced:

(11)
$$h' = u'_A F_A + v'_{A'} G_{A'} - h, \quad h'_i = u'_A F_{iA} + v'_{A'} G_{iA'} - h_i.$$

The derivatives of these variables are as follows:

$$dh' = F_A du'_A + G_{A'} dv'_{A'}, \quad dh'_i = F_{iA} du'_A + G_{iA'} dv'_{A'},$$

and then the original variables are given as

(12)
$$F_{A} = \frac{\partial h'}{\partial u'_{A}}, \quad G_{A'} = \frac{\partial h'}{\partial v'_{A'}}, \quad F_{iA} = \frac{\partial h'_{i}}{\partial u'_{A}}, \quad G_{iA'} = \frac{\partial h'_{i}}{\partial v'_{A'}}.$$

As the densities F_A and $G_{A'}$ are expressed by the distribution function (3), dropping the subscript (N, M) of f and χ for the sake of compactness, dh' and dh'_i are expressed as

$$dh' = \int_{\mathbb{R}^3} \int_0^\infty mf\left(c_A \, du'_A + \left(c^2 + \frac{2I}{m}\right)c_{A'} \, dv'_{A'}\right) I^\delta \, dI \, d\mathbf{c}$$
$$= \int_{\mathbb{R}^3} \int_0^\infty mf \, d\chi \, I^\delta \, dI \, d\mathbf{c} = d \int_{\mathbb{R}^3} \int_0^\infty mHI^\delta \, dI \, d\mathbf{c}.$$

The introduction of $H(\chi)$ which satisfy (8) indicates that $f = f(\chi)$. As a consequence,

(13)
$$h' = \int_{\mathbb{R}^3} \int_0^\infty m H I^\delta \, dI \, d\mathbf{c}.$$

Similarly, for the new flux,

(14)
$$h'_i = \int_{\mathbb{R}^3} \int_0^\infty mc_i H I^\delta \, dI \, d\mathbf{c}.$$

Therefore, inserting (13) and (14) into (11), the expressions of the entropy density and flux in (7) are deduced. For the entropy production (10) is equal to the expression in (7).

The system (4) may be rewritten with respect to the independent fields u'_{A} and $v'_{A'}$ by using (12) as follows:

(15)
$$\begin{pmatrix} J_{AB}^{0} & J_{AB'}^{1} \\ J_{A'B}^{1} & J_{A'B'}^{2} \end{pmatrix} \partial_{l} \begin{pmatrix} u'_{B} \\ v'_{B'} \end{pmatrix} + \begin{pmatrix} J_{iAB}^{0} & J_{iAB'}^{1} \\ J_{iA'B}^{1} & J_{iA'B'}^{2} \end{pmatrix} \partial_{i} \begin{pmatrix} u'_{B} \\ v'_{B'} \end{pmatrix} = \begin{pmatrix} P_{A} \\ Q_{llA'} \end{pmatrix},$$

where

$$J_{AB}^{0} = \frac{\partial^{2}h'}{\partial u'_{A}\partial u'_{B}} = \int_{\mathbb{R}^{3}} \int_{0}^{\infty} mH''c_{A}c_{B}I^{\delta} dI d\mathbf{c},$$
(16)
$$J_{AB'}^{1} = \frac{\partial^{2}h'}{\partial u'_{A}\partial v'_{B'}} = \int_{\mathbb{R}^{3}} \int_{0}^{\infty} mH''c_{A}c_{B'}\left(c^{2} + \frac{2I}{m}\right)I^{\delta} dI d\mathbf{c},$$

$$J_{A'B'}^{2} = \frac{\partial^{2}h'}{\partial v'_{A'}\partial v'_{B'}} = \int_{\mathbb{R}^{3}} \int_{0}^{\infty} mH''c_{A'}c_{B'}\left(c^{2} + \frac{2I}{m}\right)^{2}I^{\delta} dI d\mathbf{c}.$$

By the requirement that the system is symmetric hyperbolic, the coefficient matrix of $\partial_t(u'_B v'_{B'})$ must be negative definite. With any variables X_A and $X_{A'}$, the quadratic form associated to the matrix is expressed as

$$(X_A \quad X_{A'}) \begin{pmatrix} J^0_{AB} & J^1_{AB'} \\ J^1_{A'B} & J^2_{A'B'} \end{pmatrix} \begin{pmatrix} X_B \\ X_{B'} \end{pmatrix}$$

= $\int_{\mathbb{R}^3} \int_0^\infty m H'' \left(c_A X_A + \left(c^2 + \frac{2I}{m} \right) c_{A'} X_{A'} \right)^2 I^\delta \, dI \, d\mathbf{c}$

This concludes that when H'' < 0, the matrix is negative definite.

2.2.2. Maximum entropy principle. As an alternative approach to close the (N, M)-system, the maximum entropy principle (MEP) requires the distribution function $f_{(N,M)}$ to maximize the entropy h under the constraints that the moments F_A and $G_{llA'}$ are given as in (3). For the generic form of entropy density:

$$h = \int_{\mathbb{R}^3} \int_0^\infty m \Psi(f) I^\delta \, dI \, d\mathbf{c},$$

the variational problem of the functional

$$\begin{aligned} \mathscr{L}_{(N,M)}(f,\Lambda_A,\mu_{A'}) &= \int_{\mathbb{R}^3} \int_0^\infty m \Psi(f) I^\delta \, dI \, d\mathbf{c} + \Lambda_A \Big(F_A - \int_{\mathbb{R}^3} \int_0^\infty m f c_A I^\delta \, dI \, d\mathbf{c} \Big) \\ &+ \mu_{A'} \Big(G_{llA'} - \int_{\mathbb{R}^3} \int_0^\infty m f \Big(c^2 + \frac{2I}{m} \Big) c_{A'} I^\delta \, dI \, d\mathbf{c} \Big), \end{aligned}$$

where Λ_A and $\mu_{A'}$ are the Lagrange multipliers of the system. The first and second variations with respect to f are obtained as

$$\delta \mathscr{L}_{(N,M)} = \int_{\mathbb{R}^3} \int_0^\infty m \left\{ \frac{d\Psi}{df} - \Lambda_A c_A - \mu_{A'} \left(c^2 + \frac{2I}{m} \right) c_{A'} \right\} \delta f I^\delta \, dI \, d\mathbf{c},$$
$$\delta^2 \mathscr{L}_{(N,M)} = \int_{\mathbb{R}^3} \int_0^\infty m \frac{d^2 \Psi}{df^2} (\delta f)^2 I^\delta \, dI \, d\mathbf{c}.$$

As a necessary condition for a extremum,

$$\frac{d\Psi}{df} = \chi \equiv \Lambda_A c_A + \mu_{A'} \left(c^2 + \frac{2I}{m} \right) c_{A'},$$

and therefore

(17)
$$\Psi = \chi f - \int f \, d\chi$$

As a necessary condition for a maximum, the inequality $\frac{d^2\Psi}{df^2} < 0$ must be held, and from (17) the following inequality is obtained:

$$\frac{df}{d\chi} < 0.$$

As Boillat and Ruggeri have proven [9], considering that f = H', the maximization of entropy derive the same result with the method of EP. The converse is also true. The Lagrange multipliers turn out to be identified as the main field: $u'_A = \Lambda_A$ and $v'_{A'} = \mu_{A'}$.

2.2.3. The closure for classical entropy density. If it is required that *h* is the usual entropy density defined as follows:

$$h = -k \int_{\mathbb{R}^3} \int_0^\infty f \log f I^\delta \, dI \, d\mathbf{c},$$

it can be shown [1] that the sought distribution function $f_{(N,M)}$ has the following form:

(18)
$$f = \exp\left(-1 - \frac{m}{k}\chi\right).$$

In this case the entropy flux h_i and the entropy production Σ can be expressed as

$$h_i = -k \int_{\mathbb{R}^3} \int_0^\infty c_i f \log f I^\delta \, dI \, d\mathbf{c}, \quad \Sigma = -k \int_{\mathbb{R}^3} \int_0^\infty Q(f) \log f I^\delta \, dI \, d\mathbf{c}.$$

Making use of (18) and of the expressions for F_A and $G_{llA'}$, the Lagrange multipliers are evaluated in terms of F_A and $G_{llA'}$ and, plugging (18) into the last flux and production term, the system can be closed.

In this case, the symmetric conditions of the system (15) is satisfied and the coefficients (16) may be expressed as follows:

(19)
$$J_{AB}^{0} = -\frac{m^{2}}{k} \int_{\mathbb{R}^{3}} \int_{0}^{\infty} fc_{A}c_{B}I^{\delta} dI d\mathbf{c},$$
$$J_{AB'}^{1} = -\frac{m^{2}}{k} \int_{\mathbb{R}^{3}} \int_{0}^{\infty} fc_{A}c_{B'} \left(c^{2} + \frac{2I}{m}\right) I^{\delta} dI d\mathbf{c},$$
$$J_{A'B'}^{2} = -\frac{m^{2}}{k} \int_{\mathbb{R}^{3}} \int_{0}^{\infty} fc_{A'}c_{B'} \left(c^{2} + \frac{2I}{m}\right)^{2} I^{\delta} dI d\mathbf{c}.$$

2.3. The distribution function in the neighborhood of a local equilibrium state

The distribution function (18) is expanded in the neighborhood of a local equilibrium state:

$$f \approx f^{E} \left[1 - \frac{m}{k} \left(\tilde{u}_{A}' c_{A} + \left(c^{2} + \frac{2I}{m} \right) \tilde{v}_{A'}' c_{A'} \right) \right], \quad \tilde{u}_{A}' = u_{A}' - u_{A}'^{E}, \quad \tilde{v}_{A'}' = v_{A'}' - v_{A'}'^{E},$$

where the superscript "*E*" denotes that a quantity is evaluated in the equilibrium state, i.e. involving the local equilibrium distribution function f^E given as follows [17]:

(20)
$$f^E = \frac{1}{q(T)} \frac{\rho}{m} \left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left(-\frac{m}{2kT}\left(C^2 + \frac{2I}{m}\right)\right),$$

where $C^2 = C_i C_i$ with the peculiar velocity $C_i = c_i - v_i$ and the normalization function q(T) is defined as

$$q(T) = \int_0^\infty \exp\left(-\frac{I}{kT}\right) I^\delta dI = (kT)^{1+\delta} \Gamma(1+\delta),$$

and Γ denotes the gamma function. All the Lagrange multipliers (main field) at equilibrium vanish, except those corresponding to the hydrodynamic variables ρ , v_i , ε . After some manipulation [1], a linear algebraic system that permits to evaluate the main field $(u_A'^E, v_{A'}'^E)$ in terms of the densities F_A and $G_{llA'}$ is obtained:

$$\begin{pmatrix} J_{AB}^{0|E} & J_{AB'}^{1|E} \\ J_{A'B}^{1|E} & J_{A'B'}^{2|E} \end{pmatrix} \begin{pmatrix} \tilde{u}'_B \\ \tilde{v}'_{B'} \end{pmatrix} = \begin{pmatrix} F_A - F_A^E \\ G_{llA'} - G_{llA'}^E \end{pmatrix}.$$

Plugging (20) into (19), it is also possible to obtain the following useful relations:

$$\begin{split} J^{0|E}_{AB} &= J^{\mathscr{M}}_{AB}, \quad J^{1|E}_{AB'} = J^{\mathscr{M}}_{iiAB'} + 2c^2_s(1+\delta)J^{\mathscr{M}}_{AB'}, \\ J^{2|E}_{A'B'} &= J^{\mathscr{M}}_{iijjA'B'} + 4c^2_s(1+\delta)(J^{\mathscr{M}}_{iiA'B'} + c^2_s(2+\delta)J^{\mathscr{M}}_{A'B'}), \end{split}$$

where $c_s = \sqrt{\frac{k}{m}T}$, $J_{AB}^{\mathcal{M}}$ is defined as:

$$J_{AB}^{\mathscr{M}} = -\frac{m^2}{k} \int_{\mathbb{R}^3} f^{\mathscr{M}} c_A c_B \, d\mathbf{c},$$

and $f^{\mathcal{M}}$ denotes the Maxwellian.

Once the main field $(u'_A, v'_{A'})$ has been calculated in terms of F_A and $G_{llA'}$, the constitutive functions necessary to close the system are finally obtained.

2.4. Equilibrium characteristic velocities

The set of the characteristic velocities of the system (15) at equilibrium in the direction of propagation having unit vector $\mathbf{n} \equiv (n^i)$, denoted as $\lambda_{(N,M)}^E$, is the set of the roots of the characteristic polynomial $T_{(N,M)}^E$ given by:

$$T^{E}_{(N,M)} = \det \begin{bmatrix} \begin{pmatrix} J^{0|E}_{iAB} & J^{1|E}_{iAB'} \\ J^{1|E}_{iA'B} & J^{2|E}_{iA'B'} \end{pmatrix} n^{i} - \lambda^{E}_{(N,M)} \begin{pmatrix} J^{0|E}_{AB} & J^{1|E}_{AB'} \\ J^{1|E}_{A'B} & J^{2|E}_{A'B'} \end{pmatrix} \end{bmatrix} = 0.$$

Without loss of generality, for the sake of simplicity, the one-dimensional case is studied. After some manipulations [1], the previous expression can be written as:

(21)
$$T_{(N,M)}^{E} = \det \begin{pmatrix} \hat{J}_{p+r,q+s}^{\mathscr{M}} & \hat{J}_{p'+r,q'+s+1}^{\mathscr{M}} \\ \hat{J}_{p+r',q+s'+1}^{\mathscr{M}} & \hat{J}_{p'+r',q'+s'+2}^{\mathscr{M}} + 4c_{s}^{4}(1+\delta)\hat{J}_{p'+r',q'+s'}^{\mathscr{M}} \end{pmatrix} = 0,$$

being

$$J_{p+r,q+s}^{\mathscr{M}} = -\frac{m^2}{k} \int_{\mathbb{R}^3} f^{\mathscr{M}} c_1^{p+r} (c^2)^{q+s} \, d\mathbf{c}.$$

where the indexes p, q, p', and q' are the non-negative integers satisfying:

$$0 \le p + 2q \le N$$
, $0 \le p' + 2q' \le M$ $(M \le N - 1)$.

Analyzing the features of the polynomial $T^E_{(N,M)}$, it seems that, as expected, the equilibrium characteristic velocities $\lambda^E_{(N,M)}$ depend on the the parameter δ and, in turn, on the degrees of freedom *D*. Nonetheless, it can be easily seen that this is not always the case [1]. Upon inspection of the features of $T^E_{(N,M)}$, the following holds:

THEOREM 3. If M < N - 1, the equilibrium characteristic velocities of a (N, M)-system, $\lambda_{(N,M)}^E$, are independent from the degrees of freedom of a particle D. More specifically, the equilibrium characteristic velocities coincide with those of a (N)-system, $\lambda_{(N)}^E$, and those of a (M)-system, $\lambda_{(M)}^E$, of monatomic gases:

$$\lambda_{(N,M)}^E = \lambda_{(N)}^E \cup \lambda_{(M)}^E$$

Moreover, the maximum equilibrium characteristic velocity of the (N, M)-system, $\lambda_{(N,M)}^{E,\max}$, does not depend on M and coincides with the one of the (N)-system for

monatomic gases:

$$\lambda_{(N,M)}^{E,\max} = \lambda_{(N)}^{E,\max}.$$

It can be seen that Theorem 3 is true for the (N^+, M) -system with M < N where N^+ truncation order denotes that in addition to the first N tensorial equations the trace part of the N + 1 tensorial equation is considered.

Combining the results of Theorem 1 and Theorem 3, the following conclusion holds:

THEOREM 4. The (N, M)-system is Galilean invariant and its equilibrium characteristic velocities depend on the degrees of freedom D if and only if M = N - 1.

Physical examples are given by the Euler system and by the 14-moment theory, which are obtained, respectively, with N = 1, M = 0, and with N = 2, M = 1.

3. Characteristic velocities of (N, N-1)-systems

The maximum equilibrium characteristic velocities of a (N, N - 1)-system of polyatomic rarefied gases is limited by those of monatomic gases as pointed out by the following:

THEOREM 5. The maximum equilibrium characteristic velocity of a (N, N - 1)system of a polyatomic gas, $\lambda_{(N,N-1)}^{\max}$, is bounded by the maximum equilibrium characteristic velocities of the (N^+) -system and of the (N)-system of monatomic gases as follows:

$$\lambda_{(N)}^{\max} \le \lambda_{(N,N-1)}^{\max} \le \lambda_{(N^+)}^{\max}.$$

In order to prove the above Theorem, it suffices to notice that both the upper and the lower bounds are obtained from Theorem 3 and the subcharacteristic conditions [10]:

$$\begin{split} \lambda^{\max}_{(N^+)} &= \lambda^{\max}_{(N^+,M)} = \lambda^{\max}_{(N^+,N-1)} \geq \lambda^{\max}_{(N,N-1)}, \quad \forall M < N \\ \lambda^{\max}_{(N,N-1)} &\geq \lambda^{\max}_{(N,M)} = \lambda^{\max}_{(N)}, \quad \forall M < N-1. \end{split}$$

The influence of the degrees of freedom D on the characteristic velocities is described in the following.

The limit case $D \to 3$. It has been proven for the 14-moment theory in [5] and for the general theory of (N, M)-system in [8] that in the limit case $D \to 3$ the solutions of the (N, N - 1)-system for rarefied polyatomic gases (which is composed by $n_{(N,N-1)} = \frac{1}{6}(N+1)(N+2)(2N+3)$ equations) converge to those of the (N^+) -system for rarefied monatomic gases (which is composed by $n_{(N^+)} = \frac{1}{6}(N+1)(N^2+6N+6)$ equations), and the differences between the *F*-hierarchy and G-hierarchy,

$$I_{\alpha} \equiv \lim_{D \to 3} (F_{ll\alpha} - G_{ll\alpha}) \quad (0 \le \alpha \le N - 2)$$

which are governed by the $n_{(N-2)} = \frac{1}{6}(N-1)N(N+1) = n_{(N,N-1)} - n_{(N^+)}$ balance equations:

(22)
$$\partial_t I_{\alpha} + \partial_i I_{i\alpha} = \lim_{D \to 3} (P_{ll\alpha} - Q_{ll\alpha}),$$

vanish under suitable initial condition for rarefied monatomic gases, therefore the double-hierarchy is regarded as the single-hierarchy of rarefied monatomic gases. As a consequence of the convergence of the solution of polyatomic gases towards those of monatomic gases, the characteristic velocities follow the same rule. It is noted that when the characteristic polynomial (21) is calculated in this limit, the obtained characteristic velocities are those of the (N^+) -system augmented by those of (N-2)-system:

(23)
$$\lim_{D \to 3} \lambda^{E}_{(N,N-1)} = \lambda^{E}_{(N^{+})} \cup \lambda^{E}_{(N-2)}.$$

However, the characteristic velocities of the (N-2)-system are related to the balance equations (22), which vanish in this limit. It is noted (see Theorem 3) that when $D \rightarrow 3$, the maximum characteristic velocity of the (N, N-1)-system coincides with the one of the (N^+) -system for rarefied monatomic gases, which in turn coincides with that of the (N^+, M) -system for any M < N, i.e.

$$\lim_{D \to 3} \lambda_{(N,N-1)}^{\max} = \lambda_{(N^+)}^{\max} = \lambda_{(N^+,M)}^{\max}, \quad \forall M < N.$$

The limit case $D \to \infty$. In the case $D \to \infty$, the following Theorem holds [1]:

THEOREM 6. When $D \to \infty$, the $n_{(N,N-1)} = \frac{1}{6}(N+1)(N+2)(2N+3)$ characteristic velocities of the (N, N-1)-system coincide with the $n_{(N)} = \frac{1}{6}(N+1) \cdot (N+2)(N+3)$ ones of the (N)-system and with the $n_{(N-1)} = \frac{1}{6}N(N+1)(N+2)$ ones of the (N-1)-system, i.e.

$$\lim_{D\to\infty}\lambda^E_{(N,N-1)}=\lambda^E_{(N)}\cup\lambda^E_{(N-1)}.$$

In particular, the maximum characteristic velocity of the (N, N - 1)-system coincides with the one of the (N)-system for monatomic gases which is in turn coincident with the one of the (N, M)-system for any M < N - 1, i.e.

$$\lim_{D \to \infty} \lambda_{(N,N-1)}^{\max} = \lambda_{(N)}^{\max} = \lambda_{(N,M)}^{\max}, \quad \forall M < N-1.$$

The case $3 < D < \infty$. In the case $3 < D < \infty$ the following is obtained as a corollary of previous results.

THEOREM 7. For any truncation order N, the maximum equilibrium characteristic velocity of a (N, N - 1)-system of polyatomic gases is bounded as follows:

$$\lim_{D \to \infty} \lambda_{(N,N-1)}^{\max} \le \lambda_{(N,N-1)}^{\max} \le \lim_{D \to 3} \lambda_{(N,N-1)}^{\max}.$$

4. Dependence of the maximum equilibrium characteristic velocities on the truncation order

As a consequence of Theorem 5, the following result is obtained.

THEOREM 8. The maximum equilibrium characteristic velocity of a (N, N - 1)-system of polyatomic gases has the same lower bound as a (N)-system of mona-tomic gases [9]:

(24)
$$\hat{\lambda}_{(N,N-1)}^{\max} \equiv \frac{\lambda_{(N,N-1)}^{\max}}{c_0} \ge \frac{\lambda_{(N)}^{\max}}{c_0} \ge \sqrt{\frac{6}{5}\left(N - \frac{1}{2}\right)},$$

where $c_0 = \sqrt{\frac{5}{3} \frac{k}{m} T}$ is the sound velocity in the rarefied monatomic gas case at an equilibrium state.

A major consequence of the previous Theorem is that maximum equilibrium characteristic velocity is unbounded as $N \rightarrow \infty$.

In Figure 1 the dependence of $\hat{\lambda}_{(N,N-1)}^{\max}$ on N is shown for D = 50, and for the values $D \to 3$, $D \to \infty$, as well as for the lower bound given by (24). From the figure, it is evident that for a given D, $\lambda_{(N,N-1)}^{\max}$ gets closer and closer to the limit



Figure 1: Nondimensional equilibrium maximum characteristic velocity of the (N, N-1)-system, $\hat{\lambda}_{(N, N-1)}^{\max} = \lambda_{(N, N-1)}^{\max}/c_0$, as a function of N for a polyatomic gas with D = 50 (dots). The limits for $D \to 3$ and $D \to \infty$ are represented by the continuous curves immediately above and below the dots, respectively. The bottom curve represents the lower bound given by (24).

velocity corresponding to the case $D \rightarrow 3$. For what concerns the characteristic velocities, this numerical result supports the conjecture according to which as the order of the system increases, the monatomic gas model allows to describe with reasonable accuracy also polyatomic gases.

Moreover the dependence of $\lambda_{(N,N-1)}^{\max}$ on N has also the feature that—as seen from Theorem 5 and the subcharacteristic conditions—the ranges of variation of $\lambda_{(N,N-1)}^{\max}$ with respect to D, for different values of N are non-overlapping, e.g.,

$$\lambda_{(N,N-1)}^{\max} \leq \lambda_{(N+1,N)}^{\max}$$
, for any *D*.

In other words, with (23) and Theorem 6, the following inequality holds:

$$\lim_{D\to 3} \lambda_{(N,N-1)}^{\max} \leq \lim_{D\to\infty} \lambda_{(N+1,N)}^{\max}.$$

5. SUMMARY AND CONCLUSIONS

In the framework of Extended thermodynamics, the results that in recent decades have been obtained for rarefied monatomic gases are extended to rarefied polyatomic gases.

In the kinetic model of polyatomic gases adopted now, the velocity distribution function depends not only on position, velocity and time as in the monatomic gas case, but also on an internal energy parameter accounting for the energy transfer during binary collisions. Correspondingly, Extended thermodynamics of polyatomic gases is based on the balance laws obtained as moments of the velocity distribution function and consist of a *double hierarchical structure*, that is, a momentum-like and a energy-like hierarchies. One of the question of Extended thermodynamics for rarefied polyatomic gases is what is the appropriate choice of the orders of truncation for these two hierarchies? In this paper the answer has been found by means of the universal principle of Galilean invariance which restricts this relation as follows: once the order of truncation N of the momentum-like hierarchy is given, the order of truncation M of the energy-like hierarchy is automatically forced to respect the inequality $M \leq N - 1$. Moreover, by means of the requirement that the characteristic velocities of the system cannot be independent on the degrees of freedom of a particle D, it has been pointed out that once the order N is given, the order M must be exactly equal to N - 1.

The closure of the truncated system has been also discussed. The two equivalent methods, that is, the entropy principle and the maximum entropy principle, which are well-established for the monatomic gas case, are adopted also in the polyatomic gas case. For the usual entropy density, the explicit expression of the velocity distribution function is obtained and the closed set of the equations have been shown.

Moreover, an analysis on the dependence of the maximum characteristic velocity of the rarefied polyatomic gas model has been proposed: it has been pointed out that the maximum characteristic velocity of the rarefied polyatomic gas is always bounded by the limit value obtained for the rarefied monatomic gas $(D \rightarrow 3)$ and by the limit value of a gas whose particles have infinite degrees of freedom $(D \rightarrow \infty)$. The analysis of the influence of the order of truncation N of the two hierarchies on the maximum characteristic velocity suggests that as the order N increases, the maximum characteristic velocity approaches the limit value of the rarefied monatomic gas case.

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References

- T. ARIMA A. MENTRELLI T. RUGGERI, Molecular Extended Thermodynamics of Rarefied Polyatomic Gases and Wave Velocities for Increasing Number of Moments, Annals of Physics 345, 111–140 (2014)
- [2] T. ARIMA T. RUGGERI M. SUGIYAMA S. TANIGUCHI, On the six-field model of fluids based on extended thermodynamics, Meccanica 4, DOI 10.1007/s11012-014-9886-0 (2014)
- [3] T. ARIMA S. TANIGUCHI T. RUGGERI M. SUGIYAMA, *Extended thermodynamics* of dense gases, Continuum Mech. Thermodyn. 24, 271–292 (2011)
- [4] T. ARIMA S. TANIGUCHI T. RUGGERI M. SUGIYAMA, Extended thermodynamics of real gases with dynamic pressure: An extension of Meixner's theory, Phys. Lett. A 376, 2799–2803 (2012)
- [5] T. ARIMA S. TANIGUCHI T. RUGGERI M. SUGIYAMA, Monatomic Rarefied Gas as a Singular Limit of Polyatomic Gas in Extended Thermodynamics, Phys. Lett. A 377, 2136–2140 (2013)
- [6] T. ARIMA S. TANIGUCHI T. RUGGERI M. SUGIYAMA, Dispersion relation for sound in rarefied polyatomic gases based on extended thermodynamics, Continuum Mech. Thermodyn. 25, 727–737 (2013)
- [7] T. ARIMA S. TANIGUCHI M. SUGIYAMA, Light scattering in rarefied polyatomic gases based on extended thermodynamics, Proceedings of The 34th Symposium on Ultrasonic Electronics 4, 15–16 (2013)
- [8] T. ARIMA S. TANIGUCHI T. RUGGERI M. SUGIYAMA, A singular limit of rarefied polyatomic gas to monatomic gas in molecular extended thermodynamics, 3 (in preparation)
- [9] G. BOILLAT T. RUGGERI, Moment equations in the kinetic theory of gases and wave velocities, Continuum Mech. Thermodyn. 9, 205–212 (1997)
- [10] G. BOILLAT T. RUGGERI, Hyperbolic Principal Subsystems: Entropy Convexity and Subcharacteristic Conditions, Arch. Rat. Mech. Anal. 137, 305–320 (1997)
- [11] C. BORGNAKKE P. S. LARSEN, Statistical Collision Model for Monte Carlo Simulation of Polyatomic Gas Mixture, J. Comput. Phys. 18, 405–420 (1975)
- [12] J.-F. BOURGAT L. DESVILLETTES P. LE TALLEC B. PERTHAME, Microreversible collisions for polyatomic gases, Eur. J. Mech. B/Fluids 13, 237–254 (1994)

- [13] L. DESVILLETTES R. MONACO F. SALVARANI, A kinetic model allowing to obtain the energy law of polytropic gases in the presence of chemical reactions, Eur. J. Mech. B Fluids 24, 219–236 (2005)
- [14] W. DREYER, Maximization of the entropy in non-equilibrium, J. Phys. A: Math. Gen. 20, 6505–6517 (1987)
- [15] I. MÜLLER T. RUGGERI, Extended Thermodynamics, Springer Tracts in Natural Philosophy 37 (I edition), Springer-Verlag, New York (1993)
- [16] I. MÜLLER T. RUGGERI, Rational Extended Thermodynamics, Springer Tracts in Natural Philosophy 37 (II edition), Springer-Verlag, New York (1998)
- [17] M. PAVIĆ T. RUGGERI S. SIMIĆ, Maximum entropy principle for rarefied polyatomic gases, Physica A 392, 1302–1317 (2013)
- [18] T. RUGGERI, Galilean invariance and entropy principle for systems of balance laws. The structure of extended thermodynamics, Continuum Mech. Thermodyn. 1, 3–20 (1989)
- [19] M. SLEMROD, From Boltzmann to Euler: Hilberts 6th problem revisited, Computers and Mathematics with Applications 65, 1497–1501 (2013)
- [20] S. TANIGUCHI T. ARIMA T. RUGGERI M. SUGIYAMA, Effect of dynamic pressure on the shock wave structure in a rarefied polyatomic gas, Phys. Fluids 26, 016103 (2014)
- [21] S. TANIGUCHI T. ARIMA T. RUGGERI M. SUGIYAMA, Thermodynamic theory of the shock wave structure in a rarefied polyatomic gas: Beyond the Bethe-Teller theory, Phys. Rev. E 89, 013025 (2014)

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