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

Takashi Arima 1,† and Tommaso Ruggeri 2,*,†

1 Department of Engineering for Innovation, National Institute of Technology, Tomakomai College, Tomakomai, Hokkaido 059-1275, Japan; arima@tomakomai-ct.ac.jp
2 Department of Mathematics and Alma Mater Research Center on Applied Mathematics AM 2, University of Bologna, 40126 Bologna, Italy
* Correspondence: tommaso.ruggeri@unibo.it
† These authors contributed equally to this work.

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

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):

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

where the state of the gas can be described by the distribution function $f(x, \xi, t)$, being $x \equiv (x_1, \xi \equiv (\xi_i)$, $t$ 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):

$$F_{k_1k_2...k_n}(x,t) = m \int_{\mathbb{R}^3} f(x, \xi, t) \xi_{k_1} \xi_{k_2} ... \xi_{k_n} \, d\xi,$$

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

$$\frac{\partial F_{k_1k_2...k_n}}{\partial t} + \frac{\partial F_{k_1k_2...k_n\xi_{k_{n+1}}}}{\partial x_{k_{n+1}}} = P_{k_1k_2...k_n}, \quad n = 0, 1, \ldots,$$

where

$$P_{k_1k_2...k_n} = m \int_{\mathbb{R}^3} Q(f) \xi_{k_1} \xi_{k_2} ... \xi_{k_n} \, d\xi,$$

$P = P_k = P_{kk} = 0.$
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, Majdarević, 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: $(F, F_{k_1}, F_{k_1k_2}, F_{k_1k_1})$ (so-called ET13). 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 ET14) [18] by adopting a new scalar field $F_{jjkk}$ in addition to the previous 13 fields: $(F, F_{k_1}, F_{k_1k_2}, F_{k_1k_1}, F_{jjkk})$.

For the case with many fields such as (2) truncated at a generic tensorial order $\tilde{N}$, 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]:

$$p^a \partial_a f = Q,$$

in which the distribution function $f$ depends on $(x^a, p^\beta)$, where $x^a$ are the space-time coordinates, $p^a$ is the four-momentum $(p_a p^a = m^2 c^2)$, $\partial_a = \partial / \partial x^a$, $c$ 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

\[
\partial_a A^{\alpha_1 \cdots \alpha_n} = I^{\alpha_1 \cdots \alpha_n} \quad \text{with} \quad n = 0, \cdots, N
\]  

with

\[
A^{\alpha_1 \cdots \alpha_n} = \frac{c}{m^{n-1}} \int_{\Omega^3} f p^\alpha p^{\alpha_1} \cdots p^{\alpha_n} \, dP, \quad I^{\alpha_1 \cdots \alpha_n} = \frac{c}{m^{n-1}} \int_{\Omega^3} Q p^{\alpha_1} \cdots p^{\alpha_n} \, dP,
\]

and

\[
dP = \frac{dp^1 \, dp^2 \, dp^3}{p^0}.
\]

When \( n = 0 \), the tensor in (5) reduces to \( A^\alpha \). Moreover, the production tensor in (5) 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 \( A^{\alpha \beta} = c^2 A^\alpha \) and therefore only 14 equations of (6) are independent):

\[
\partial_a A^\alpha = 0, \quad \partial_a A^{\alpha \beta} = 0, \quad \partial_a A^{\alpha \beta \gamma} = I^{\beta \gamma}, \quad (\beta, \gamma = 0, 1, 2, 3; I^{\alpha \gamma} = 0).
\]  

The surprising result was that the LMR theory converges, in the classical limit, to Kremer’s monatomic ET\(_{14} \) theory, not Grad’s theory (thus ET\(_{13} \)) 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 tentative papers [30,31], Arima, Taniguchi, Ruggeri and Sugiyama [32] proposed a binary hierarchy of field equations with 14 fields (polyatomic ET\(_{14} \)) 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:

\[
\begin{align*}
\frac{dF}{dt} + \frac{dF_i}{dx_i} &= 0, \\
\frac{dF_j}{dt} + \frac{dF_{ij}}{dx_j} &= 0, \\
\frac{dF_{ij}}{dt} + \frac{dF_{ijk}}{dx_k} &= P_{ij}, \\
\frac{dG_{ij}}{dt} + \frac{dG_{ijl}}{dx_l} &= 0, \\
\frac{dG_{ijl}}{dt} + \frac{dG_{ijkl}}{dx_l} &= Q_{ijl},
\end{align*}
\]

where \( F(= \rho) \) is the mass density, \( F_i(= \rho v_i) \) is the momentum density, \( G_{ij} = \rho v^2 + 2 \rho \epsilon \) is twice times the energy density, \( F_{ij} \) is the momentum flux, and \( G_{ijkl} \) is the energy flux. As usual, \( v_i \) denotes the components of velocity, and \( \epsilon \) is the specific internal energy. \( F_{ijk} \) and \( G_{ijkl} \) are the fluxes of \( F_{ij} \) and \( G_{ijl} \), respectively, and \( P_{ij} \) (\( P_{ij} \neq 0 \)) and \( Q_{ijl} \) are the productions with respect to \( F_{ij} \) and \( G_{ijl} \), 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 \( f(x, \xi, t, I) \) is assumed to depend on an additional non-negative internal energy parameter \( I \) 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:

\[
\frac{\partial F_{k_1 k_2 \ldots k_n}}{\partial t} + \frac{\partial F_{k_1 k_2 \ldots k_n k_{n+1}}}{\partial x_{k_{n+1}}} = P_{k_1 k_2 \ldots k_n},
\]

\[
\frac{\partial G_{ll k_1 k_2 \ldots k_n k_{n+1}}}{\partial t} + \frac{\partial G_{lll k_1 k_2 \ldots k_n k_{n+1}}}{\partial x_{k_{n+1}}} = Q_{l_l l k_1 k_2 \ldots k_n},
\]

with the following definition of moments of polyatomic gases \((\xi^2 = |\xi|^2 = \tilde{\xi}_j \tilde{\xi}_j)\):

\[
F_{k_1 k_2 \ldots k_n} = m \int_{\mathbb{R}^3} \int_0^{+\infty} f(\mathbf{x}, \mathbf{\xi}, t, \mathcal{I}) \xi_{k_1} \xi_{k_2} \ldots \xi_{k_n} \varphi(\mathcal{I}) \, d\mathcal{I} \, d\xi,
\]

\[
G_{ll k_1 k_2 \ldots k_n} = \int_{\mathbb{R}^3} \int_0^{+\infty} \left( m\xi^2 + 2\mathcal{I} \right) f(\mathbf{x}, \mathbf{\xi}, t, \mathcal{I}) \xi_{k_1} \xi_{k_2} \ldots \xi_{k_n} \varphi(\mathcal{I}) \, d\mathcal{I} \, d\xi,
\]

\[
G_{llk_1 k_2 \ldots k_n} = \int_{\mathbb{R}^3} \int_0^{+\infty} \left( m\xi^2 + 2\mathcal{I} \right) f(\mathbf{x}, \mathbf{\xi}, t, \mathcal{I}) \xi_{k_1} \xi_{k_2} \ldots \xi_{k_n} \varphi(\mathcal{I}) \, d\mathcal{I} \, d\xi,
\]

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 fluxes in both hierarchies together with the production terms are functions to be determined by the closure of all densities \((F_{k_1 k_2 \ldots k_n}, G_{ll k_1 k_2 \ldots k_n})\). The index \(n = 0, 1, \ldots, N\) and \(m = 0, 1, \ldots, M\). Moreover, \(P = P_k = Q_{ll} = 0\) 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 \(N\) and \(M\), in the sense of the Galilean invariance and the characteristic velocity, is \(M = N - 1\).

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:

\[
A^{a_1 \ldots a_n} = \frac{c}{m^{n-1}} \int_{\mathbb{R}^3} \int_0^{+\infty} f(p^a p^{a_1} \ldots p^{a_n}) \left( 1 + n \frac{\mathcal{I}}{m c^2} \right) \varphi(\mathcal{I}) \, d\mathcal{I} \, dp,
\]

\[
I^{a_1 \ldots a_n} = \frac{c}{m^{n-1}} \int_{\mathbb{R}^3} \int_0^{+\infty} Q(p^{a_1} \ldots p^{a_n}) \left( 1 + n \frac{\mathcal{I}}{m c^2} \right) \varphi(\mathcal{I}) \, d\mathcal{I} \, dp,
\]

with a distribution function \(f(x^a, p^\beta, \mathcal{I})\) 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

\[
H_{llmm} = 2G_{llmm} - F_{llmm}
\]
is involved. In the case that \( N > 2 \), the new hierarchy contains, in addition to the \( F' \)s and \( G' \)s hierarchies (8) with \( n = 0, 1, \ldots N \) and \( m = 0, 1, \ldots N - 1 \), 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 ET\(_{14} \) 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 (ET\(_{15} \)):

\[
\begin{align*}
\frac{\partial F}{\partial t} + \frac{\partial F_k}{\partial x_k} &= 0, \\
\frac{\partial F_i}{\partial t} + \frac{\partial F_{ik}}{\partial x_k} &= 0, \\
\frac{\partial F_{ij}}{\partial t} + \frac{\partial F_{ijk}}{\partial x_k} &= P_{ij}, \\
\frac{\partial G_{ll}}{\partial t} + \frac{\partial G_{llk}}{\partial x_k} &= 0, \\
\frac{\partial G_{lli}}{\partial t} + \frac{\partial G_{llik}}{\partial x_k} &= Q_{lli}, \\
\frac{\partial H_{llmm}}{\partial t} + \frac{\partial H_{llmmk}}{\partial x_k} &= R_{llmm},
\end{align*}
\]

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 ET\(_{14} \) theory as a principal subsystem, the monatomic ET\(_{14} \) theory in the monatomic singular limit, and the NSF theory as its parabolic limit. To show the difference with the polyatomic ET\(_{14} \) and the role of the new field \( H_{llmm} \), we study the dispersion relation of the linear waves and compare the result of ET\(_{14} \).

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 (\( p, \varepsilon, \rho, T \) 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 \( D = 3 \) )

\[
p = \frac{k_B}{m} \rho T, \quad \varepsilon = \frac{D}{2} \frac{k_B}{m} T
\]
in [35,39] and in the present case of non-polytropic gas

\[ p = p(\rho, T) = \frac{k_B}{m} \rho T, \quad \epsilon \equiv \epsilon_E(T) \]  \hspace{1cm} (12)

in [36,40]:

\[ f_E = f_K^E f_I^E, \]  \hspace{1cm} (13)

where \( f_K^E \) is the Maxwellian distribution function and \( f_I^E \) is the distribution function of the internal mode:

\[ f_K^E = \frac{\rho}{m} \left( \frac{m}{2\pi k_B T} \right)^{3/2} \exp \left( -\frac{mC_i^2}{2k_B T} \right), \quad f_I^E = \frac{1}{A(T)} \exp \left( -\frac{\mathcal{I}}{k_B T} \right), \]  \hspace{1cm} (14)

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

\[ A(T) = \int_0^{+\infty} \exp \left( -\frac{\mathcal{I}}{k_B T} \right) \varphi(\mathcal{I}) d\mathcal{I}, \]  \hspace{1cm} (15)

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

\[ \int_0^{+\infty} f_I^E \varphi(\mathcal{I}) d\mathcal{I} = 1. \]  \hspace{1cm} (16)

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

\[ \epsilon = \epsilon_E(T) = \epsilon_K^E(T) + \epsilon_I^E(T) = \frac{1}{2\rho} \int f_K^E \mathcal{I} f_I^E(T) d\mathcal{I} dC, \]  \hspace{1cm} (17)

where \( \epsilon_K^E \) and \( \epsilon_I^E \) are the equilibrium kinetic (translational) and internal specific energies defined by

\[ \epsilon_K^E(T) = \frac{1}{2\rho} \int f_K^E \mathcal{I} f_K^E(T) d\mathcal{I} dC = \frac{1}{2\rho} \int f_K^E \mathcal{I} d\mathcal{I} = \frac{3}{2} \frac{k_B T}{m}, \quad \epsilon_I^E(T) = \frac{1}{m} \int f_I^E \mathcal{I} f_I^E(T) d\mathcal{I} = \frac{1}{m} \int f_I^E d\mathcal{I} = \frac{k_B T^2}{m} \frac{d \log A(T)}{dT}. \]  \hspace{1cm} (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 \( \epsilon_I^E(T) \) from (18)\textsubscript{2} (see for more details [36]). Vice versa, if the caloric equation of state is known, from (18)\textsubscript{2}, we can evaluate the function \( A(T) \) in integral form with respect to \( T \) as follows:

\[ A(T) = A_0 \exp \left( \frac{m}{k_B T_0} \int_{T_0}^T \frac{\epsilon_I^E(T')}{T'^2} dT' \right), \]

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]:

\[ \varphi(\mathcal{I}) = \mathcal{I}^{\frac{\omega-3}{2}}. \]  \hspace{1cm} (19)
It was proved in [36] that
\[ \frac{1}{m^2} \int_0^\infty \mathcal{I}^2 f^I E \phi(\mathcal{I}) \, d\mathcal{I} = \frac{p^2}{\rho^2} \bar{e}_v^I + \varepsilon^I (T)^2, \] (20)

where
\[ \bar{e}_v^I = m \frac{c_v}{k_B}, \quad \text{and} \quad c_v = \frac{d \varepsilon^I (T)}{dT} \]
is the specific heat of the internal mode. We remark that the relation between the pressure and the translational internal energy is as follows:
\[ p = \frac{2}{3} \rho \varepsilon^K (T). \]

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
\[ s^K (\rho, T) \equiv -\frac{k_B}{\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} f E \log f^E \phi(\mathcal{I}) \, d\mathcal{I} \, dC, \]
\[ = \frac{k_B}{m} \log \left( \frac{T^{3/2}}{\rho} \right) + \frac{\varepsilon^K (T)}{m} - \frac{k_B}{m} \log \left[ \frac{1}{m} \left( \frac{m}{2\pi k_B} \right)^{3/2} \right], \]
\[ s^I (T) \equiv \frac{k_B}{\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} f E \log f^I \phi(\mathcal{I}) \, d\mathcal{I} \, dC, \]
\[ = \frac{k_B}{m} \log A(T) + \frac{\varepsilon^I (T)}{T}. \]

2.1. System of Balance Equations for 15 Fields

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

\[
\begin{pmatrix}
F \\
F_i \\
F_{ij} \\
F_{ijk}
\end{pmatrix} = \int_{\mathbb{R}^3} \int_0^{+\infty} \left( \begin{array}{c}
\frac{1}{\xi^i} \\
\frac{1}{\xi^i \xi^j} \\
\frac{1}{\xi^i \xi^j \xi^k}
\end{array} \right) f \phi(\mathcal{I}) \, d\mathcal{I} \, d\xi,
\]
\[\begin{pmatrix}
G_{ll} \\
G_{lll} \\
G_{llmm}
\end{pmatrix} = \int_{\mathbb{R}^3} \int_0^{+\infty} (m \xi^2 + 2 \mathcal{I}) \left( \begin{array}{c}
\frac{1}{\xi^i} \\
\frac{1}{\xi^i \xi^j} \\
\frac{1}{\xi^i \xi^j \xi^k}
\end{array} \right) f \phi(\mathcal{I}) \, d\mathcal{I} \, d\xi, \]
\[\begin{pmatrix}
H_{llmm} \\
H_{llm} \\
H_{ll}
\end{pmatrix} = \int_{\mathbb{R}^3} \int_0^{+\infty} (m \xi^2 + 4 \mathcal{I}) \xi^2 \left( \begin{array}{c}
\frac{1}{\xi^i} \\
\frac{1}{\xi^i \xi^j} \\
\frac{1}{\xi^i \xi^j \xi^k}
\end{array} \right) f \phi(\mathcal{I}) \, d\mathcal{I} \, d\xi, \]

and the production terms
\[ f \equiv \begin{pmatrix}
P_{ij} \\
Q_{ll} \\
R_{llmm}
\end{pmatrix} = \int_{\mathbb{R}^3} \int_0^{+\infty} \left( \begin{array}{c}
\frac{m \xi^i \xi^j}{(m \xi^2 + 2 \mathcal{I}) \xi^i} \\
\frac{m \xi^i \xi^j}{(m \xi^2 + 4 \mathcal{I}) \xi^2}
\end{array} \right) Q(f) \phi(\mathcal{I}) \, d\mathcal{I} \, d\xi. \] (22)
Since the intrinsic (velocity independent) variables are the moments in terms of the peculiar velocity $\mathbf{v}$ instead of $\xi_i$, the velocity dependence of the densities is obtained as follows:

\[
\begin{align*}
F &= \rho, \\
F_i &= \rho v_i, \\
F_{ij} &= \delta_{ij} \rho v_i v_j, \\
G_{ij} &= \delta_{ij} \rho v_i v_j, \\
G_{III} &= \delta_{III} + \rho v_i v_j, \\
H_{lmm} &= \hat{H}_{llmm} + 4 \hat{G}_{lll} v_i + 2 \hat{G}_{lll} v_i^2 + 4 \hat{F}_{ij} v_i v_j + \rho \sigma^4,
\end{align*}
\]

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

mass density:
\[
\rho = \int_{\mathbb{R}^3} \int_{0}^{+\infty} m f (\mathcal{I}) d\mathcal{I} d\mathbf{C} = \int_{\mathbb{R}^3} \int_{0}^{+\infty} m f_E (\mathcal{I}) d\mathcal{I} d\mathbf{C},
\]

velocity:
\[
v_i = \frac{1}{\rho} \int_{\mathbb{R}^3} \int_{0}^{+\infty} m \mathcal{C}_i f (\mathcal{I}) d\mathcal{I} d\mathbf{C} = \frac{1}{\rho} \int_{\mathbb{R}^3} \int_{0}^{+\infty} m \mathcal{C}_i f_E (\mathcal{I}) d\mathcal{I} d\mathbf{C},
\]

specific internal energy density:
\[
\varepsilon = \varepsilon^K + \varepsilon^I = \frac{1}{2\rho} \int_{\mathbb{R}^3} \int_{0}^{+\infty} (m C^2 + 2 T) f (\mathcal{I}) d\mathcal{I} d\mathbf{C},
\]

specific translational energy density:
\[
\varepsilon^K = \frac{1}{2\rho} \int_{\mathbb{R}^3} \int_{0}^{+\infty} m C^2 f (\mathcal{I}) d\mathcal{I} d\mathbf{C},
\]

total nonequilibrium pressure:
\[
\mathcal{P} = \frac{2}{3} \rho \varepsilon^K = \frac{1}{3} \int_{\mathbb{R}^3} \int_{0}^{+\infty} m C^2 f (\mathcal{I}) d\mathcal{I} d\mathbf{C},
\]

dynamic pressure:
\[
\Pi = \mathcal{P} - p = \frac{1}{3} \int_{\mathbb{R}^3} \int_{0}^{+\infty} m C^2 (f - f_E) (\mathcal{I}) d\mathcal{I} d\mathbf{C},
\]

shear stress:
\[
\sigma_{ij} = - \int_{\mathbb{R}^3} \int_{0}^{+\infty} m C_i C_j f (\mathcal{I}) d\mathcal{I} d\mathbf{C},
\]

heat flux:
\[
q_i = \frac{1}{\rho} \int_{\mathbb{R}^3} \int_{0}^{+\infty} (m C^2 + 2 T) C_i f (\mathcal{I}) d\mathcal{I} d\mathbf{C},
\]

are related to the intrinsic moments as follows:

\[
\begin{align*}
\hat{G}_{ll} &= 2 \rho \varepsilon = \rho (\varepsilon^K + \varepsilon^I), \\
\hat{F}_{ll} &= 3 \mathcal{P} = 3 (p + \Pi), \\
\hat{F}_{ij} &= - \sigma_{ij}, \\
\hat{C}_{llll} &= 2 \rho \varepsilon^I,
\end{align*}
\]

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

\[
\varepsilon = \varepsilon_E(T).
\]

Let us decompose the intrinsic part of $H_{lmm}$ into the equilibrium part and the nonequilibrium part $\Delta$ as follows:

\[
\hat{H}_{lmm} = \int_{\mathbb{R}^3} \int_{0}^{+\infty} (m C^2 + 4 T) C_i f (\mathcal{I}) d\mathcal{I} d\mathbf{C} = 12 \frac{\rho^2}{\rho} (5 + 4 y^I) + \Delta,
\]

where

\[
y^I = \frac{\rho \varepsilon^I}{\rho \varepsilon_E}(T),
\]

and $\Delta$ is defined by

\[
\Delta = \int_{\mathbb{R}^3} \int_{0}^{+\infty} (m C^2 + 4 T) C_i (f - f_E) f (\mathcal{I}) d\mathcal{I} d\mathbf{C}.
\]
Similarly, the velocity dependences of the fluxes and productions are obtained as follows:

\[
F_{ijk} = \hat{f}_{ijk} + \hat{f}_{ij} v_k + \hat{f}_{ik} v_j + \hat{f}_{ki} v_j + \rho v_j v_k v_i,
\]

\[
G_{llik} = \hat{G}_{llik} + \hat{G}_{llj} v_k + \hat{G}_{llk} v_i + 2 \hat{G}_{llik} v_i v_k + \hat{G}_{llj} v_k v_i + 2 \hat{G}_{llj} v_j v_k + \hat{G}_{llk} v_i v_j + \rho v_i v_j v_k,
\]

\[
H_{llmmnk} = \frac{d}{d t} \hat{H}_{llmmnk} + \hat{H}_{llmmn} v_k + 4 \hat{G}_{llik} v_i + 2 \hat{G}_{llj} v_j + 4 \hat{G}_{llik} v_i v_j + 2 \hat{G}_{llj} v_j v_i + 4 \hat{f}_{ijk} v_i v_j + 4 \hat{f}_{ijk} v_j v_i + 4 \hat{f}_{ijk} v_i v_j v_k + \rho v^3 v_i v_j v_k,
\]

\[
P_{ij} = \hat{P}_{ij},
\]

\[
Q_{lli} = 2 v_i \hat{P}_{ii} + \hat{Q}_{lli},
\]

\[
R_{llmm} = 4 v_i v_j \hat{P}_{ij} + 4 v_i \hat{Q}_{lii} + \hat{R}_{llmm}.
\]

The velocity dependences of moments (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:

\[
\hat{F}_{ijk} = \int_{\mathbb{R}^3} \int_0^{+\infty} m C_i C_j C_k f \varphi(I) dI d\xi,
\]

\[
\hat{G}_{lljk} = \int_{\mathbb{R}^3} \int_0^{+\infty} (m C_j^2 + 2 I) C_i C_k f \varphi(I) dI d\xi,
\]

\[
\hat{H}_{llmmnk} = \int_{\mathbb{R}^3} \int_0^{+\infty} (m C_j^2 + 4 I) C_i C_k f \varphi(I) dI d\xi,
\]

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

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

under the constraints that the density moments \( I, F_i, F_{ij}, G_{lij}, G_{lli}, H_{llmm} \) 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

\[
\mathcal{L}(f) = -k_B \int_{\mathbb{R}^3} \int_0^{+\infty} f \log f \varphi(I) dI d\xi
\]

\[+ \lambda \left( F - \int_{\mathbb{R}^3} \int_0^{+\infty} m f \varphi(I) dI d\xi \right) + \lambda_i \left( F_i - \int_{\mathbb{R}^3} \int_0^{+\infty} m C_i f \varphi(I) dI d\xi \right)
\]

\[+ \lambda_{ij} \left( F_{ij} - \int_{\mathbb{R}^3} \int_0^{+\infty} m C_i C_j f \varphi(I) dI d\xi \right) + \mu \left( G_{llij} - \int_{\mathbb{R}^3} \int_0^{+\infty} (m C_i C_j^2 + 2 I) f \varphi(I) dI d\xi \right)
\]

\[+ \mu_i \left( G_{lli} - \int_{\mathbb{R}^3} \int_0^{+\infty} (m C_i^2 + 2 I) C_j f \varphi(I) dI d\xi \right) + \xi \left( H_{llmm} - \int_{\mathbb{R}^3} \int_0^{+\infty} (m C_i^2 + 4 I) C_j^2 f \varphi(I) dI d\xi \right),
\]

where \( \lambda, \lambda_{ij}, \lambda_i, \mu, \mu_i, \) and \( \xi \) 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]):

\[
\begin{align*}
\lambda &= \hat{\lambda} - \lambda_i v_i + \hat{\lambda}_{ij} v_i v_j + \hat{\mu} v^2 - \mu_i v^2 v_i + \hat{\xi} v^4, \\
\lambda_i &= \hat{\lambda}_i - 2\hat{\lambda}_{ij} v_j - 2\hat{\mu}_i v_i + 3\hat{\mu}_i v^2 - 4\hat{\xi} v^2 v_i, \\
\lambda_{ij} &= \hat{\lambda}_{ij} - 2\hat{\mu}_i v_j + 4\hat{\xi} v_i v_j, \\
\mu &= \hat{\mu} - \mu_i v_i + 2\hat{\xi} v^2, \\
\mu_i &= \hat{\mu}_i - 4\hat{\xi} v_i, \\
\zeta &= \hat{\xi}.
\end{align*}
\]

The distribution function \( f \), which satisfies \( \delta L/\delta f = 0 \), is

\[
f_{15} = \exp \left( -1 - \frac{m}{k_B} \chi \right), \quad \text{with} \quad \chi = \hat{\lambda} + C\hat{\lambda}_i + C_i\hat{\lambda}_{ij} + \left( C^2 + \frac{2\mathcal{T}}{m} \right) \hat{\mu} + \left( C^2 + \frac{2\mathcal{T}}{m} \right) \hat{\mu}_i + \left( C^2 + \frac{4\mathcal{T}}{m} \right) C^2 \hat{\xi}. \tag{31}
\]

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 \( G_{II} \) 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

\[
\begin{align*}
\lambda_E &= \frac{1}{T} \left( -g + \frac{v_i^2}{2} \right), \quad \lambda_{iE} = -\frac{v_i}{T}, \quad \lambda_{iiE} = 0, \quad \lambda_{ij} = 0, \quad \mu_E = \frac{1}{2\mathcal{T}}, \quad \mu_{iE} = 0, \quad \zeta_E = 0, \tag{32}
\end{align*}
\]

where \( g(= \epsilon_E(T) + p/\rho - Ts) \) 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 \( \chi \) in (31) 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., \( \overline{N} = 2N \). 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:

\[
\begin{align*}
\tilde{f}_{15} &\simeq f_E \left( 1 - \frac{m}{k_B} \tilde{\chi} \right), \\
\tilde{\chi} &= \tilde{\lambda} + C\tilde{\lambda}_i + C_i\tilde{\lambda}_{ij} + \left( C^2 + \frac{2\mathcal{T}}{m} \right) \tilde{\mu} + \left( C^2 + \frac{2\mathcal{T}}{m} \right) \tilde{\mu}_i + \left( C^2 + \frac{4\mathcal{T}}{m} \right) C^2 \tilde{\xi}, \tag{33}
\end{align*}
\]

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 \( (\rho, T, \Pi, \sigma_{ij}, q_i, \Delta) \) up to the first order with respect to the nonequilibrium fields, \( \Pi, \sigma_{ij}, q_i \) and \( \Delta \). The derivation is given in the Appendix A. Instead of \( \Delta \), it may be useful to introduce the following nonequilibrium field:

\[
\tilde{\Pi} = \frac{1}{3(4\hat{c}_l^2 + 5)} \left\{ 12\Pi(y^l + 1) - \frac{\rho}{\hat{c}^2} \Delta \right\},
\]

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

\[
\tilde{\lambda} = \frac{3(\hat{c}_l^2 - y^l)}{2\hat{c}_l^2 \rho T} \Pi + \frac{3(4y^l + 5)}{8\rho T} \hat{C}_l,
\]

\[
\tilde{\lambda}_i = \frac{2y^l + 5}{p T(2\hat{c}_l^2 + 5)} q_i,
\]

\[
\tilde{\lambda}_{ll} = -\frac{3(2\hat{c}_l^2 + 3)}{4\hat{c}_l^2 p T} \Pi - \frac{3(y^l + 1)}{2p T} \hat{C}_l,
\]

\[
\tilde{\lambda}_{ij} = \frac{\sigma_{ij}}{2p T},
\]

\[
\tilde{\lambda}_i = \frac{3}{4\hat{c}_l^2 p T} \Pi - \frac{3}{4p T} \hat{C}_l,
\]

\[
\tilde{\mu} = \frac{\rho}{p^2 T(2\hat{c}_l^2 + 5)} q_i,
\]

\[
\tilde{\zeta} = \frac{\rho}{8p^2 T} \hat{C}_l.
\]

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

\[
\mathbf{u}' \equiv (\lambda, \lambda_i, \lambda_{ij}, \mu, \mu_i, \zeta)
\]

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:

\[
\tilde{F}_{ijk} = \frac{2}{2\hat{c}_l^2 + 5} (q_k \delta_{ij} + q_i \delta_{jk} + q_j \delta_{ik}),
\]

\[
\tilde{G}_{llij} = (2y^l + 5) \frac{\rho^2}{\rho} \delta_{ij} + (2y^l + 7) \frac{\rho}{\rho} \Pi \delta_{ij} - (2\hat{c}_l^2 + 5) \frac{\rho}{\rho} \hat{C}_l \delta_{ij} - (2y^l + 7) \frac{\rho}{\rho} \sigma_{ij},
\]

\[
\tilde{H}_{llmmk} = \frac{20}{\rho} \frac{2y^l + 2\hat{c}_l^2 + 7}{2\hat{c}_l^2 + 5} q_k.
\]

2.4. Nonequilibrium Temperatures and Generalized BGK Model

2.4.1. Nonequilibrium Temperatures

We recall that \( \varepsilon^K \) and \( \varepsilon^I \) given in (24) are nonequilibrium variables while their sum is an equilibrium variable. Then, we can define two nonequilibrium temperatures \( (\theta^K, \theta^I) \)
such that, by inserting them into the caloric equation of state (12) instead of $T$, the nonequilibrium internal energies $(\varepsilon^K, \varepsilon^I)$ are obtained, i.e.:

$$\varepsilon^K = \varepsilon^E_{K}(\theta^K) = \frac{3}{2} k_B \rho^K, \quad \varepsilon^I = \varepsilon^E_{I}(\theta^I).$$ (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), the total nonequilibrium pressure is expressed by the thermal equation of state (12) with $\theta^K$ as follows:

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

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

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

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 $\tau_K$: 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 $\theta^K$, 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 $\tau$ 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:

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

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

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

Specifically, $f^K$ is the Maxwellian with $\rho(I)$ and $\theta^K$ given by

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

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

\[
\dot{p}_{ii} = -\frac{3}{\tau} \Pi, \quad \dot{p}_{(ij)} = \left( \frac{1}{\tau} + \frac{1}{\tau} \right) \sigma_{(ij)}, \quad \dot{Q}_{ll} = -2 \left( \frac{1}{\tau} + \frac{1}{\tau} \right) q_{ll},
\]

\[
\hat{R}_{llmm} = -\left( \frac{1}{\tau} + \frac{1}{\tau} \right) \Delta + \frac{1}{\tau} \frac{p}{2} \Pi \left( 12y' + 12 - 3 \Pi \right).
\]

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

\[
\hat{R}_{llmm} = -\left( \frac{1}{\tau} + \frac{1}{\tau} \right) \Delta + \frac{12}{\tau} \frac{p}{2} \left( y' + 1 \right) \Pi.
\]

2.5. Closed Field Equations

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

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} \left( \rho v \right) = 0,
\]

\[
\frac{\partial \rho v}{\partial t} + \frac{\partial}{\partial x} \left( \rho v^2 \right) = 0,
\]

\[
\frac{\partial}{\partial t} \left( \rho v^2 + (p + \Pi) \sigma_{ij} - \rho v_{ij} \right) = 0,
\]

\[
\frac{\partial}{\partial t} \left( 3(p + \Pi) + \rho v^2 \right) + \frac{\partial}{\partial x} \left\{ 2\rho \left( 2y' + 5 \right) + 12 \Pi (y' + 1) - \frac{p}{\rho} \left( \frac{2(2y' + 7)}{3(4y' + 5)} \left( 12 \Pi (y' + 1) - \frac{p}{\rho} \right) \sigma_{ij} - (2y' + 7) \frac{p}{\rho} \sigma_{ij} \right) 
\]

\[+ \frac{2}{2y' + 7} \rho \dot{q} \sigma_{ij} + 4 \frac{2y' + 7}{2y' + 5} \left( q_{ij} v_{ik} + q_{ik} v_{ij} \right) \right\} = -2 \Pi \frac{1}{\tau} v_{ij} + 2 \left( \frac{1}{\tau} + \frac{1}{\tau} \right) \sigma_{ij} v_{ij} - 2 \left( \frac{1}{\tau} + \frac{1}{\tau} \right) q_{ij}.
\]

\[
\frac{\partial}{\partial t} \left\{ 4y' + 5 \right\} + \Delta + 8q_{ij} + 2\Pi \left( 2y' + 5 \right) + 2 \Pi - 4v_{ij} \sigma_{ij} + \rho v^2 \sigma_{ij} \right\} +
\]

\[
- \frac{20p}{\rho} \left( 2y' + 7 \right) \frac{2y' + 7}{2y' + 5} \left( q_{ij} v_{ik} + q_{ik} v_{ij} \right) - 4 \left( 2y' + 7 \right) \frac{p}{\rho} \sigma_{ij} v_{ij} + 8 \left( \frac{1}{\tau} + \frac{1}{\tau} \right) q_{ij} v_{ij} - \left( \frac{1}{\tau} + \frac{1}{\tau} \right) \Delta + \frac{12}{\tau} \frac{p}{2} \left( y' + 1 \right) \Pi.
\]

where, from (34),

\[
\Delta = 3 \frac{p}{\rho} \left( 4y' + 1 \right) \Pi - (4y' + 5) \Pi.
\]

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 \(\tau\) and \(T\).

We remark that the field equations of \(\rho, v, T, \Pi, \sigma_{(ij)}\) are the same as the ones of polyatomic 14 field theory and the presence of \(\Delta\) 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 $\varphi_i$ and $\Sigma$ are, respectively, the non-convective entropy flux and the entropy production which are defined below.

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

$$h = \rho - \frac{3(2\epsilon^0 + 3)}{8\epsilon^0 p^T} \Pi^2 - \frac{3(4\epsilon^0 + 5)}{16p^T} \Pi^2 - \frac{1}{4p^T} \sigma_{(ij)}\sigma_{(ij)} - \frac{\rho}{(2\epsilon^0 + 5)p^T} \rho_i q_i.$$

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:

$$\varphi_i = -2\epsilon^0 \int_0^{+\infty} C_i f \log f \varphi(I) d\mathcal{I} d\mathcal{C}$$

$$= \frac{1}{\tau} q_i + \frac{2}{p^T(2\epsilon^0 + 5)} q_i \sigma_{(i)} - \frac{2}{p^T(2\epsilon^0 + 5)} q_i \Pi + \frac{1}{p^T} q_i \Pi,$$

The entropy production $\Sigma$ 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

$$\Sigma = u' \cdot f = \Sigma = \sum u' \cdot \hat{f} = \frac{1}{3} \Pi^2 \Gamma - \frac{1}{3} \Pi^2 \Gamma + 2 \hat{\varphi}_i \hat{q}_i + \hat{\xi} \Delta$$

$$= \frac{3(2\epsilon^0 + 3)}{4\epsilon^0 p^T} \Pi^2 + \frac{3(4\epsilon^0 + 5)}{8p^T} \left( \frac{1}{\tau} \frac{1}{1} \right) \Pi^2 + \frac{1}{2p^T} \left( \frac{1}{\tau} \frac{1}{1} \right) \Pi^2 + \frac{2p^T(2\epsilon^0 + 5)}{1} \left( \frac{1}{\tau} \frac{1}{1} \right) q_i q_i.$$

It is noteworthy that the entropy production is positive with the provided positive relaxation times and $\epsilon^0 \geq 0$.

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:

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

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]):

$$\frac{\partial}{\partial t} \rightarrow -V \delta, \quad \frac{\partial}{\partial x^i} \rightarrow n_i \delta, \quad f \rightarrow 0,$$

where $n_i$ denotes the $i$-component of the unit normal to the wavefront, $f$ is the production terms and $\delta$ 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 $(\rho, v = v_1, T, \Pi, \sigma = \sigma_{(11)}, q = q_1, \Delta)$. After some
cumbersome calculations, it is possible to prove that the system has the following 7 real characteristic velocities evaluated in equilibrium:

\[
\begin{align*}
V^{(1)} &= v - U_{1st}^E \sqrt{\frac{k_B}{m} T}, \\
V^{(2)} &= v - U_{2nd}^E \sqrt{\frac{k_B}{m} T}, \\
V^{(3)} &= V^{(4)} = V^{(5)} = v, \\
V^{(6)} &= v + U_{2nd}^E \sqrt{\frac{k_B}{m} T}, \\
V^{(7)} &= v + U_{1st}^E \sqrt{\frac{k_B}{m} T},
\end{align*}
\]

(44)

with the normalized characteristic speeds of the first mode \(U_{1st}^E\) and the second mode \(U_{2nd}^E\) defined by

\[
\begin{align*}
U_{1st}^E &= \frac{1}{\sqrt{6(4\hat{c}_v - 1)(\hat{c}_v + 1)}} \sqrt{8\hat{c}_v(7\hat{c}_v + 11) - 13 + 4\hat{c}_v \{64\hat{c}_v^2(\hat{c}_v + 16) + 897\hat{c}_v - 482\} + 349}, \\
U_{2nd}^E &= \frac{1}{\sqrt{6(4\hat{c}_v - 1)(\hat{c}_v + 1)}} \sqrt{8\hat{c}_v(7\hat{c}_v + 11) - 13 - 4\hat{c}_v \{64\hat{c}_v^2(\hat{c}_v + 16) + 897\hat{c}_v - 482\} + 349},
\end{align*}
\]

(45)

(46)

where \(\hat{c}_v = 3/2 + \hat{c}_I\) is the dimensionless specific heat. It is easy to prove that \(U_{1st}^E\) given by (45) and \(U_{2nd}^E\) 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 \(U_{1st}^E\) is larger than the corresponding one of the polyatomic ET\(_{14}\) theory, and this indicates that the subcharacteristic condition [50] is satisfied due to the convexity of entropy (43). In the limit of monatomic gases (\(\hat{c}_v = 3/2\), \(U_{1st}^E \sim 2.27655\) and \(U_{2nd}^E \sim 1.16218\), which coincide with the ones of monatomic ET\(_{14}\). In the limit that \(\hat{c}_v \to \infty\), \(U_{1st}^E \to \sqrt{3}\) which is the same as the one predicted by polyatomic ET\(_{14}\) 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 (ET\(_{10}\)) in which \((F, F_i, F_{ij})\) are the only independent fields. On the other hand, in this limit, \(U_{2nd}^E \to \sqrt{5/3}\) is different from the one of ET\(_{14}\) but is the same as the equilibrium sound velocity (the characteristic speed of Euler system) of monatomic gases in which \((F, F_i, F_{ll})\) are the only independent fields. While, \(U_{2nd}^E\) of ET\(_{14}\) approaches to 1 which is the characteristic speed of ET theory with 4 moments (ET\(_{4}\)) 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 \(U_{1st}^E, U_{2nd}^E\) depend only on the degrees of freedom \(D\). The dependences are shown in Figure 1.
Figure 1. Dependence of the normalized characteristic speeds $U_{1st}^E$ (left) and $U_{2nd}^E$ (right) with respect to $D$. The solid and dashed lines are, respectively, the normalized characteristic speeds of Extended Thermodynamics (ET)\textsubscript{15} and polyatomic ET\textsubscript{14}. The limit value of the normalized characteristic speeds of $D \to 3$ and $D \to \infty$ are indicated with dotted lines. In the limit that $D \to 3$, $U_{1st}^E$ and $U_{2nd}^E$ of ET\textsubscript{15} and ET\textsubscript{14} coincide with the monatomic ET\textsubscript{10}. In the limit that $D \to \infty$, both of $U_{1st}^E$ of ET\textsubscript{15} and ET\textsubscript{14} approach to the one of monatomic ET\textsubscript{10}, and $U_{2nd}^E$ of ET\textsubscript{15} and ET\textsubscript{14} approach, respectively, to monatomic Euler and ET\textsubscript{4}.

2.8. Maxwellian Iteration and Phenomenological Coefficients

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

$$\Pi = -\nu \frac{4\ell^l}{6\ell^l + 9} \frac{\partial v_i}{\partial x_i}, \quad \sigma_{(ij)} = 2\mu \frac{\partial v_{ij}}{\partial x_j}, \quad q_i = -\kappa \frac{2\ell^l + 5k_B}{2m} \frac{\partial T}{\partial x_i},$$

(47)

and

$$\Delta = -\tau_{\Delta} \frac{16\ell^l}{2\ell^l + 3} \rho \left(y^l + 1\right) \left(1 + \frac{\tau}{\tau_K}\right) \frac{\partial v_i}{\partial x_i},$$

(48)

where

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

Recalling the definitions of the bulk viscosity $\nu$, shear viscosity $\mu$, and heat conductivity $\kappa$ in the NFS theory:

$$\Pi = -\nu \frac{\partial v_i}{\partial x_i}, \quad \sigma_{(ij)} = 2\mu \frac{\partial v_{ij}}{\partial x_j}, \quad q_i = -\kappa \frac{\partial T}{\partial x_i},$$

(49)

we have from (47)

$$\nu = \frac{4\ell^l}{6\ell^l + 9} \rho \tau_v, \quad \mu = \rho \tau_\sigma, \quad \kappa = \frac{2\ell^l + 5k_B}{2m} \rho \tau_q.$$

(50)

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

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

This result seems similar to the case of monatomic ET\textsubscript{14} in which the nonequilibrium scalar field is equal to 0 in the Maxwellian iteration \cite{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 $\tau, \tau_v,$
and \( \tau_q \) as functions of \( \rho \) and \( T \), and estimate them by using the experimental data on \( \nu, \mu \) and \( \kappa \). On the other hand, \( \tau_\lambda \) and \( \tau_\kappa \) 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,

\[ \Delta = 12 \frac{\rho \Pi}{\rho} \left( y^l + 1 \right), \]

and (41)\(_7\) is ignored.

2.10. Monatomic Gas Limit

The monatomic gases are described in the limit \( \varepsilon^l \to 0 \) (\( y^l \to 0 \)) and therefore \( \varepsilon^l_0 \to 0 \).

In the limit, the equation for \( \Pi \) obtained by subtracting (41)\(_3\) from (41)\(_4\) and by using the conservation laws (41)\(_1,2,3\) becomes

\[ \frac{\partial \Pi}{\partial t} + \nu_k \frac{\partial \Pi}{\partial x_k} = - \left( \frac{1}{\nu_1} + \frac{\partial \nu_k}{\partial x_k} \right) \Pi. \]  

(51)

This is the first-order quasi-linear partial differential equation with respect to \( \Pi \). 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

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

(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 \( \hat{F}_M^{ij...in} \) (see (A2) for their explicit expressions) as follows:

\[
\hat{F}_{ij} = p \delta_{ij} - \sigma_{(ij)} = \hat{F}_M^{ij}, \\
\hat{F}_{ijk} = \frac{2}{5} \left( q_i \delta_{jk} + q_j \delta_{ik} + q_k \delta_{ij} \right) = \hat{F}_M^{ijk}, \\
\hat{C}_{ll} = \hat{F}_{ll} = 2pK = 3p = \hat{F}_M^{ll}, \\
\hat{C}_{lli} = \hat{F}_{lli} = 2q_i = \hat{F}_M^{lli}, \\
\hat{C}_{llij} = \frac{5p^2}{\rho} \delta_{ij} + \frac{1}{3} \Delta \delta_{ij} - \frac{7}{3} \frac{p}{\rho} \sigma_{(ij)} = \hat{F}_M^{llij}, \\
\hat{H}_{llmm} = 15 \frac{p^2}{\rho} + \Delta = \hat{G}_{llmm} = \hat{F}_M^{llmm}, \\
\hat{H}_{llmmk} = 28 \frac{p}{\rho} q_k = \hat{F}_M^{llmmk}.
\]

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 ET\(_{15}\) converge to those of the monatomic 14 theory by Kremer [18].

3. Dispersion Relation

The difference between ET\(_{15}\) and ET\(_{14}\) 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 \( u = (\rho, v_i, T, \sigma_{(ij)}, q, \Delta) \) with the angular frequency \( \omega \) and the complex wave number \( k \) such that

\[
u = w e^{i(\omega t - kx_1)},
\]

where \( w \) is a constant amplitude vector. We assume a longitudinal wave:

\[
v_i \equiv \begin{pmatrix} v \\ 0 \\ 0 \end{pmatrix}, \quad \sigma_{(ij)} \equiv \begin{pmatrix} \sigma & 0 & 0 \\ 0 & -\frac{1}{2} \sigma & 0 \\ 0 & 0 & -\frac{1}{2} \sigma \end{pmatrix}, \quad q_i \equiv \begin{pmatrix} q \\ 0 \end{pmatrix},
\]

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 \( \alpha \) and the attenuation per wavelength \( \alpha_\lambda \) are calculated as the functions of the frequency \( \omega \) by using the following relations:

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

where \( \lambda \) 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 $\Omega$ and $\hat{\tau}_K$ does not depend on $\rho$, 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 $c_0$:

$$c_0 = \sqrt{\frac{2c_I^2 + 5 k_B}{2c_I^2 + 3 m}}$$

and the attenuation per wavelength on the dimensionless frequency of the first mode in Figure 2 in the case with $c_I^2 = 2$. Around $\Omega \sim 10^0 (\omega \sim \tau^{-1})$, we can observe a change of $v_{ph}$ and a peak of $\alpha_\lambda$. Since this is due to the relaxation of internal mode relating to $\Pi$, both of the predictions by $ET_{14}$ and $ET_{15}$ 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 $\alpha_\lambda$. Since this is due to the relaxation of $\sigma$, $q$, and $\Delta$, 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 $ET_{14}$ 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 $ET_{15}$ or many moment theory to describe the experimental data.

![Figure 2](https://example.com/figure2.png)

**Figure 2.** Typical dependence of the dimensionless phase velocity $v_{ph}/c_0$ (left) and the attenuation per wavelength $\alpha_\lambda$ (right) on the dimensionless frequency $\Omega$ predicted by the $ET_{15}$ and polyatomic $ET_{14}$ 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 $ET_{14}$ theory obtained by Kremer $[18]$ in the monatomic singular limit. Moreover, we proved that the polyatomic $ET_{14}$ theory is a principal subsystem of the present one, and according to the general results, the spectrum of characteristic speeds of $ET_{15}$ includes the spectrum of eigenvalues of $ET_{14}$. Finally, we have evaluated the dispersion relation proving that, in the low-frequency region, the predictions by $ET_{14}$ and $ET_{15}$ 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\textsubscript{14} is enough to describe the experimental fact. On the other hand, to capture the structure of shock waves, ET\textsubscript{15} is needed because the theory has a larger maximum characteristic speed than the one of ET\textsubscript{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:

\[
\begin{align*}
\hat{\lambda} \rho &+ \frac{1}{3} \lambda_{i} F_{ij}^{E} + \mu C_{ij}^{E} + \xi H_{iijm}^{E} = 0, \\
\hat{\lambda}_{i} F_{ij}^{E} + \mu_{i} C_{ij}^{E} = 0, \\
\hat{\lambda} C_{iijm}^{E} + \frac{1}{3} \lambda_{i} C_{iijm}^{E} + \mu H_{iijm}^{E} + \xi \left( F_{iijm}^{E} + 3 I_{iijm}^{E} + 2 I_{ij}^{E} \right) = 0, \\
\lambda_{i} F_{ij}^{E} + \mu_{i} C_{ij}^{E} + \xi \left( F_{iijm}^{E} + 2 I_{iijm}^{E} + I_{ij}^{E} \right) = -\frac{k_{B}}{m} \left( \Pi_{ij} - \sigma_{ij} \right), \\
\hat{\lambda}_{i} C_{iijm}^{E} + \mu_{i} \left( F_{iijm}^{E} + 2 I_{iijm}^{E} + I_{ij}^{E} \right) = -\frac{k_{B}}{m} q_{i}, \\
\hat{\lambda} \left( F_{iijm}^{E} + 2 I_{ij}^{E} \right) + \frac{1}{3} \lambda_{i} \left( F_{iijm}^{E} + 2 I_{iijm}^{E} + 3 I_{iijm}^{E} + 2 I_{ij}^{E} \right) + \mu \left( F_{iijm}^{E} + 2 I_{iijm}^{E} + 2 I_{ij}^{E} \right) + \xi \left( F_{iijm}^{E} + 2 I_{iijm}^{E} + I_{ij}^{E} \right) = -\frac{k_{B}}{m} \Delta,
\end{align*}
\]

(A1)

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

\[
\begin{align*}
\hat{f}_{k_{1}k_{2}\cdots k_{s}}^{1} & = \hat{G}_{k_{1}k_{2}\cdots k_{s}}^{E} - \hat{G}_{k_{1}k_{2}\cdots k_{s}}^{M} = \int_{\mathbb{R}^{3}} \int_{0}^{+\infty} 2 C_{k_{1}k_{2}\cdots k_{s}} f_{E} I \varphi(I) dI dC, \\
\hat{f}_{k_{1}k_{2}\cdots k_{t}}^{2} & = -\int_{\mathbb{R}^{3}} \int_{0}^{+\infty} m C_{k_{1}k_{2}\cdots k_{s}} f_{E} \left( \frac{2T}{m} \right)^{2} \varphi(I) dI dC.
\end{align*}
\]

Taking into account the moments of $f_{E}^{1}$, i.e., (16), (18) and (20), we obtain the following relation:

\[
\begin{align*}
\hat{f}_{k_{1}k_{2}\cdots k_{t}}^{E} & = \hat{f}_{k_{1}k_{2}\cdots k_{t}}^{M}, \\
\hat{f}_{k_{1}k_{2}\cdots k_{s}}^{1} & = \frac{2}{\rho} v f_{k_{1}k_{2}\cdots k_{t}}^{E}, \\
\hat{f}_{k_{1}k_{2}\cdots k_{t}}^{2} & = \frac{4}{\rho} \left( \frac{e^{l}}{v} + y^{l} \right) f_{k_{1}k_{2}\cdots k_{t}}^{M}.
\end{align*}
\]
where $\hat{f}^M_{k_1k_2...k_r}$ is the equilibrium moments for monatomic gas defined by

$$\hat{f}^M_{k_1k_2...k_r} = m \int_{\mathbb{R}^3} f^E_{k_1} C_{k_2} \cdots C_{k_r} dC.$$  \hspace{1cm} (A2)

Since $f^E_k$ is the Maxwell distribution function (14), $\hat{f}^M_{k_1k_2...k_r}$ are easily calculated, e.g.,

$$\hat{f}^M = \rho,$$  

$$\hat{f}_{ij}^M = p \delta_{ij},$$  

$$\hat{f}_{ijrs}^M = \frac{p^2}{\rho} \left( \delta_{ij} \delta_{rs} + \delta_{ir} \delta_{js} + \delta_{is} \delta_{jr} \right),$$  

$$\hat{f}_{lijrs}^M = 7 \frac{p^3}{\rho^2} \left( \delta_{ij} \delta_{rs} + \delta_{ir} \delta_{js} + \delta_{is} \delta_{jr} \right),$$  

$$\hat{f}_{kkllmmnn}^M = 945 \frac{p^4}{\rho^3}.$$

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

References

60. Arima, T.; Ruggeri, T.; Sugiyama, M. Extended Thermodynamics of Rarefied Polyatomic Gases: 15-Field Theory Incorporating Relaxation Processes of Molecular Rotation and Vibration. Entropy 2018, 20, 301. [CrossRef]


