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Molecular Extended Thermodynamics of Rarefied Polyatomic Gases with a New Hierarchy of Moments

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Abstract: The aim of this paper is to construct the molecular extended thermodynamics for classical rarefied polyatomic gases with a new hierarchy, which is absent in the previous procedures of moment equations. The new hierarchy is deduced recently from the classical limit of the relativistic theory of moments associated with the Boltzmann–Chernikov equation. The field equations for 15 moments of the distribution function, in which the internal degrees of freedom of a molecule are taken into account, are closed with the maximum entropy principle. It is shown that the theory contains, as a principal subsystem, the previously polyatomic 14 fields theory, and in the monatomic limit, in which the dynamical pressure vanishes, the differential system converges, instead of to the Grad 13-moment system, to the Kremer 14-moment system.

Keywords: extended thermodynamics; maximum entropy principle; rarefied polyatomic gas; moments equation

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1. Introduction

It is well-known that the appropriate theory of the monatomic gas is the Boltzmann equation (as usual, the repeated indices denote the summation):

$$\frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial x_i} = Q(f), \quad (1)$$

where the state of the gas can be described by the distribution function $f(\mathbf{x}, \boldsymbol{\xi}, t)$, being $\mathbf{x} \equiv (x_i)$, $\boldsymbol{\xi} \equiv (\xi_i)$, t the space coordinates, the microscopic velocity and the time, respectively, and Q denotes the collisional term. A huge literature background exists on the Boltzmann equation in which very important mathematical contributions were given by Cercignani [1,2]. Associated to the distribution function, we can construct macroscopic observable quantities that are called moments (m is the atomic mass):

$$F_{k_1 k_2 \dots k_n}(\mathbf{x}, t) = m \int_{\mathbb{R}^3} f(\mathbf{x}, \boldsymbol{\xi}, t) \xi_{k_1} \xi_{k_2} \dots \xi_{k_n} d\boldsymbol{\xi}, \quad k_1, k_2, \dots, k_n = 1, 2, 3 \quad \text{and} \quad n = 0, 1, 2, \dots,$$

where the moment with $n = 0$ is denoted as F and is the mass density ρ . As a consequence of the Boltzmann equation (1), we have an infinite hierarchy of moment equations that are in the form of balance laws:

$$\frac{\partial F_{k_1 k_2 \dots k_n}}{\partial t} + \frac{\partial F_{k_1 k_2 \dots k_n k_{n+1}}}{\partial x_{k_{n+1}}} = P_{k_1 k_2 \dots k_n}, \quad n = 0, 1, \dots, \quad (2)$$

where

$$P_{k_1 k_2 \dots k_n} = m \int_{\mathbb{R}^3} Q(f) \xi_{k_1} \xi_{k_2} \dots \xi_{k_n} d\boldsymbol{\xi}, \quad P = P_{k_1} = P_{kk} = 0.$$

For a small Knudsen number $K_n < 0.1$, the continuum approach with the classical constitutive equations of Navier–Stokes and Fourier (NSF) gives a satisfactory theory and is applicable to a larger class of fluids, such as polyatomic and dense gases, compared to the Boltzmann equation.

Beyond the assumption of the local thermodynamic equilibrium which determines the application range of the NSF theory, many different approaches of nonequilibrium thermodynamics start from different points of view, such as the Extended Irreversible Thermodynamics (EIT) [3], the Rational Extended Thermodynamics (RET) [4–7], GENERIC, an acronym for the General Equation for Non-Equilibrium Reversible-Irreversible Coupling proposed in [8–10]. A tentative list of some different approaches in nonequilibrium thermodynamics was presented by Cimmelli, Jou, Ruggeri, and Ván (see [11] and references cited therein), and in the recent papers by Jou [12], by Öttinger, Struchtrup and Torrilhon [13], and by Kovács, Madjarević, Simić and Ván [14].

This paper belongs to the approach of RET. In this theory, dissipative fluxes, such as the viscous stress and the heat flux, are adopted as independent variables in addition to the usual hydrodynamic variables, and a system of balance equations with local-type constitutive equations is assumed. The main idea of RET is to consider, for sufficient large Knudsen number $K_n > 0.1$, a structure of balance laws that has the form dictated by the moments (2) truncated at some level. Then, the main problem is to obtain an optimal closure procedure. The first approach was purely phenomenological, which adopts the structure of balance laws of moments but forgets that the F 's are moments of a distribution function. The phenomenological closure was obtained by using the universal principles of continuum thermomechanics—I the Galilean invariance and the objectivity principle, II the entropy principle, and III the causality and thermodynamic stability (i.e., the convexity of the entropy)—to select admissible constitutive equations.

The first paper with this procedure was given by Liu and Müller [15] motivated by a paper of Ruggeri [16], considering 13 moments in the form of (2) with $n = 0, 1, 2, 3$ and taking only the trace part of the triple tensor with respect to two indexes: $(F, F_{k_1}, F_{k_1 k_2}, F_{k_1 k k})$ (so-called ET_{13}). It was surprising that the macroscopic closure obtained only by adopting the previous universal principles gives the same system obtained by Grad [17] using a completely different closure at the kinetic level. Successively, Kremer presented a refined model with 14 fields (monatomic ET_{14}) [18] by adopting a new scalar field F_{jjkk} in addition to the previous 13 fields: $(F, F_{k_1}, F_{k_1 k_2}, F_{k_1 k k}, F_{jjkk})$.

For the case with many fields such as (2) truncated at a generic tensorial order $\bar{N}$, to avoid the complexity of the phenomenological approach, the so-called molecular extended thermodynamics has been proposed in which the macroscopic quantities are moments of a distribution function [4]. For the closure, we adopt as a technique the variational procedure of Maximum Entropy Principle (MEP) introduced first in the theory of moments by Kogan [19] and resumed in the case with 13 moments by Dreyer [20]. The MEP for the system with many moments is studied in the first edition of Müller and Ruggeri's book [4], and it was proved that the closed system is symmetric hyperbolic. See also on this subject the mathematical revisiting due to Levermore [21]. It was also proved that the MEP closure is equivalent to the closure using an entropy principle by Boillat and Ruggeri [22]. A huge literature exists on the closure problem of moments for monatomic gas (see, for example, the book of Struchtrup [23]).

The first relativistic version of the modern RET was given by Liu, Müller and Ruggeri (LMR) [24] considering the Boltzmann–Chernikov relativistic equation [25–27]:

$$p^\alpha \partial_\alpha f = Q, \quad (3)$$

in which the distribution function f depends on (x^α, p^β) , where x^α are the space-time coordinates, p^α is the four-momentum ($p_\alpha p^\alpha = m^2 c^2$), $\partial_\alpha = \partial/\partial x^\alpha$, c denotes the light

velocity, m denotes the particle mass in the rest frame and $\alpha, \beta = 0, 1, 2, 3$. The relativistic moment equations associated with (3), truncated at tensorial index $N + 1$, are now

$$\partial_\alpha A^{\alpha\alpha_1\cdots\alpha_n} = I^{\alpha_1\cdots\alpha_n} \quad \text{with} \quad n = 0, \dots, N \quad (4)$$

with

$$A^{\alpha\alpha_1\cdots\alpha_n} = \frac{c}{m^{n-1}} \int_{\mathbb{R}^3} f p^\alpha p^{\alpha_1} \cdots p^{\alpha_n} d\mathbf{P}, \quad I^{\alpha_1\cdots\alpha_n} = \frac{c}{m^{n-1}} \int_{\mathbb{R}^3} Q p^{\alpha_1} \cdots p^{\alpha_n} d\mathbf{P}, \quad (5)$$

and

$$d\mathbf{P} = \frac{dp^1 dp^2 dp^3}{p^0}.$$

When $n = 0$, the tensor in (5)₁ reduces to A^α . Moreover, the production tensor in (5)₂ is zero for $n = 0, 1$, because the first 5 equations represent the conservation laws of the particle number and the energy-momentum, respectively.

When $N = 1$, we have the relativistic Euler system, and when $N = 2$, we have the LMR theory of a relativistic gas with 14 fields (in the monatomic case, from (5), we have $A^{\alpha\beta}_\beta = c^2 A^\alpha$ and therefore only 14 equations of (6) are independent):

$$\partial_\alpha A^\alpha = 0, \quad \partial_\alpha A^{\alpha\beta} = 0, \quad \partial_\alpha A^{\alpha\beta\gamma} = I^{\beta\gamma}, \quad (\beta, \gamma = 0, 1, 2, 3; I^\alpha_\alpha = 0). \quad (6)$$

The surprising result was that the LMR theory converges, in the classical limit, to Kremer's monatomic ET₁₄ theory, not Grad's theory (thus ET₁₃) as was expected [5,28,29].

For many years, the applicability range of RET was only limited to monatomic gases both in the classical and relativistic regime. For rarefied polyatomic gases, after some previous tentatives [30,31], Arima, Taniguchi, Ruggeri and Sugiyama [32] proposed a binary hierarchy of field equations with 14 fields (polyatomic ET₁₄) because now there is also, as a new field, the dynamical pressure relating to the relaxation of the molecular internal modes which is identical to zero in monatomic gases:

$$\begin{aligned} \frac{\partial F}{\partial t} + \frac{\partial F_i}{\partial x_i} &= 0, \\ \frac{\partial F_j}{\partial t} + \frac{\partial F_{ij}}{\partial x_i} &= 0, \\ \frac{\partial F_{ij}}{\partial t} + \frac{\partial F_{ijk}}{\partial x_k} &= P_{ij}, & \frac{\partial G_{ll}}{\partial t} + \frac{\partial G_{llk}}{\partial x_k} &= 0, \\ & & \frac{\partial G_{lli}}{\partial t} + \frac{\partial G_{llik}}{\partial x_k} &= Q_{lli}, \end{aligned} \quad (7)$$

where $F(= \rho)$ is the mass density, $F_i(= \rho v_i)$ is the momentum density, $G_{ll} = \rho v^2 + 2\rho\varepsilon$ is two times the energy density, F_{ij} is the momentum flux, and G_{llk} is the energy flux. As usual, v_i denotes the components of velocity, and ε is the specific internal energy. F_{ijk} and G_{llik} are the fluxes of F_{ij} and G_{lli} , respectively, and P_{ij} ($P_{ll} \neq 0$) and Q_{lli} are the productions with respect to F_{ij} and G_{lli} , respectively. This theory converges to the NSF theory in the parabolic limit, and in the monatomic singular limit, it converges to the Grad's theory [7,33,34].

This hierarchy was justified from the kinetic consideration in [35–37] by using the kinetic model of polyatomic gases. In the kinetic model, the distribution function $f(\mathbf{x}, \boldsymbol{\xi}, t, \mathcal{I})$ is assumed to depend on an additional non-negative internal energy parameter $\mathcal{I}$ that takes into account the influence of the internal degrees of freedom of a molecule on energy transfer during collisions and to obey the same form of Boltzmann equation (1). This model was introduced at a numerical level by Borgnakke and Larsen [38] and the theoretical description was given by Bourgat et al. in [39]. Another description of polyatomic gases consists of a semi-classical approach, which describes the internal structure of a molecule

with discrete energy levels and treats the gas as a sort of mixture of monatomic components. In the regime of RET, at least for the case with the smallest set of independent fields, it has been shown that the approaches with the continuous energy parameter and with discrete energy levels give the same differential system of macroscopic fields [40].

The theory with generic number of moments was also developed in [35,37,41] of which the system of moments equations is the following:

$$\begin{aligned} \frac{\partial F_{k_1 k_2 \dots k_n}}{\partial t} + \frac{\partial F_{k_1 k_2 \dots k_n k_{n+1}}}{\partial x_{k_{n+1}}} &= P_{k_1 k_2 \dots k_n}, \\ \frac{\partial G_{ll k_1 k_2 \dots k_m}}{\partial t} + \frac{\partial G_{ll k_1 k_2 \dots k_m k_{m+1}}}{\partial x_{k_{m+1}}} &= Q_{ll k_1 k_2 \dots k_m}, \end{aligned} \quad (8)$$

with the following definition of moments of polyatomic gases ($\xi^2 = |\xi|^2 = \xi_j \xi_j$):

$$\begin{aligned} F_{k_1 k_2 \dots k_n} &= m \int_{\mathbb{R}^3} \int_0^{+\infty} f(\mathbf{x}, \xi, t, \mathcal{I}) \xi_{k_1} \xi_{k_2} \dots \xi_{k_n} \varphi(\mathcal{I}) d\mathcal{I} d\xi, \\ P_{k_1 k_2 \dots k_n} &= m \int_{\mathbb{R}^3} \int_0^{+\infty} Q(f) \xi_{k_1} \xi_{k_2} \dots \xi_{k_n} \varphi(\mathcal{I}) d\mathcal{I} d\xi, \\ G_{ll k_1 k_2 \dots k_m} &= \int_{\mathbb{R}^3} \int_0^{+\infty} (m \xi^2 + 2\mathcal{I}) f(\mathbf{x}, \xi, t, \mathcal{I}) \xi_{k_1} \xi_{k_2} \dots \xi_{k_m} \varphi(\mathcal{I}) d\mathcal{I} d\xi, \\ Q_{ll k_1 k_2 \dots k_m} &= \int_{\mathbb{R}^3} \int_0^{+\infty} (m \xi^2 + 2\mathcal{I}) Q(f) \xi_{k_1} \xi_{k_2} \dots \xi_{k_m} \varphi(\mathcal{I}) d\mathcal{I} d\xi, \end{aligned}$$

where $\varphi(\mathcal{I})$ is the state density corresponding to $\mathcal{I}$, i.e., $\varphi(\mathcal{I})d\mathcal{I}$ represents the number of internal state between $\mathcal{I}$ and $\mathcal{I} + d\mathcal{I}$. The measure $\varphi(\mathcal{I})$ is necessary to recover the caloric equation of state of internal energy for polyatomic gases as observed first in [39]. In Section 2, the derivation of $\varphi(\mathcal{I})$ is discussed. We need to remark that the two blocks of hierarchies in (8) are not separated because the last fluxes in both hierarchies together with the production terms are functions to be determined by the closure of all densities ($F_{k_1 k_2 \dots k_n}, G_{ll k_1 k_2 \dots k_m}$). The index $n = 0, 1, \dots, \mathcal{N}$ and $m = 0, 1, \dots, \mathcal{M}$. Moreover, $P = P_{k_1} = Q_{ll} = 0$ since the first 4 equations of the F 's hierarchy and the first scalar equation of G 's hierarchy represent the mass, momentum, and energy conservations, respectively. It was studied in [37] that the physically meaningful choice of the truncated order $\mathcal{N}$ and $\mathcal{M}$, in the sense of the Galilean invariance and the characteristic velocity, is $\mathcal{M} = \mathcal{N} - 1$.

Recently, Pennisi and Ruggeri first constructed a relativistic version of polyatomic ET theory in the case of $N = 2$ [42]. Then, in [29], they studied the classical limit of generic moments equations (4) for a fixed N both in monatomic gas of which moments are (5) and in polyatomic gas of which moments are given by:

$$\begin{aligned} A^{\alpha \alpha_1 \dots \alpha_n} &= \frac{c}{m^{n-1}} \int_{\mathbb{R}^3} \int_0^{+\infty} f p^\alpha p^{\alpha_1} \dots p^{\alpha_n} \left(1 + n \frac{\mathcal{I}}{m c^2}\right) \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{p}, \\ I^{\alpha_1 \dots \alpha_n} &= \frac{c}{m^{n-1}} \int_{\mathbb{R}^3} \int_0^{+\infty} Q p^{\alpha_1} \dots p^{\alpha_n} \left(1 + n \frac{\mathcal{I}}{m c^2}\right) \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{p}, \end{aligned}$$

with a distribution function $f(x^\alpha, p^\beta, \mathcal{I})$ depends on the extra energy variable $\mathcal{I}$, similar to the classical one. They proved that there is a unique possible choice of classical moments for a prescribed truncation index N of (4). The moment system $N = 1$ is the Euler system with 5 moments for both cases of monatomic and polyatomic gases. For $N = 2$, which is the case for viscous heat-conducting fluids, in the monatomic case, we have the monatomic 14-moment equations according to the old result of [28]. Instead, in the polyatomic case, for $N = 2$, we have 15 moments in which, in addition to the previous polyatomic 14-moment equations (7), one equation for a mixed type moment H_{llmm} defined by

$$H_{llmm} = 2G_{llmm} - F_{llmm} \quad (9)$$

is involved. In the case that $N > 2$, the new hierarchy contains, in addition to the F 's and G 's hierarchies (8) with $n = 0, 1, \dots, N$ and $m = 0, 1, \dots, N - 1$, more complex $N + 1$ hierarchies for the mixed type of moments (see [29]), and these are absent in not only the previous studies of RET [34] but also other moment theories [43]. For more details on RET beyond the monatomic gas, see the new book of Ruggeri and Sugiyama [7].

The motivation for the present paper arises from the following considerations: (i) every classical theory must be the limit of a relativistic theory, and therefore, the theory with the binary hierarchy for polyatomic gases is regarded as an approximation of a more general model; (ii) the second reason, which is typical of RET in general, is that the more moments are taken into account, the more proximity to the kinetic theory which corresponds to the limit of infinite moments is obtained. Although there is still no theorem, as we have seen for monatomic gas in [5], it is needed to take many moments to have an optimal agreement with the experiments on such as the high-frequency sound wave, low-angle light scattering, or shock wave with a high Mach number. In the case of polyatomic gases, when the bulk viscosity is very high compared to the shear viscosity, the ET₁₄ gives excellent results concerning shock waves [44–46] and sound waves with high-frequency [47]. However, when the order of the bulk viscosity is the same or smaller the one of the shear viscosity, we have a similar situation to monatomic gases, and we expect the necessity of more moments.

Therefore, we think it is interesting to consider the new hierarchy of the moment comparing to the previous binary hierarchy (8). As a tentative and the most simple case, we consider the case with $N = 2$, that is, the system with 15-moment equations (ET₁₅):

$$\begin{aligned} \frac{\partial F}{\partial t} + \frac{\partial F_k}{\partial x_k} &= 0, \\ \frac{\partial F_i}{\partial t} + \frac{\partial F_{ik}}{\partial x_k} &= 0, \\ \frac{\partial F_{ij}}{\partial t} + \frac{\partial F_{ijk}}{\partial x_k} &= P_{ij}, \quad \frac{\partial G_{ll}}{\partial t} + \frac{\partial G_{llk}}{\partial x_k} = 0, \\ &\quad \frac{\partial G_{lli}}{\partial t} + \frac{\partial G_{llik}}{\partial x_k} = Q_{lli}, \\ &\quad \frac{\partial H_{llmm}}{\partial t} + \frac{\partial H_{llmmk}}{\partial x_k} = R_{llmm}, \end{aligned} \quad (10)$$

where H_{llmmk} is the flux of H_{llmm} given by (9), and R_{llmm} is the production with respect to H_{llmm} . In the following, after presenting equilibrium properties of the distribution function, we close the system (10) using MEP. As the collisional term, we introduce the generalized BGK model for relaxation processes of molecular internal modes [36]. We show that the closed set of the moment equations involves the polyatomic ET₁₄ theory as a principal subsystem, the monatomic ET₁₄ theory in the monatomic singular limit, and the NSF theory as its parabolic limit. To show the difference with the polyatomic ET₁₄ and the role of the new field H_{llmm} , we study the dispersion relation of the linear waves and compare the result of ET₁₄.

2. Molecular Extended Thermodynamics with 15-Field

First, we recall the equilibrium distribution function for polyatomic gases that was deduced first in the polytropic case (p, ε, ρ, T denote as usual the equilibrium pressure, the equilibrium specific internal energy, the mass density and the absolute temperature, while k_B is the Boltzmann constant and the constant $D = 3 + f_i$, where f_i is the degrees of freedom; in the monatomic gas $D = 3$)

$$p = \frac{k_B}{m} \rho T, \quad \varepsilon = \frac{D}{2} \frac{k_B}{m} T \quad (11)$$

in [35,39] and in the present case of non-polytropic gas

$$p = p(\rho, T) = \frac{k_B}{m} \rho T, \quad \varepsilon \equiv \varepsilon_E(T) \quad (12)$$

in [36,40]:

$$f_E = f_E^K f_E^I, \quad (13)$$

where f_E^K is the Maxwellian distribution function and f_E^I is the distribution function of the internal mode:

$$f_E^K = \frac{\rho}{m} \left(\frac{m}{2\pi k_B T} \right)^{3/2} \exp\left(-\frac{mC^2}{2k_B T}\right), \quad f_E^I = \frac{1}{A(T)} \exp\left(-\frac{\mathcal{I}}{k_B T}\right), \quad (14)$$

with the peculiar velocity $C_i = \xi_i - v_i$ ($C^2 = C_j C_j$) and the normalization factor (partition function) $A(T)$ defined by

$$A(T) = \int_0^{+\infty} \exp\left(-\frac{\mathcal{I}}{k_B T}\right) \varphi(\mathcal{I}) d\mathcal{I}, \quad (15)$$

where the average of the internal energy parameter $\mathcal{I}$ is made with respect to $\varphi(\mathcal{I}) d\mathcal{I}$. From (14)₂ and (15), the equilibrium distribution function of internal mode satisfies

$$\int_0^{+\infty} f_E^I \varphi(\mathcal{I}) d\mathcal{I} = 1. \quad (16)$$

The specific internal energy is the moment of f_E as follows:

$$\varepsilon = \varepsilon_E(T) = \varepsilon_E^K(T) + \varepsilon_E^I(T) = \frac{1}{2\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} (mC^2 + 2\mathcal{I}) f_E \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}, \quad (17)$$

where ε_E^K and ε_E^I are the equilibrium kinetic (translational) and internal specific energies defined by

$$\begin{aligned} \varepsilon_E^K(T) &= \frac{1}{2\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} mC^2 f_E \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C} = \frac{1}{2\rho} \int_{\mathbb{R}^3} mC^2 f_E^K d\mathbf{C} = \frac{3}{2} \frac{k_B}{m} T, \\ \varepsilon_E^I(T) &= \frac{1}{\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} \mathcal{I} f_E \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C} = \frac{1}{m} \int_0^{+\infty} \mathcal{I} f_E^I d\mathcal{I} = \frac{k_B}{m} T^2 \frac{d \log A(T)}{dT}. \end{aligned} \quad (18)$$

The identities (18) are obtained by taking into account (13)–(15) and by evaluating the derivative of (15) with respect to T . Therefore, if we know the partition function $A(T)$ by a statistical-mechanical analysis, we can evaluate $\varepsilon_E^I(T)$ from (18)₂ (see for more details [36]). Vice versa, if the caloric equation of state is known, from (18)₂, we can evaluate the function $A(T)$ in integral form with respect to T as follows:

$$A(T) = A_0 \exp\left(\frac{m}{k_B} \int_{T_0}^T \frac{\varepsilon_E^I(T')}{T'^2} dT'\right),$$

where A_0 and T_0 are the inessential constants. Then, the measure $\varphi(\mathcal{I})$ is determined via the inverse Laplace transformation of (15). For example, in the case of polytropic gases of which caloric equation of state is given in (11), we obtain $\varphi(\mathcal{I})$ explicitly as follows [39]:

$$\varphi(\mathcal{I}) = \mathcal{I}^{\frac{D-5}{2}}. \quad (19)$$

It was proved in [36] that

$$\frac{1}{m^2} \int_0^\infty \mathcal{I}^2 f_E^I \varphi(\mathcal{I}) d\mathcal{I} = \frac{p^2}{\rho^2} \hat{c}_v^I + \varepsilon_E^I(T)^2, \quad (20)$$

where

$$\hat{c}_v^I = m \frac{c_v^I}{k_B}, \quad \text{and} \quad c_v^I = \frac{d\varepsilon_E^I(T)}{dT}$$

is the specific heat of the internal mode. We remark that the relation between the pressure and the translational internal energy is as follows:

$$p = \frac{2}{3} \rho \varepsilon_E^K(T).$$

The specific entropy density in equilibrium is expressed by

$$s = s(\rho, T) = s^K(\rho, T) + s^I(T),$$

with its translational part s^K and internal part s^I which are given by

$$\begin{aligned} s^K(\rho, T) &\equiv -\frac{k_B}{\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} f_E \log f_E^K \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}, \\ &= \frac{k_B}{m} \log \left(\frac{T^{3/2}}{\rho} \right) + \frac{\varepsilon_E^K(T)}{T} - \frac{k_B}{m} \log \left[\frac{1}{m} \left(\frac{m}{2\pi k_B} \right)^{3/2} \right], \\ s^I(T) &\equiv -\frac{k_B}{\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} f_E \log f_E^I \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}, \\ &= \frac{k_B}{m} \log A(T) + \frac{\varepsilon_E^I(T)}{T}. \end{aligned}$$

2.1. System of Balance Equations for 15 Fields

The macroscopic quantities in (10) are defined as the moments of f as follows:

$$\begin{aligned} \begin{pmatrix} F \\ F_i \\ F_{ij} \\ F_{ijk} \end{pmatrix} &= \int_{\mathbb{R}^3} \int_0^{+\infty} m \begin{pmatrix} 1 \\ \xi_i \\ \xi_i \xi_j \\ \xi_i \xi_j \xi_k \end{pmatrix} f \varphi(\mathcal{I}) d\mathcal{I} d\boldsymbol{\xi}, \\ \begin{pmatrix} G_{ll} \\ G_{lli} \\ G_{llik} \end{pmatrix} &= \int_{\mathbb{R}^3} \int_0^{+\infty} (m\tilde{\xi}^2 + 2\mathcal{I}) \begin{pmatrix} 1 \\ \xi_i \\ \xi_i \xi_k \end{pmatrix} f \varphi(\mathcal{I}) d\mathcal{I} d\boldsymbol{\xi}, \\ \begin{pmatrix} H_{llmm} \\ H_{llmmi} \end{pmatrix} &= \int_{\mathbb{R}^3} \int_0^{+\infty} (m\tilde{\xi}^2 + 4\mathcal{I}) \tilde{\xi}^2 \begin{pmatrix} 1 \\ \xi_i \end{pmatrix} f \varphi(\mathcal{I}) d\mathcal{I} d\boldsymbol{\xi}, \end{aligned} \quad (21)$$

and the production terms

$$\mathbf{f} \equiv \begin{pmatrix} P_{ij} \\ Q_{lli} \\ R_{llmm} \end{pmatrix} = \int_{\mathbb{R}^3} \int_0^{+\infty} \begin{pmatrix} m\tilde{\xi}_i \tilde{\xi}_j \\ (m\tilde{\xi}^2 + 2\mathcal{I}) \tilde{\xi}_i \\ (m\tilde{\xi}^2 + 4\mathcal{I}) \tilde{\xi}^2 \end{pmatrix} Q(f) \varphi(\mathcal{I}) d\mathcal{I} d\boldsymbol{\xi}. \quad (22)$$

Since the intrinsic (velocity independent) variables are the moments in terms of the peculiar velocity C_i instead of ξ_i , the velocity dependence of the densities is obtained as follows:

$$\begin{aligned} F &= \rho, \\ F_i &= \rho v_i, \\ F_{ij} &= \hat{F}_{ij} + \rho v_i v_j, \\ G_{ll} &= \hat{G}_{ll} + \rho v^2, \\ G_{lli} &= \hat{G}_{lli} + \hat{G}_{ll} v_i + 2\hat{F}_{li} v_l + \rho v^2 v_i, \\ H_{llmm} &= \hat{H}_{llmm} + 4\hat{G}_{lli} v_i + 2\hat{G}_{ll} v^2 + 4\hat{F}_{ij} v_i v_j + \rho v^4, \end{aligned} \quad (23)$$

where a hat on a quantity indicates its velocity independent part. The conventional fields, i.e.,

$$\begin{aligned} \text{mass density :} \quad \rho &= \int_{\mathbb{R}^3} \int_0^{+\infty} m f \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C} = \int_{\mathbb{R}^3} \int_0^{+\infty} m f_E \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}, \\ \text{velocity :} \quad v_i &= \frac{1}{\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} m \xi_i f \varphi(\mathcal{I}) d\mathcal{I} d\boldsymbol{\xi} = \frac{1}{\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} m \xi_i f_E \varphi(\mathcal{I}) d\mathcal{I} d\boldsymbol{\xi}, \\ \text{specific internal energy density :} \quad \varepsilon &= \varepsilon^K + \varepsilon^I = \frac{1}{2\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} (mC^2 + 2\mathcal{I}) f \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}, \\ \text{specific translational energy density :} \quad \varepsilon^K &= \frac{1}{2\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} mC^2 f \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}, \\ \text{specific internal energy density :} \quad \varepsilon^I &= \frac{1}{\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} \mathcal{I} f \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}, \\ \text{total nonequilibrium pressure :} \quad \mathcal{P} &= \frac{2}{3} \rho \varepsilon^K = \frac{1}{3} \int_{\mathbb{R}^3} \int_0^{+\infty} mC^2 f \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}, \\ \text{dynamic pressure :} \quad \Pi &= \mathcal{P} - p = \frac{1}{3} \int_{\mathbb{R}^3} \int_0^{+\infty} mC^2 (f - f_E) \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}, \\ \text{shear stress :} \quad \sigma_{\langle ij \rangle} &= - \int_{\mathbb{R}^3} \int_0^{+\infty} m C_{\langle i} C_{j \rangle} f \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}, \\ \text{heat flux :} \quad q_i &= \frac{1}{2} \int_{\mathbb{R}^3} \int_0^{+\infty} (mC^2 + 2\mathcal{I}) C_i f \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}, \end{aligned} \quad (24)$$

are related to the intrinsic moments as follows:

$$\hat{G}_{ll} = 2\rho\varepsilon = 2\rho(\varepsilon^K + \varepsilon^I), \quad \hat{F}_{ll} = 3\mathcal{P} = 3(p + \Pi), \quad \hat{F}_{\langle ij \rangle} = -\sigma_{\langle ij \rangle}, \quad \hat{G}_{lli} = 2q_i, \quad (25)$$

where the temperature of the system T is introduced through the caloric equation of state

$$\varepsilon = \varepsilon_E(T). \quad (26)$$

Let us decompose the intrinsic part of H_{llmm} into the equilibrium part and the nonequilibrium part Δ as follows:

$$\hat{H}_{llmm} = \int_{\mathbb{R}^3} \int_0^{+\infty} (mC^2 + 4\mathcal{I}) C^2 f \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C} = 12 \frac{p^2}{\rho} (5 + 4y^I) + \Delta,$$

where

$$y^I = \frac{\rho}{p} \varepsilon_E^I(T),$$

and Δ is defined by

$$\Delta = \int_{\mathbb{R}^3} \int_0^{+\infty} (mC^2 + 4\mathcal{I}) C^2 (f - f_E) \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}. \quad (27)$$

Similarly, the velocity dependences of the fluxes and productions are obtained as follows:

$$\begin{aligned}
 F_{ijk} &= \hat{F}_{ijk} + \hat{F}_{ij}v_k + \hat{F}_{jk}v_i + \hat{F}_{ki}v_j + \rho v_i v_j v_k, \\
 G_{llik} &= \hat{G}_{llik} + \hat{G}_{lli}v_k + \hat{G}_{llk}v_i + 2\hat{F}_{lik}v_l + 2\hat{F}_{kl}v_l v_i + 2\hat{F}_{il}v_l v_k + \hat{F}_{ik}v^2 + \hat{G}_{ll}v_i v_k + \rho v^2 v_i v_k, \\
 H_{llmmk} &= \hat{H}_{llmmk} + \hat{H}_{llmm}v_k + 4\hat{G}_{llik}v_i + 2\hat{G}_{llk}v^2 + 4\hat{G}_{lli}v_i v_k + 4\hat{F}_{ijk}v_i v_j + 2\hat{G}_{ll}v^2 v_k + 4\hat{F}_{ik}v^2 v_i + 4\hat{F}_{ij}v_i v_j v_k + \rho v^4 v_k, \\
 P_{ij} &= \hat{P}_{ij}, \\
 Q_{lli} &= 2v_l \hat{P}_{il} + \hat{Q}_{lli}, \\
 R_{llmm} &= 4v_i v_j \hat{P}_{ij} + 4v_i \hat{Q}_{lli} + \hat{R}_{llmm}.
 \end{aligned} \tag{28}$$

The velocity dependences of moments (23) and (28) ensure that the system (10) is Galilean invariant, and this fact is in agreement with the general theorem on the Galilean invariance for a generic system of balance laws (see [48]).

The constitutive quantities are now the following moments:

$$\begin{aligned}
 \hat{F}_{ijk} &= \int_{\mathbb{R}^3} \int_0^{+\infty} m C_i C_j C_k f \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}, \\
 \hat{G}_{llik} &= \int_{\mathbb{R}^3} \int_0^{+\infty} (m C^2 + 2\mathcal{I}) C_i C_k f \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}, \\
 \hat{H}_{llmmk} &= \int_{\mathbb{R}^3} \int_0^{+\infty} (m C^2 + 4\mathcal{I}) C^2 C_k f \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C},
 \end{aligned}$$

that are needed to be determined for the closure of the differential system together with the production terms P_{ij} , Q_{lli} and R_{llmm} .

2.2. Nonequilibrium Distribution Function Derived from MEP

To close the system (10), we need the nonequilibrium distribution function f , which is derived from the MEP. According to the principle, the most suitable distribution function f of the truncated system (10) is the one that maximizes the entropy density

$$h = -k_B \int_{\mathbb{R}^3} \int_0^{+\infty} f \log f \varphi(\mathcal{I}) d\mathcal{I} d\boldsymbol{\xi},$$

under the constraints that the density moments $F, F_i, F_{ij}, G_{ll}, G_{lli}, H_{llmm}$ are prescribed as in (21) [5,20]. Therefore, the best-approximated distribution function f_{15} is obtained as the solution of an unconstrained maximum of

$$\begin{aligned}
 \mathcal{L}(f) &= -k_B \int_{\mathbb{R}^3} \int_0^{+\infty} f \log f \varphi(\mathcal{I}) d\mathcal{I} d\boldsymbol{\xi} \\
 &+ \lambda \left(F - \int_{\mathbb{R}^3} \int_0^{+\infty} m f \varphi(\mathcal{I}) d\mathcal{I} d\boldsymbol{\xi} \right) + \lambda_i \left(F_i - \int_{\mathbb{R}^3} \int_0^{+\infty} m \xi_i f \varphi(\mathcal{I}) d\mathcal{I} d\boldsymbol{\xi} \right) \\
 &+ \lambda_{ij} \left(F_{ij} - \int_{\mathbb{R}^3} \int_0^{+\infty} m \xi_i \xi_j f \varphi(\mathcal{I}) d\mathcal{I} d\boldsymbol{\xi} \right) + \mu \left(G_{ll} - \int_{\mathbb{R}^3} \int_0^{+\infty} (m \xi^2 + 2\mathcal{I}) f \varphi(\mathcal{I}) d\mathcal{I} d\boldsymbol{\xi} \right) \\
 &+ \mu_i \left(G_{lli} - \int_{\mathbb{R}^3} \int_0^{+\infty} (m \xi^2 + 2\mathcal{I}) \xi_i f \varphi(\mathcal{I}) d\mathcal{I} d\boldsymbol{\xi} \right) + \zeta \left(H_{llmm} - \int_{\mathbb{R}^3} \int_0^{+\infty} (m \xi^2 + 4\mathcal{I}) \xi^2 f \varphi(\mathcal{I}) d\mathcal{I} d\boldsymbol{\xi} \right),
 \end{aligned} \tag{29}$$

where $\lambda, \lambda_i, \lambda_{ij}, \mu, \mu_i$, and ζ are the corresponding Lagrange multipliers of the constraints. As $\mathcal{L}$ is a scalar independent of frame proceeding as in [48], we can evaluate the right side

of (29) in the rest frame of the fluid ($v_i = 0$), and in this way we have the following velocity dependence of the Lagrange multipliers (according with the general theorem given in [48]):

$$\begin{aligned}\lambda &= \hat{\lambda} - \hat{\lambda}_i v_i + \hat{\lambda}_{ij} v_i v_j + \hat{\mu} v^2 - \hat{\mu}_i v^2 v_i + \hat{\zeta} v^4, \\ \lambda_i &= \hat{\lambda}_i - 2\hat{\lambda}_{ij} v_j - 2\hat{\mu} v_i + 3\hat{\mu}_i v^2 - 4\hat{\zeta} v^2 v_i, \\ \lambda_{ij} &= \hat{\lambda}_{ij} - 2\hat{\mu}_i v_i + 4\hat{\zeta} v_i v_j, \\ \mu &= \hat{\mu} - \hat{\mu}_i v_i + 2\hat{\zeta} v^2, \\ \mu_i &= \hat{\mu}_i - 4\hat{\zeta} v_i, \\ \zeta &= \hat{\zeta}.\end{aligned}\quad (30)$$

The distribution function f , which satisfies $\delta\mathcal{L}/\delta f = 0$, is

$$\begin{aligned}f_{15} &= \exp\left(-1 - \frac{m}{k_B}\chi\right), \quad \text{with} \\ \chi &= \hat{\lambda} + C_i \hat{\lambda}_i + C_i C_j \hat{\lambda}_{ij} + \left(C^2 + \frac{2\mathcal{I}}{m}\right)\hat{\mu} + \left(C^2 + \frac{2\mathcal{I}}{m}\right)C_i \hat{\mu}_i + \left(C^2 + \frac{4\mathcal{I}}{m}\right)C^2 \hat{\zeta}.\end{aligned}\quad (31)$$

Recalling the usual thermodynamical definition of the equilibrium as the state for which the entropy production vanishes and hence attains its minimum value, it is possible to prove the theorem [49,50] that the components of the Lagrange multipliers of the balance laws of nonequilibrium variables vanish, and only the Lagrange multipliers corresponding to the conservation laws (Euler System) remain. On the other hand, in [35], it was proved that the distribution function maximizes the entropy density with the constraints of 5 moments F, F_i and G_{ll} of the equilibrium subsystem is given by (13). Therefore, in equilibrium, f_{15} coincides with the equilibrium distribution function (13) with Lagrange multipliers given by

$$\lambda_E = \frac{1}{T}\left(-g + \frac{v^2}{2}\right), \quad \lambda_{iE} = -\frac{v_i}{T}, \quad \lambda_{llE} = 0, \quad \lambda_{\langle ij \rangle E} = 0, \quad \mu_E = \frac{1}{2T}, \quad \mu_{iE} = 0, \quad \zeta_E = 0, \quad (32)$$

where $g(= \varepsilon_E(T) + p/\rho - Ts)$ is the chemical potential. We remark that $\lambda_E, \lambda_{iE}, \mu_E$ in (32) are the main field that symmetrize the Euler system as was proved first by Godunov (see [34,51]).

We observe that the highest power of peculiar velocity in χ in (31)₂ is even, i.e., C^4 . In general, the highest power is the same as the highest tensorial order of the system, and it is revealed in [29] that the highest tensorial order of the system obtained in the classical limit is always even, i.e., $\bar{N} = 2N$. This fact indicates that, in principle, the moments can be integrable with the distribution function f_{15} (concerning the integrability of moments see [21,22]). Nevertheless, there remain problematics noticed first by Junk [52] that the domain of definition of the flux in the last moment equation is not convex, the flux has a singularity, and the equilibrium state lies on the border of the domain of definition of the flux. To avoid these difficulties in the molecular extended thermodynamics approach, we consider, as usual, the processes near equilibrium. Then, we expand (31) around an equilibrium state in the following form:

$$\begin{aligned}f_{15} &\simeq f_E\left(1 - \frac{m}{k_B}\tilde{\chi}\right), \\ \tilde{\chi} &= \tilde{\lambda} + C_i \tilde{\lambda}_i + C_i C_j \tilde{\lambda}_{ij} + \left(C^2 + \frac{2\mathcal{I}}{m}\right)\tilde{\mu} + \left(C^2 + \frac{2\mathcal{I}}{m}\right)C_i \tilde{\mu}_i + \left(C^2 + \frac{4\mathcal{I}}{m}\right)C^2 \tilde{\zeta},\end{aligned}\quad (33)$$

where a tilde on a quantity indicates its nonequilibrium part. In the following, for simplicity, we use the notation f instead of f_{15} . Although the expansion of the exponential (31) is truncated at the first order with respect to the nonequilibrium variables, it is possible to construct RET theories with high expansion as was presented first by Brini and Ruggeri

in [53]. The high order expansion has the advantage of having a larger hyperbolicity domain [54,55] and reducing the magnitude of the sub-shock formation in the shock structure [46].

From (33) with (24) and (27), the intrinsic nonequilibrium Lagrange multipliers are evaluated as functions of $(\rho, T, \Pi, \sigma_{\langle ij \rangle}, q_i, \Delta)$ up to the first order with respect to the nonequilibrium fields, Π , $\sigma_{\langle ij \rangle}$, q_i and Δ . The derivation is given in the Appendix A. Instead of Δ , it may be useful to introduce the following nonequilibrium field:

$$\tilde{\Pi} = \frac{1}{3(4\hat{c}_v^I + 5)} \left\{ 12\Pi(y^I + 1) - \frac{\rho}{p}\Delta \right\}. \quad (34)$$

Then, we obtain as the solution of (A1):

$$\begin{aligned} \tilde{\lambda} &= \frac{3(\hat{c}_v^I - y^I)}{2\hat{c}_v^I \rho T} \Pi + \frac{3(4y^I + 5)}{8\rho T} \tilde{\Pi}, \\ \tilde{\lambda}_i &= \frac{2y^I + 5}{pT(2\hat{c}_v^I + 5)} q_i, \\ \tilde{\lambda}_{ll} &= -\frac{3(2\hat{c}_v^I + 3)}{4\hat{c}_v^I pT} \Pi - \frac{3(y^I + 1)}{2pT} \tilde{\Pi}, \\ \tilde{\lambda}_{\langle ij \rangle} &= \frac{\sigma_{\langle ij \rangle}}{2pT}, \\ \tilde{\mu} &= \frac{3}{4\hat{c}_v^I pT} \Pi - \frac{3}{4pT} \tilde{\Pi}, \\ \tilde{\mu}_i &= -\frac{\rho}{p^2 T(2\hat{c}_v^I + 5)} q_i, \\ \tilde{\zeta} &= \frac{\rho}{8p^2 T} \tilde{\Pi}. \end{aligned} \quad (35)$$

Inserting (32) and (35) into (30), we can write down the explicit form of the Lagrange multipliers. As is well known, the multipliers coincide with the main field

$$\mathbf{u}' \equiv (\lambda, \lambda_i, \lambda_{ij}, \mu, \mu_i, \zeta) \quad (36)$$

by which the system (10) becomes symmetric hyperbolic. Therefore we have the well-posed Cauchy problem (local in time) [6,22], and in some circumstances for small initial data, there exist global smooth solutions for all time (see [7,34] and references therein).

2.3. Constitutive Equations

By using the distribution function (33) with (35), we obtain the constitutive equations for the fluxes up to the first order with respect to the nonequilibrium variables as follows:

$$\begin{aligned} \hat{F}_{ijk} &= \frac{2}{2\hat{c}_v^I + 5} (q_k \delta_{ij} + q_j \delta_{ik} + q_i \delta_{jk}), \\ \hat{G}_{llij} &= (2y^I + 5) \frac{p^2}{\rho} \delta_{ij} + (2y^I + 7) \frac{p}{\rho} \Pi \delta_{ij} - (2\hat{c}_v^I + 5) \frac{p}{\rho} \tilde{\Pi} \delta_{ij} - (2y^I + 7) \frac{p}{\rho} \sigma_{\langle ij \rangle}, \\ \hat{H}_{llmmk} &= 20 \frac{p}{\rho} \frac{2y^I + 2\hat{c}_v^I + 7}{2\hat{c}_v^I + 5} q_k. \end{aligned} \quad (37)$$

2.4. Nonequilibrium Temperatures and Generalized BGK Model

2.4.1. Nonequilibrium Temperatures

We recall that ε^K and ε^I given in (24) are nonequilibrium variables while their sum is an equilibrium variable. Then, we can define two nonequilibrium temperatures (θ^K, θ^I)

such that, by inserting them into the caloric equation of state (12)₂ instead of T , the nonequilibrium internal energies ($\varepsilon^K, \varepsilon^I$) are obtained, i.e.,:

$$\varepsilon^K = \varepsilon_E^K(\theta^K) = \frac{3}{2} \frac{k_B}{m} \theta^K, \quad \varepsilon^I = \varepsilon_E^I(\theta^I). \quad (38)$$

The present definition of the nonequilibrium temperature is usually adopted in the kinetic theory. It has been shown that the nonequilibrium temperatures are equivalent to those defined through the generalized Gibbs relation in the context of RET for the case of the small set of independent fields [56]. There also have been many other attempts to obtain well-defined nonequilibrium temperatures. For example, see [57].

Recalling $2\rho\varepsilon^K = 3\mathcal{P}$ and (18) with (38)₁, the total nonequilibrium pressure is expressed by the thermal equation of state (12)₁ with θ^K as follows:

$$\mathcal{P} = p(\rho, \theta^K) = \frac{k_B}{m} \rho \theta^K.$$

Since $\mathcal{P} = p + \Pi$, we have the following relation between the nonequilibrium temperature θ^K and the dynamical pressure Π :

$$\theta^K = T \left(1 + \frac{\Pi}{p(\rho, T)} \right).$$

Moreover, we have the relation among three temperatures from (17) and (26) as follows:

$$\varepsilon_E^I(\theta^I) - \varepsilon_E^I(T) = \varepsilon_E^K(T) - \varepsilon_E^K(\theta^K).$$

2.4.2. Generalized BGK Model

In polyatomic gases, we may introduce two characteristic times corresponding to two relaxation processes caused by the molecular collision:

(i) Relaxation time τ_K : This characterizes the relaxation process within the translational mode (mode K) of molecules. The process shows the tendency to approach an equilibrium state of the mode K with the distribution function f^K having the temperature θ^K , an explicit expression of which is shown below. However, the internal mode I remains, in general, in nonequilibrium. This process also exists in monatomic gases.

(ii) Relaxation time τ of the second stage: After the relaxation process of the translational mode K, two modes, K and I, eventually approach a local equilibrium state characterized by f_E with a common temperature T . Naturally, we have assumed the condition: $\tau > \tau_K$.

To describe the above two separated relaxation processes, we adopt the following generalized BGK collision term [43,58] (see also [36,59,60]) which treats the translational relaxation and internal relaxation separately:

$$Q(f) = -\frac{1}{\tau_K} (f - f^K) - \frac{1}{\tau} (f - f_E), \quad (39)$$

where the distribution functions f^K is the equilibrium function with respect to the mode K with the temperature θ^K and the mass density $\rho^I(\mathcal{I})$ under the frozen energy $\mathcal{I}$ defined by

$$\rho^I(\mathcal{I}) = \int_{\mathbb{R}^3} m f d\boldsymbol{\xi}.$$

Specifically, f^K is the Maxwellian with $\rho^I(\mathcal{I})$ and θ^K given by

$$f^K = \frac{\rho^I(\mathcal{I})}{m} \left(\frac{m}{2\pi k_B \theta^K} \right)^{3/2} \exp \left(-\frac{mC^2}{2k_B \theta^K} \right).$$

2.4.3. Production Terms

From the generalized BGK model (39), the production terms given by (22) are evaluated as follows:

$$\begin{aligned}\hat{P}_{ll} &= -\frac{3}{\tau}\Pi, \quad \hat{P}_{\langle ij \rangle} = \left(\frac{1}{\tau_K} + \frac{1}{\tau}\right)\sigma_{\langle ij \rangle}, \quad \hat{Q}_{lli} = -2\left(\frac{1}{\tau_K} + \frac{1}{\tau}\right)q_i, \\ \hat{R}_{llmm} &= -\left(\frac{1}{\tau_K} + \frac{1}{\tau}\right)\Delta + \frac{1}{\tau_K}\frac{p}{\rho}\Pi\left(12y^I + 12 - 3\frac{\Pi}{p}\right).\end{aligned}\quad (40)$$

Since we consider the linear constitutive equations, we neglect the quadratic term in the last expression of (40):

$$\hat{R}_{llmm} = -\left(\frac{1}{\tau_K} + \frac{1}{\tau}\right)\Delta + \frac{12}{\tau_K}\frac{p}{\rho}(y^I + 1)\Pi.$$

2.5. Closed Field Equations

Using the constitutive equations above, we obtain the closed system of field equations for the 15 independent fields $(\rho, v_i, T, \Pi, \sigma_{\langle ij \rangle}, q_i, \Delta)$:

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho v_i) &= 0, \\ \frac{\partial \rho v_j}{\partial t} + \frac{\partial}{\partial x_i} \{ [p + \Pi]\delta_{ij} - \sigma_{\langle ij \rangle} + \rho v_i v_j \} &= 0, \\ \frac{\partial}{\partial t} \{ p(2y^I + 3) + \rho v^2 \} + \frac{\partial}{\partial x_i} \{ 2q_i + [p(2y^I + 5) + 2\Pi]v_i - 2\sigma_{\langle li \rangle}v_l + \rho v^2 v_i \} &= 0, \\ \frac{\partial}{\partial t} \{ 3(p + \Pi) + \rho v^2 \} + \frac{\partial}{\partial x_k} \left\{ \frac{10}{2\hat{c}_v^I + 5}q_k + 5(p + \Pi)v_k - 2\sigma_{\langle lk \rangle}v_l + \rho v^2 v_k \right\} &= -\frac{3\Pi}{\tau}, \\ \frac{\partial}{\partial t} (-\sigma_{\langle ij \rangle} + \rho v_{\langle i} v_{j \rangle}) + \frac{\partial}{\partial x_k} \left\{ \frac{2}{1 + \hat{c}_v}q_{\langle i} \delta_{j \rangle k} + 2[p + \Pi]v_{\langle i} \delta_{j \rangle k} - \sigma_{\langle ij \rangle}v_k - 2\sigma_{\langle k(i} v_{j \rangle)} + \rho v_{\langle i} v_{j \rangle}v_k \right\} &= \left(\frac{1}{\tau_K} + \frac{1}{\tau}\right)\sigma_{\langle ij \rangle}, \\ \frac{\partial}{\partial t} \{ 2q_i + [p(2y^I + 5) + 2\Pi]v_i - 2\sigma_{\langle li \rangle}v_l + \rho v^2 v_i \} + \\ + \frac{\partial}{\partial x_k} \left\{ (2y^I + 5)\frac{p^2}{\rho}\delta_{ik} + (2y^I + 7)\frac{p}{\rho}\Pi\delta_{ik} - \frac{p}{\rho}\frac{2\hat{c}_v^I + 5}{3(4\hat{c}_v^I + 5)}\left(12\Pi(y^I + 1) - \frac{\rho}{p}\Delta\right)\delta_{ik} - (2y^I + 7)\frac{p}{\rho}\sigma_{\langle ik \rangle} \right. \\ + \frac{2}{2\hat{c}_v^I + 5}q_l v_l \delta_{ik} + 4\frac{\hat{c}_v^I + 3}{2\hat{c}_v^I + 5}(q_i v_k + q_k v_i) + (p + \Pi)v^2 \delta_{ik} + [(2y^I + 7)p + 4\Pi]v_i v_k \\ \left. - \sigma_{\langle ik \rangle}v^2 - 2\sigma_{\langle lk \rangle}v_l v_i - 2v_l v_k \sigma_{\langle il \rangle} + \rho v^2 v_i v_k \right\} &= -2\frac{\Pi}{\tau}v_i + 2\left(\frac{1}{\tau_K} + \frac{1}{\tau}\right)\sigma_{\langle il \rangle}v_l - 2\left(\frac{1}{\tau_K} + \frac{1}{\tau}\right)q_i, \\ \frac{\partial}{\partial t} \left\{ 3\frac{p^2}{\rho}(4y^I + 5) + \Delta + 8v_i q_i + 2v^2[p(2y^I + 5) + 2\Pi] - 4v_i v_j \sigma_{\langle ij \rangle} + \rho v^4 \right\} + \\ + \frac{\partial}{\partial x_k} \left\{ \frac{20p}{\rho(2\hat{c}_v^I + 5)}(2\hat{c}_v^I + 2y^I + 7)q_k + 5(4y^I + 7)\frac{p^2}{\rho}v_k + 20(y^I + 2)\frac{p}{\rho}\Pi v_k - \frac{5p(4\hat{c}_v^I + 7)}{3\rho(4\hat{c}_v^I + 5)}\left[12\Pi(y^I + 1) - \frac{\rho}{p}\Delta\right]v_k \right. \\ - 4(2y^I + 7)\frac{p}{\rho}\sigma_{\langle ik \rangle}v_i + \frac{4(2\hat{c}_v^I + 7)}{2\hat{c}_v^I + 5}(q_k v^2 + 2q_i v_i v_k) - 4\sigma_{\langle ik \rangle}v^2 v_i - 4\sigma_{\langle ij \rangle}v_i v_j v_k + 2[p(2y^I + 7) + 4\Pi]v^2 v_k + \rho v^4 v_k \left. \right\} \\ = -4v^2 \frac{\Pi}{\tau} + 4\left(\frac{1}{\tau_K} + \frac{1}{\tau}\right)v_{\langle i} v_{j \rangle} \sigma_{\langle ij \rangle} + 8\left(\frac{1}{\tau_K} + \frac{1}{\tau}\right)v_i q_i - \left(\frac{1}{\tau_K} + \frac{1}{\tau}\right)\Delta + \frac{12}{\tau_K}\frac{p}{\rho}(y^I + 1)\Pi.\end{aligned}\quad (41)$$

where, from (34),

$$\Delta = 3\frac{p}{\rho}\left\{4(y^I + 1)\Pi - (4\hat{c}_v^I + 5)\tilde{\Pi}\right\}.\quad (42)$$

In conclusion: the system (41) formed by 15 equations in the 15 unknown is closed with the provided equilibrium state function (12) and relaxation times τ and τ_K .

We remark that the field equations of ρ, v_i, T, Π and $\sigma_{\langle ij \rangle}$ are the same as the ones of polyatomic 14 field theory and the presence of Δ involves only the last two equations of (41).

2.6. Entropy Density, Flux, and Production

The entropy density h satisfies the entropy balance equation:

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x_i}(hv_i + \varphi_i) = \Sigma,$$

where φ_i and Σ are, respectively, the non-convective entropy flux and the entropy production which are defined below.

By adopting (33) with (35), we obtain the entropy density within the second order with respect to the nonequilibrium variables as follows:

$$h = \rho s - \frac{3(2\hat{c}_v^I + 3)}{8\hat{c}_v^I p T} \Pi^2 - \frac{3(4\hat{c}_v^I + 5)}{16pT} \tilde{\Pi}^2 - \frac{1}{4pT} \sigma_{\langle ij \rangle} \sigma_{\langle ij \rangle} - \frac{\rho}{(2\hat{c}_v^I + 5)p^2 T} q_i q_i. \quad (43)$$

This means that the entropy density is convex and reaches the maximum at equilibrium, then the system (41) provides the symmetric form in the main field components.

Similarly, the entropy flux is obtained as follows:

$$\begin{aligned} \varphi_i &= -k_B \int_{\mathbb{R}^3} \int_0^{+\infty} C_i f \log f \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C} \\ &= \frac{1}{T} q_i + \frac{2}{pT(2\hat{c}_v^I + 5)} q_j \sigma_{\langle ij \rangle} - \frac{2}{pT(2\hat{c}_v^I + 5)} q_i \Pi + \frac{1}{pT} q_i \tilde{\Pi}, \end{aligned}$$

The entropy production Σ according to the symmetrization theorem [6,7,34] is obtained as the scalar product between the main field given by (36) and the production vector given by (22). By taking into account (40) and (35), we have

$$\begin{aligned} \Sigma = \mathbf{u}' \cdot \mathbf{f} = \hat{\Sigma} = \hat{\mathbf{u}}' \cdot \hat{\mathbf{f}} &= \frac{\hat{\lambda}_{II}}{3} \Pi - \hat{\lambda}_{\langle ij \rangle} \sigma_{\langle ij \rangle} + 2\hat{\mu}_i q_i + \hat{\xi} \Delta \\ &= \frac{3(2\hat{c}_v^I + 3)}{4\hat{c}_v^I p T} \frac{1}{\tau} \Pi^2 + \frac{3(4\hat{c}_v^I + 5)}{8pT} \left(\frac{1}{\tau_K} + \frac{1}{\tau} \right) \tilde{\Pi}^2 + \frac{1}{2pT} \left(\frac{1}{\tau_K} + \frac{1}{\tau} \right) \sigma_{\langle ij \rangle} \sigma_{\langle ij \rangle} + \frac{2\rho}{p^2 T(2\hat{c}_v^I + 5)} \left(\frac{1}{\tau_K} + \frac{1}{\tau} \right) q_i q_i. \end{aligned}$$

It is noteworthy that the entropy production is positive with the provided positive relaxation times and $\hat{c}_v^I \geq 0$.

2.7. Hyperbolicity and Characteristic Speeds

First of all, we want to prove that the differential system is hyperbolic in the equilibrium state by evaluating the characteristic velocities of the differential system. The equilibrium characteristic velocities of the differential system play an important role in several processes such as the determination of the phase velocity of linear waves in the high-frequency limit [61], the propagation of acceleration waves [62,63], and the sub-shock formation [49].

Since the differential system (41) is a particular case of a generic balance law system:

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{F}^i(\mathbf{u})}{\partial x^i} = \mathbf{f}(\mathbf{u}),$$

it is well known that the characteristic velocities V associated with a hyperbolic system of equations can be obtained by using the operator chain rule (see [34]):

$$\frac{\partial}{\partial t} \rightarrow -V\delta, \quad \frac{\partial}{\partial x_i} \rightarrow n_i \delta, \quad \mathbf{f} \rightarrow 0,$$

where n_i denotes the i -component of the unit normal to the wavefront, $\mathbf{f}$ is the production terms and δ is a differential operator.

Let us consider only one dimensional space-variable, and the system (41) reduces to only 7 scalar equations for the 7 unknown $(\rho, v = v_1, T, \Pi, \sigma = \sigma_{\langle 11 \rangle}, q = q_1, \Delta)$. After some

cumbersome calculations, it is possible to prove that the system has the following 7 real characteristic velocities evaluated in equilibrium:

$$\begin{aligned} V^{(1)} &= v - U_E^{1st} \sqrt{\frac{k_B}{m}} T, & V^{(2)} &= v - U_E^{2nd} \sqrt{\frac{k_B}{m}} T, \\ V^{(3)} &= V^{(4)} = V^{(5)} = v, \\ V^{(6)} &= v + U_E^{2nd} \sqrt{\frac{k_B}{m}} T, & V^{(7)} &= v + U_E^{1st} \sqrt{\frac{k_B}{m}} T, \end{aligned} \quad (44)$$

with the normalized characteristic speeds of the first mode U_E^{1st} and the second mode $U_E^{2nd} (< U_E^{1st})$ defined by

$$U_E^{1st} = \frac{1}{\sqrt{6(4\hat{c}_v - 1)(\hat{c}_v + 1)}} \sqrt{8\hat{c}_v(7\hat{c}_v + 11) - 13 + \sqrt{4\hat{c}_v\{64\hat{c}_v^2(\hat{c}_v + 16) + 897\hat{c}_v - 482\} + 349}}, \quad (45)$$

$$U_E^{2nd} = \frac{1}{\sqrt{6(4\hat{c}_v - 1)(\hat{c}_v + 1)}} \sqrt{8\hat{c}_v(7\hat{c}_v + 11) - 13 - \sqrt{4\hat{c}_v\{64\hat{c}_v^2(\hat{c}_v + 16) + 897\hat{c}_v - 482\} + 349}}, \quad (46)$$

where $\hat{c}_v = 3/2 + \hat{c}_v^I$ is the dimensionless specific heat. It is easy to prove that U_E^{1st} given by (45) and U_E^{2nd} by (46) are real because $\hat{c}_v \geq 3/2$, and therefore the characteristic speeds (44) are all real in agreement that any symmetric systems are hyperbolic.

Note that the fastest speed U_E^{1st} is larger than the corresponding one of the polyatomic ET₁₄ theory, and this indicates that the subcharacteristic condition [50] is satisfied due to the convexity of entropy (43). In the limit of monatomic gases ($\hat{c}_v = 3/2$), $U_E^{1st} \sim 2.27655$ and $U_E^{2nd} \simeq 1.16218$, which coincide with the ones of monatomic ET₁₄. In the limit that $\hat{c}_v \rightarrow \infty$, $U_E^{1st} \rightarrow \sqrt{3}$ which is the same as the one predicted by polyatomic ET₁₄ in this limit. Recalling the general discussion of the dependence of the characteristic speeds on the degrees of freedom [37], this limiting value corresponds to the characteristic speed of monatomic ET theory with 10 moments (ET₁₀) in which (F, F_i, F_{ij}) are the only independent fields. On the other hand, in this limit, $U_E^{2nd} \rightarrow \sqrt{5/3}$ is different from the one of ET₁₄ but is the same as the equilibrium sound velocity (the characteristic speed of Euler system) of monatomic gases in which (F, F_i, F_{II}) are the only independent fields. While, U_E^{2nd} of ET₁₄ approaches to 1 which is the characteristic speed of ET theory with 4 moments (ET₄) in which (F, F_i) are the only independent fields.

In the case of the polytropic gases of which equations of state are given in (11), $\hat{c}_v = D/2$, the normalized characteristic speeds U_E^{1st}, U_E^{2nd} depend only on the degrees of freedom D . The dependences are shown in Figure 1.

Figure 1. Dependence of the normalized characteristic speeds U_E^{1st} (left) and U_E^{2nd} (right) with respect to D . The solid and dashed lines are, respectively, the normalized characteristic speeds of Extended Thermodynamics (ET)₁₅ and polyatomic ET₁₄. The limit value of the normalized characteristic speeds of $D \rightarrow 3$ and $D \rightarrow \infty$ are indicated with dotted lines. In the limit that $D \rightarrow 3$, U_E^{1st} and U_E^{2nd} of ET₁₅ coincide with the monatomic ET₁₄. In the limit that $D \rightarrow \infty$, both of U_E^{1st} of ET₁₅ and ET₁₄ approach to the one of monatomic ET₁₀, and U_E^{2nd} of ET₁₅ and ET₁₄ approach, respectively, to monatomic Euler and ET₄.

2.8. Maxwellian Iteration and Phenomenological Coefficients

The NSF theory is obtained by carrying out the Maxwellian iteration [64] on (41) in which only the first order terms with respect to the relaxation times are retained. Then we obtain

$$\Pi = -p\tau \frac{4\hat{c}_v^I}{6\hat{c}_v^I + 9} \frac{\partial v_k}{\partial x_k}, \quad \sigma_{\langle ij \rangle} = 2p\tau_\sigma \frac{\partial v_{\langle i}}{\partial x_{j \rangle}}, \quad q_i = -p\tau_q \frac{2\hat{c}_v^I + 5}{2} \frac{k_B}{m} \frac{\partial T}{\partial x_i}, \quad (47)$$

and

$$\Delta = -\tau_\Delta \frac{16\hat{c}_v^I}{2\hat{c}_v^I + 3} \frac{p^2}{\rho} (y^I + 1) \left(1 + \frac{\tau}{\tau_K}\right) \frac{\partial v_I}{\partial x_I}, \quad (48)$$

where

$$\frac{1}{\tau_\sigma} = \frac{1}{\tau_q} = \frac{1}{\tau_\Delta} = \frac{1}{\tau_K} + \frac{1}{\tau}.$$

Recalling the definitions of the bulk viscosity ν , shear viscosity μ , and heat conductivity κ in the NFS theory:

$$\Pi = -\nu \frac{\partial v_i}{\partial x_i}, \quad \sigma_{\langle ij \rangle} = 2\mu \frac{\partial v_{\langle i}}{\partial x_{j \rangle}}, \quad q_i = -\kappa \frac{\partial T}{\partial x_i}, \quad (49)$$

we have from (47)

$$\nu = \frac{4\hat{c}_v^I}{6\hat{c}_v^I + 9} p\tau, \quad \mu = p\tau_\sigma, \quad \kappa = \frac{2\hat{c}_v^I + 5}{2} \frac{k_B}{m} p\tau_q. \quad (50)$$

We note that Δ and $\tilde{\Pi}$ are not present in the conservation laws of mass, momentum and energy. In particular, (48) indicates with (42)

$$\tilde{\Pi} = 0.$$

This result seems similar to the case of monatomic ET₁₄ in which the nonequilibrium scalar field is equal to 0 in the Maxwellian iteration [18].

As usual in the BGK model, the Prandtl number predicted by the present model is not satisfactory. To avoid this difficulty, one possibility is to regard the relaxation times τ , τ_σ ,

and τ_q as functions of ρ and T , and estimate them by using the experimental data on ν , μ and κ . On the other hand, τ_Δ and τ_K are not related to such phenomenological coefficients and the kinetic theory is needed for their estimation, or we may determine these relaxation times as parameters to have a better agreement with some experimental data as it has been usually done for the bulk viscosity.

To summarize, we have the following result: With the Maxwellian iteration procedure, the hyperbolic system (41) converges (in a similar way to the 14 fields theory) to the classical parabolic system of NFS formed by the first five equations of (41) with the constitutive equations (49) with the bulk and shear viscosities and heat conductivity related to the relaxation times by (50).

2.9. Principal Subsystem

Since ET_{15} includes a large set of the field equations compared to the polyatomic ET_{14} , it is natural to expect that the polyatomic ET_{14} is a special case of ET_{15} , although both theories are based on the different entropy densities which maximize the corresponding system. In fact, ET_{15} includes ET_{14} as its special case dictated by its principal subsystem.

The concept of the principal subsystem for a general system of the hyperbolic system of balance laws was introduced in [50]. By definition, some components of the main field are put as a constant, and the corresponding balance laws are deleted. In this way, we have a small set of the field equations from a large set of the field equations that have the property that the entropy principle is preserved and the sub-characteristic conditions are satisfied, i.e., the spectrum of characteristic eigenvalues of the small system is contained in the spectrum of the larger one. As a consequence, in the moment theory, the maximum characteristic speed increases with the number of moments [22].

In the present case, the polyatomic ET_{14} is obtained as a principal subsystem of ET_{15} under the condition $\zeta = 0$, i.e., from (35)₇,

$$\tilde{\Pi} = 0,$$

or, in other words,

$$\Delta = 12 \frac{p}{\rho} \Pi (y^I + 1),$$

and (41)₇ is ignored.

2.10. Monatomic Gas Limit

The monatomic gases are described in the limit $\varepsilon^I \rightarrow 0$ ($y^I \rightarrow 0$) and therefore $\hat{c}_v^I \rightarrow 0$. In the limit, the equation for Π obtained by subtracting (41)₃ from (41)₄ and by using the conservation laws (41)_{1,2,3} becomes

$$\frac{\partial \Pi}{\partial t} + v_k \frac{\partial \Pi}{\partial x_k} = - \left(\frac{1}{\tau_\Pi} + \frac{\partial v_k}{\partial x_k} \right) \Pi. \quad (51)$$

This is the first-order quasi-linear partial differential equation with respect to Π . As it has been studied in [33], the initial condition for (51) must be compatible with the case of monatomic gas, i.e., $\Pi(0, x) = 0$, and, assuming the uniqueness of the solution, the possible solution of Equation (51) is given by

$$\Pi(t, x) = 0 \quad (\text{for any } t). \quad (52)$$

If we insert the solution (52) into (25) and (37) with $y^I = 0$ and $\hat{c}_v^I = 0$, the velocity independent moments are expressed by the velocity independent moments of monatomic gas $\hat{F}_{i_1 i_2 \dots i_n}^M$ (see (A2) for their explicit expressions) as follows:

$$\begin{aligned}\hat{F}_{ij} &= p\delta_{ij} - \sigma_{\langle ij \rangle} = \hat{F}_{ij}^M, \\ \hat{F}_{ijk} &= \frac{2}{5} (q_i \delta_{jk} + q_j \delta_{ik} + q_k \delta_{ij}) = \hat{F}_{ijk}^M, \\ \hat{G}_{ll} &= \hat{F}_{ll} = 2\rho\epsilon^K = 3p = \hat{F}_{ll}^M, \\ \hat{G}_{lli} &= \hat{F}_{lli} = 2q_i = \hat{F}_{lli}^M, \\ \hat{G}_{llij} &= \frac{5p^2}{\rho} \delta_{ij} + \frac{1}{3} \Delta \delta_{ij} - 7 \frac{p}{\rho} \sigma_{\langle ij \rangle} = \hat{F}_{llij}^M, \\ \hat{H}_{llmm} &= 15 \frac{p^2}{\rho} + \Delta = \hat{G}_{llmm} = \hat{F}_{llmm}^M, \\ \hat{H}_{llmmk} &= 28 \frac{p}{\rho} q_k = \hat{F}_{llmmk}^M.\end{aligned}$$

Then, the F 's hierarchy coincides with the monatomic F 's hierarchy and G 's and H 's hierarchies coincide with the corresponding monatomic F 's hierarchy. This indicates that, in this singular limit, the triple hierarchies for 15 moments in (10) converges to the single hierarchy of monatomic gases, and solutions of ET₁₅ converge to those of the monatomic 14 theory by Kremer [18].

3. Dispersion Relation

The difference between ET₁₅ and ET₁₄ is studied through the study of the dispersion relation.

Phase Velocity and Attenuation per Wavelength

Let us confine our study within the one-dimensional problem, and we study a harmonic wave propagating in the positive x_1 -direction for the fields $\mathbf{u} = (\rho, v_i, T, \Pi, \sigma_{\langle ij \rangle}, q_i, \Delta)$ with the angular frequency ω and the complex wave number k such that

$$\mathbf{u} = \mathbf{w} e^{i(\omega t - kx_1)}, \quad (53)$$

where $\mathbf{w}$ is a constant amplitude vector. We assume a longitudinal wave:

$$v_i \equiv \begin{pmatrix} v \\ 0 \\ 0 \end{pmatrix}, \quad \sigma_{\langle ij \rangle} \equiv \begin{pmatrix} \sigma & 0 & 0 \\ 0 & -\frac{1}{2}\sigma & 0 \\ 0 & 0 & -\frac{1}{2}\sigma \end{pmatrix}, \quad q_i \equiv \begin{pmatrix} q \\ 0 \\ 0 \end{pmatrix}. \quad (54)$$

From Equation (10) with (54) and (53), the dispersion relation $k = k(\omega)$ is obtained as it has been studied in [5]. The phase velocity v_{ph} , the attenuation factor α and the attenuation per wavelength α_λ are calculated as the functions of the frequency ω by using the following relations:

$$v_{ph} = \frac{\omega}{\text{Re}(k)}, \quad \alpha = -\text{Im}(k), \quad \alpha_\lambda(\omega) = \alpha\lambda = \frac{2\pi v_{ph} \alpha}{\omega} = -2\pi \frac{\text{Im}(k)}{\text{Re}(k)},$$

where λ is the wavelength.

By introducing the following dimensionless parameters:

$$\Omega = \tau\omega, \quad \hat{\tau}_K = \frac{\tau_K}{\tau},$$

the dispersion relation depends on these parameters and the dimensionless specific heat of internal mode $\hat{c}_v^I$ which depends only on the temperature. We notice that $k = k(\omega)$

with fixed Ω and $\hat{\tau}_K$ does not depend on ρ , and its temperature dependence is determined through the dimensionless specific heat.

Although the theory predicts seven modes of the linear waves, the first mode is usually observed in experiments in gases. Therefore, hereafter, we focus our study on the first mode. As an example, we adopt $\hat{\tau}_K = 0.001$ which indicates the existence of the slow relaxation of internal mode [47,59,65]. We show the dependence of the phase velocity normalized by the equilibrium sound velocity c_0 :

$$c_0 = \sqrt{\frac{2\hat{c}_v^I + 5}{2\hat{c}_v^I + 3} \frac{k_B}{m} T},$$

and the attenuation per wavelength on the dimensionless frequency of the first mode in Figure 2 in the case with $\hat{c}_v^I = 2$. Around $\Omega \sim 10^0$ ($\omega \sim \tau^{-1}$), we can observe a change of v_{ph} and a peak of α_λ . Since this is due to the relaxation of internal mode relating to Π , both of the predictions by ET₁₄ and ET₁₅ coincide with each other. Around $\Omega \sim 10^3$ ($= \hat{\tau}_K^{-1}$), we can observe a steep change of v_{ph} and a large peak of α_λ . Since this is due to the relaxation of σ, q , and Δ , the difference between the two theories emerges.

We remark that the experimental data of sound waves are usually obtained in a relatively low-frequency region less than $\Omega = 10^3$ (see [47,59,65]) (In [47,65], the comparisons with the experimental data are made with the dimensionless frequency $\tau_\sigma \omega$ which is not the one of the present paper.). This fact ensures that ET₁₄ is enough to describe the experimental data of sound waves of low frequency even though the moment theory usually needs many moments to have good agreement with experimental facts. On the other hand, for the sound waves with high frequency and nonlinear waves, we need ET₁₅ or many moment theory to describe the experimental data.

Figure 2. Typical dependence of the dimensionless phase velocity v_{ph}/c_0 (left) and the attenuation per wavelength α_λ (right) on the dimensionless frequency Ω predicted by the ET₁₅ and polyatomic ET₁₄ theories.

4. Conclusions

According to the general results of Pennisi and Ruggeri [29], the classical limit of the relativistic theory of moments provides a more complex hierarchy than the F' and G' 's binary hierarchy. In this paper, we have studied the case of $N = 2$ in which the classical limit dictates 15 fields for a non-polytropic polyatomic gas. We have obtained the closure by using the MEP. The closed field equations include the classical NSF theory as its parabolic limit and converge to those of the monatomic ET₁₄ theory obtained by Kremer [18] in the monatomic singular limit. Moreover, we proved that the polyatomic ET₁₄ theory is a principal subsystem of the present one, and according to the general results, the spectrum of characteristic speeds of ET₁₅ includes the spectrum of eigenvalues of ET₁₄. Finally, we have evaluated the dispersion relation proving that, in the low-frequency region, the predictions by ET₁₄ and ET₁₅ theories coincide with each other. In contrast,

in the high-frequency region, the difference between the two theories emerges due to the existence of the additional higher-order moment.

Since the experimental data of sound waves is usually obtained in the low-frequency region in the sense of the present dimensionless frequency, ET_{14} is enough to describe the experimental fact. On the other hand, to capture the structure of shock waves, ET_{15} is needed because the theory has a larger maximum characteristic speed than the one of ET_{14} . The study of the shock waves is left for future study.

We finally remark that, in the present approach, we treat the internal modes as a whole; however, in principle, we can generalize the theory with two internal modes, one for the rotational and one for the vibrational motion of a molecule, as was done in the paper [59,60].

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Appendix A. Derivation of the Nonequilibrium Part of Lagrange Multipliers

Inserting (33) into (24) and (27), we obtain the following algebraic relation for Lagrange multipliers:

$$\begin{aligned} \tilde{\lambda}\rho + \frac{1}{3}\tilde{\lambda}_{ll}\hat{F}_{ll}^E + \tilde{\mu}\hat{G}_{ll}^E + \tilde{\zeta}\hat{H}_{llmm}^E &= 0, \\ \tilde{\lambda}_i\hat{F}_{ij}^E + \tilde{\mu}_i\hat{G}_{lij}^E &= 0, \\ \tilde{\lambda}\hat{G}_{ll}^E + \frac{1}{3}\tilde{\lambda}_{ll}\hat{G}_{llmm}^E + \tilde{\mu}\hat{H}_{llmm}^E + \tilde{\zeta}\left(\hat{F}_{llmmnn}^E + 3\hat{f}_{llmm}^{1|E} + 2\hat{f}_{ll}^{2|E}\right) &= 0, \\ \tilde{\lambda}\hat{F}_{ij}^E + \tilde{\lambda}_{rs}\hat{F}_{ijrs}^E + \tilde{\mu}\hat{G}_{llij}^E + \tilde{\zeta}\left(\hat{F}_{llmmij}^E + 2\hat{f}_{llij}^{1|E}\right) &= -\frac{k_B}{m}\left(\Pi\delta_{ij} - \sigma_{(ij)}\right), \\ \tilde{\lambda}_i\hat{G}_{llij}^E + \tilde{\mu}_i\left(\hat{F}_{llmmij}^E + 2\hat{f}_{llij}^{E|1} + \hat{f}_{ij}^{E|2}\right) &= -2\frac{k_B}{m}q_j, \\ \tilde{\lambda}\left(\hat{F}_{llmm}^E + 2\hat{f}_{ll}^{E|1}\right) + \frac{1}{3}\tilde{\lambda}_{ll}\left(\hat{F}_{llmmnn}^E + 2\hat{f}_{llmm}^{E|1}\right) + \tilde{\mu}\left(\hat{F}_{llmmnn}^E + 3\hat{f}_{llmm}^{E|1} + 2\hat{f}_{ll}^{E|2}\right) + \tilde{\zeta}\left(\hat{F}_{kkllmmmm}^E + 4\hat{f}_{llmmnn}^{E|1} + 4\hat{f}_{llmm}^{E|2}\right) &= -\frac{k_B}{m}\Delta, \end{aligned} \quad (A1)$$

where E with a quantity indicates the moment evaluated by the equilibrium distribution function, and

$$\begin{aligned} \hat{f}_{k_1k_2\cdots k_s}^{1|E} &= \hat{G}_{llk_1k_2\cdots k_s}^E - \hat{F}_{llk_1k_2\cdots k_s}^E = \int_{\mathbf{R}^3} \int_0^{+\infty} 2C_{k_1}C_{k_2}\cdots C_{k_s}f_E \mathcal{I} \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}, \\ \hat{f}_{k_1k_2\cdots k_t}^{2|E} &= \int_{\mathbf{R}^3} \int_0^{+\infty} mC_{k_1}C_{k_2}\cdots C_{k_t}f_E \left(\frac{2\mathcal{I}}{m}\right)^2 \varphi(\mathcal{I}) d\mathcal{I} d\mathbf{C}. \end{aligned}$$

Taking into account the moments of f_E^I , i.e., (16), (18) and (20), we obtain the following relation:

$$\begin{aligned} \hat{F}_{k_1k_2\cdots k_r}^E &= \hat{F}_{k_1k_2\cdots k_r}^M, \\ \hat{f}_{k_1k_2\cdots k_s}^{1|E} &= 2\frac{p}{\rho}y^I\hat{F}_{k_1k_2\cdots k_s}^M, \\ \hat{f}_{k_1k_2\cdots k_t}^{2|E} &= 4\frac{p}{\rho}\left(\hat{c}_v^I + y^{I^2}\right)\hat{F}_{k_1k_2\cdots k_t}^M, \end{aligned}$$

where $\hat{F}_{k_1 k_2 \dots k_r}^M$ is the equilibrium moments for monatomic gas defined by

$$\hat{F}_{k_1 k_2 \dots k_r}^M = m \int_{\mathbb{R}^3} f_E^K C_{k_1} C_{k_2} \dots C_{k_r} dC. \quad (\text{A2})$$

Since f_E^K is the Maxwell distribution function (14)₁, $\hat{F}_{k_1 k_2 \dots k_r}^M$ are easily calculated, e.g.,

$$\begin{aligned} \hat{F}^M &= \rho, \quad \hat{F}_{ij}^M = p \delta_{ij}, \quad \hat{F}_{ijrs}^M = \frac{p^2}{\rho} (\delta_{ij} \delta_{rs} + \delta_{ir} \delta_{js} + \delta_{is} \delta_{jr}), \\ \hat{F}_{llijrs}^M &= 7 \frac{p^3}{\rho^2} (\delta_{ij} \delta_{rs} + \delta_{ir} \delta_{js} + \delta_{is} \delta_{jr}), \\ \hat{F}_{kkllmmnn}^M &= 945 \frac{p^4}{\rho^3}. \end{aligned}$$

As the solutions of (A1), the nonequilibrium parts of the Lagrange multipliers are obtained as (35).

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