

# Article **Molecular Extended Thermodynamics of Rarefied Polyatomic Gases with a new Hierarchy of Moments**

Takashi Arima <sup>1,‡</sup> and Tommaso Ruggeri <sup>2,‡</sup>\*

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

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Abstract: Recently, Pennisi and Ruggeri [J Stat Phys 179, 231–246 (2020)] consider the classical limit of the relativistic theory of moments associated with the Boltzmann-Chernikov equation truncated at a tensorial index N + 1 and they proved that there exists a unique possible choice of the moments in the classical case for a given N both for monatomic and polyatomic gases. In particular, in polyatomic gases, there exists a new hierarchy of moments that is more general than the one considered in the recent literature. As consequence, when N = 2, in the classical limit, there is a theory with 15 fields. In this paper, we consider this system of moments, and we close the system using 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 to Grad 13-moments system to the 14 moments theory proposed by Kremer [Annales de l'I.H.P. Physique théorique, 45, 419-440 (1986)]. 10 **Keywords:** Extended thermodynamics; Maximum entropy principle; Rarefied polyatomic gas; Moments equation;

#### 1. Introduction 12

It is well known that when the Knudsen number  $K_n$  is very high, the appropriate theory of the monatomic gas is the Boltzmann equation<sup>1</sup>

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

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 exists on the Boltzmann equation in which very important mathematical contributions were given by Cercignani [1,2]. Associating to the distribution function, we can construct macroscopic observable quantities that are called moments  $(m \text{ is the atomic mass})^2$ :

$$F_{k_1k_2...k_n}(\mathbf{x},t) = m \int_{\mathbb{R}^3} f(\mathbf{x},\,\boldsymbol{\xi},t)\,\xi_{k_1}\xi_{k_2}\ldots\xi_{k_n}\,d\boldsymbol{\xi}, \qquad k_1,k_2,\ldots,k_n = 1,2,3 \quad \text{and} \quad n = 0,1,2,\ldots$$

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As usual, the repeated indices denote the summation.

<sup>2</sup> When n = 0, we have the mass density  $F = \rho$ .

As a consequence of the Boltzmann equation (1), we have an infinite hierarchy of moment equations that are in the form of balance laws:

$$\frac{\partial F_{k_1k_2\dots k_n}}{\partial t} + \frac{\partial F_{k_1k_2\dots k_nk_{n+1}}}{\partial x_{k_{n+1}}} = P_{k_1k_2\dots k_n}, \qquad n = 0, 1, \dots$$
(2)

where

$$P_{k_1k_2...k_n} = m \int_{\mathbb{R}^3} Q(f) \,\xi_{k_1}\xi_{k_2}\ldots\xi_{k_n} \,d\xi, \qquad P = P_{k_1} = P_{k_k} = 0.$$

Instead, for small  $K_n$ , the continuum approach with the classical constitutive equations of Navier–Stokes and Fourier (NSF) gives a satisfactory theory and is applicable for a more large class of fluids, such as polyatomic and dense gases.

Beyond the assumption of the local thermodynamic equilibrium which determines the application range of the 16 the NSF theory, the Rational Extended Thermodynamics (RET) has been developed [3–5]. In the theory, dissipative 17 fluxes, such as viscous stress and heat flux, are adopted as independent variables in addition to the usual hydrodynamic 18 variables, and we assume a system of balance equations with local-type constitutive equations. More precisely, 19 the main idea of RET is to consider for sufficient large Knudsen number a structure of balance laws that have the 20 form dictated by the moments (2) truncated at some level. The main problem is in this case that we need a closure 21 procedure. The first approach was pure phenomenological which adopts the structure of moments but forgets that 22 the F's are moments of a distribution function. The phenomenological closure was obtained by using the universal 23 principles of continuum thermomechanics—(I) the Galilean invariance and the objectivity principle, (II) the entropy 24 principle, and (III) the causality and thermodynamic stability (i.e., convexity of the entropy)—to select admissible 25 constitutive equations. 26 The first paper with this procedure was given by Liu and Müller [6] motivated by a paper of Ruggeri [7] 27

considering 13 moments of the form (2) with n = 0, 1, 2, 3 and taking only the trace of the triple tensor with respect 28 two indexes:  $(F, F_{k_1}, F_{k_1k_2}, F_{k_1k_2})$ . It was surprising that the macroscopic closure obtained only by adopting the 29 previous universal principles gives the same system obtained by Grad [8] using a complete different closure at kinetic 30 level. Successively, Kremer presented a refined model with 14 fields (monatomic  $ET_{14}$ ) [9] by adopting a new scalar 31 field  $F_{jjkk}$  in addition to the previous 13 fields:  $(F, F_{k_1}, F_{k_1k_2}, F_{k_1kk}, F_{jjkk})$ . 32 For the case with many fields such as (2) truncated at a tensorial order  $\bar{N}$ , to avoid the complexity of the 33 phenomenological approach, the so-called *molecular extended thermodynamics* has been proposed in which the 34 macroscopic quantities are moments of the distribution function [10]. For the closure, we adopt as technique the 35

variational procedure of Maximum Entropy Principle (MEP) introduced first in the theory of moments by Kogan [11]

and resumed in 13 moments by Dreyer [12] and for many moments in the first edition of Müller and Ruggeri book in

<sup>38</sup> which it was proved that the closed system is symmetric hyperbolic [10]. See also on this subject the contribution of

<sup>39</sup> Boillat and Ruggeri [13] in which they proved that in the molecular approach the MEP closure is equivalent to the

<sup>40</sup> closure using an entropy principle.

The first relativistic version of the modern RET was give by Liu, Müller and Ruggeri (LMR) [14] considering the Boltzmann-Chernikov relativistic equation [15–17]:

$$p^{\alpha}\partial_{\alpha}f = Q. \tag{3}$$

in which now the distribution function f depends on  $(x^{\alpha}, p^{\beta})$ , where  $x^{\alpha}$  are the space-time coordinates,  $p^{\alpha}$  is the four-momentum  $p_{\alpha}p^{\alpha} = m^2c^2$ ,  $\partial_{\alpha} = \partial/\partial x^{\alpha}$ , c denotes the light velocity, m the 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<sup>3</sup>:

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

with

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

and

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

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 <sup>4</sup>:

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

<sup>41</sup> The surprising results was that the LMR theory converges, in the classical limit, to the monatomic ET<sub>14</sub> theory by

<sup>42</sup> Kremer for monatomic gas not the Grad theory  $(ET_{13})$  as was expected [3,18,19].

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 [20,21], Arima, Taniguchi, Ruggeri and Sugiyama [22] 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 identically to zero in monatomic gases:

$$\frac{\partial F}{\partial t} + \frac{\partial F_{i}}{\partial x_{i}} = 0,$$

$$\frac{\partial F_{j}}{\partial t} + \frac{\partial F_{ij}}{\partial x_{i}} = 0,$$

$$\frac{\partial F_{ij}}{\partial t} + \frac{\partial F_{ijk}}{\partial x_{k}} = P_{ij},$$

$$\frac{\partial G_{ll}}{\partial t} + \frac{\partial G_{llk}}{\partial x_{k}} = 0,$$

$$\frac{\partial G_{lli}}{\partial t} + \frac{\partial G_{llik}}{\partial x_{k}} = Q_{lli}.$$
(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  $\varepsilon$  is the 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. In the parabolic limit, this theory converges to the NSF theory, and in the monatomic singular limit, it converges to the Grad system [4,5,23]. This hierarchy was justified at kinetic level in [24–26] using the same form of Boltzmann equation (1) but with a distribution function  $f(\mathbf{x}, \boldsymbol{\xi}, t, \boldsymbol{J})$  that depends on a non-negative *internal energy parameter I*, that takes into account the influence of the internal degrees

<sup>&</sup>lt;sup>3</sup> When n = 0, the tensor reduces to  $A^{\alpha}$ . Moreover, the production tensor in the right-side of (5) is zero for n = 0, 1, because the first 5 equations represent the conservation laws of the particles number and the energy-momentum, respectively.

<sup>&</sup>lt;sup>4</sup> 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.

of freedom of a molecule on energy transfer during collisions [27,28]. The theory with many moments was also developed in [24,26,29]:

$$\frac{\partial F_{k_1k_2\dots k_n}}{\partial t} + \frac{\partial F_{k_1k_2\dots k_nk_{n+1}}}{\partial x_{k_{n+1}}} = P_{k_1k_2\dots k_n},$$

$$\frac{\partial G_{llk_1k_2\dots k_m}}{\partial t} + \frac{\partial G_{llk_1k_2\dots k_nk_{m+1}}}{\partial x_{k_{m+1}}} = Q_{llk_1k_2\dots k_m},$$
(8)

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

$$F_{k_{1}k_{2}...k_{n}} = m \int_{\mathbb{R}^{3}} \int_{0}^{+\infty} f(\mathbf{x}, \boldsymbol{\xi}, t, I) \, \xi_{k_{1}}\xi_{k_{2}} \dots \xi_{k_{n}} \, \varphi(I) \, dI \, d\boldsymbol{\xi},$$

$$P_{k_{1}k_{2}...k_{n}} = m \int_{\mathbb{R}^{3}} \int_{0}^{+\infty} Q(f)\xi_{k_{1}}\xi_{k_{2}} \dots \xi_{k_{n}} \, \varphi(I) \, dI \, d\boldsymbol{\xi},$$

$$G_{llk_{1}k_{2}...k_{m}} = \int_{\mathbb{R}^{3}} \int_{0}^{+\infty} \left(m\xi^{2} + 2I\right) f(\mathbf{x}, \boldsymbol{\xi}, t, I) \, \xi_{k_{1}}\xi_{k_{2}} \dots \xi_{k_{m}} \, \varphi(I) \, dI \, d\boldsymbol{\xi},$$

$$Q_{llk_{1}k_{2}...k_{m}} = \int_{\mathbb{R}^{3}} \int_{0}^{+\infty} \left(m\xi^{2} + 2I\right) Q(f) \, \xi_{k_{1}}\xi_{k_{2}} \dots \xi_{k_{m}} \, \varphi(I) \, dI \, d\boldsymbol{\xi},$$

where  $\varphi(I)$  is the state density corresponding to I, i.e.,  $\varphi(I)dI$  represents the number of internal state between I

- and I + dI. We need to remark that the two blocks of hierarchies in (8) are not separated because the last fluxes in
- <sup>45</sup> both hierarchies together with the productions terms are functions to be determined by the closure of all densities
- <sup>46</sup>  $(F_{k_1k_2...k_n}, G_{llk_1k_2...k_m})$ . The index n = 0, 1, ..., N and m = 0, 1, ..., M. Moreover,  $P = P_{k_1} = Q_{ll} = 0$  since the
- $_{47}$  first 4 equations of the F' hierarchy and the first scalar equation of G's hierarchy represent the mass, momentum and
- <sup>48</sup> energy conservation, respectively. It was studied in [26] that the physically meaning full choice of the truncated order
- <sup>49</sup>  $\mathcal{N}$  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 gas in the case of N = 2 [30]. Then, in [19], 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:

$$A^{\alpha\alpha_{1}\cdots\alpha_{n}} = \frac{c}{m^{n-1}} \int_{\mathbb{R}^{3}} \int_{0}^{+\infty} f p^{\alpha} p^{\alpha_{1}} \cdots p^{\alpha_{n}} \left(1 + n \frac{I}{m c^{2}}\right) \varphi(I) \, dI \, dP$$
$$I^{\alpha_{1}\cdots\alpha_{n}} = \frac{c}{m^{n-1}} \int_{\mathbb{R}^{3}} \int_{0}^{+\infty} Q \, p^{\alpha_{1}} \cdots p^{\alpha_{n}} \left(1 + n \frac{I}{m c^{2}}\right) \varphi(I) \, dI \, dP,$$

with a distribution functions  $f(x^{\alpha}, p^{\beta}, I)$  depends on the extra energy variable 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). In particular, for N = 2, in the monatomic case, we have in the classical limit the monatomic 14-moment equations by Kremer [9] according with the old results of [18]. Instead, in the polyatomic case, for N = 2, we have, as classical limit, 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

$$H_{llmm} = 2G_{llmm} - F_{llmm} \tag{9}$$

<sup>50</sup> is involved. For many moments, the new hierarchy contains, in addition to the F's and G's hierarchies (8) with

- n = 0, 1, ..., N and m = 0, 1, ..., N 1, more complex N + 1 hierarchies for mixed type of moments (see [19]). For
- <sup>52</sup> more details on RET beyond the monatomic gas, see the new book of Ruggeri and Sugiyama [5].

The aim of the present paper is to study the closure of the most simple case of this new hierarchy, that is the system with 15 equations  $(ET_{15})$ :

$$\frac{\partial F}{\partial t} + \frac{\partial F_k}{\partial x_k} = 0,$$

$$\frac{\partial F_i}{\partial t} + \frac{\partial F_{ik}}{\partial x_k} = 0,$$

$$\frac{\partial F_{ij}}{\partial t} + \frac{\partial F_{ijk}}{\partial x_k} = P_{ij},$$

$$\frac{\partial G_{lli}}{\partial t} + \frac{\partial G_{llik}}{\partial x_k} = Q_{lli},$$

$$\frac{\partial H_{llmm}}{\partial t} + \frac{\partial H_{llmmk}}{\partial x_k} = R_{llmm},$$
(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 a equilibrium properties of the distribution function, we close the system (10) by means of MEP. As the collisional term, we introduce the generalized BGK model for a relaxation processes of molecular internal modes [25]. We show that the derived closed set of the moment equations involves the polyatomic ET<sub>14</sub> theory as a principal subsystem, the monatomic ET<sub>14</sub> theory in the monatomic singular limit, and the NSF theory as its parabolic limit.

# 58 2. Molecular Extended Thermodynamics with 15-field

First, we recall the equilibrium distribution function for polyatomic gas 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  $f_i$  are the degree of freedom; in the monatomic gas D = 3)

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

in [24,28] and in the present case of non polytropic gas

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

in [25,31]:

$$f_E = f_E^K f_E^I, \tag{13}$$

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

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

with A(T) is the normalization factor (partition function):

$$A(T) = \int_0^{+\infty} \varphi(I) \mathrm{e}^{-\beta_E I} \mathrm{d}I, \qquad \beta_E = 1/(k_B T), \tag{15}$$

<sup>59</sup> and we have put with  $C_i = \xi_i - v_i (C^2 = C_j C_j)$  the peculiar velocity.

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

$$\varepsilon = \varepsilon_E(T) = \varepsilon_E^K(T) + \varepsilon_E^I(T) = \frac{1}{2\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} (mC^2 + 2I) f_E \varphi(I) \, dI \, dC, \tag{16}$$

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

$$\varepsilon_E^K(T) = \frac{1}{2\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} mC^2 f_E \varphi(I) \, dI \, dC = \frac{1}{2\rho} \int_{\mathbb{R}^3} mC^2 f_E^K \, dC = \frac{3}{2} \frac{k_B}{m} T,$$
  

$$\varepsilon_E^I(T) = \frac{1}{\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} I f_E \varphi(I) \, dI \, dC = \frac{1}{m} \int_0^{+\infty} I f_E^I \, dI = \frac{k_B}{m} T^2 \frac{d\log A(T)}{dT},$$
(17)

where the following relation is taking into account by  $(14)_2$  and (15)

$$\int_0^\infty f_E^I \varphi(I) \, dI = 1. \tag{18}$$

<sup>60</sup> The partition function is obtained by integrating  $(17)_2$  if the caloric equations of state is given. Then the measure

 $\varphi(I)$  is determined via the inverse Laplace transformation of (15). Vice versa, if the partition functions A(T) is

 $_{62}$  given, for example, by a statistical-mechanical analysis, we obtain the equilibrium energies of internal mode from  $_{63}$  (17)<sub>2</sub> (see for more details [25]).

It was proved in [25] that

$$\frac{1}{m^2} \int_0^\infty I^2 f_E^I dI = \frac{p^2}{\rho^2} \hat{c}_v^I + \varepsilon_E^I(T)^2,$$
(19)

where

$$\hat{c}_{v}^{I}=mrac{c_{v}^{I}}{k_{B}}, \quad ext{and} \quad c_{v}^{I}=rac{darepsilon_{E}^{I}(T)}{dT}$$

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

$$s^{K}(\rho,T) \equiv -\frac{k_{B}}{\rho} \int_{\mathbb{R}^{3}} \int_{0}^{+\infty} f_{E} \log f_{E}^{K} \varphi(I) dI dC,$$
  
$$= \frac{k_{B}}{m} \log\left(\frac{T^{3/2}}{\rho}\right) + \frac{\varepsilon_{E}^{K}(T)}{T} - \frac{k_{B}}{m} \log\left[\frac{1}{m}\left(\frac{m}{2\pi k_{B}}\right)^{3/2}\right],$$
  
$$s^{I}(T) \equiv -\frac{k_{B}}{\rho} \int_{\mathbb{R}^{3}} \int_{0}^{+\infty} f_{E} \log f_{E}^{I} \varphi(I) dI dC,$$
  
$$= \frac{k_{B}}{m} \log A(T) + \frac{\varepsilon_{E}^{I}(T)}{T}.$$

# 64 2.1. System of balance equations for 15 fields

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

$$\begin{pmatrix} F \\ F_i \\ F_{ij} \\ F_{ijk} \end{pmatrix} = \int_{\mathbb{R}^3} \int_0^{+\infty} m \begin{pmatrix} 1 \\ \xi_i \\ \xi_i \xi_j \\ \xi_i \xi_j \xi_k \end{pmatrix} f \varphi(I) dI d\xi,$$

$$\begin{pmatrix} G_{ll} \\ G_{lli} \\ G_{llik} \end{pmatrix} = \int_{\mathbb{R}^3} \int_0^{+\infty} (m\xi^2 + 2I) \begin{pmatrix} 1 \\ \xi_i \\ \xi_i \xi_k \end{pmatrix} f \varphi(I) dI d\xi,$$

$$\begin{pmatrix} H_{llmm} \\ H_{llmmi} \end{pmatrix} = \int_{\mathbb{R}^3} \int_0^{+\infty} (m\xi^2 + 4I) \xi^2 \begin{pmatrix} 1 \\ \xi_i \end{pmatrix} f \varphi(I) dI d\xi,$$

$$(20)$$

and the production terms

$$\mathbf{f} \equiv \begin{pmatrix} P_{ij} \\ Q_{lli} \\ R_{llmm} \end{pmatrix} = \int_{\mathbb{R}^3} \int_0^{+\infty} \begin{pmatrix} m\xi_i\xi_j \\ (m\xi^2 + 2I)\xi_i \\ (m\xi^2 + 4I)\xi^2 \end{pmatrix} Q(f)\varphi(I) \, dId\xi.$$
(21)

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

$$F = \rho, F_{i} = \rho v_{i}, F_{ij} = \hat{F}_{ij} + \rho v_{i} v_{j}, G_{ll} = \hat{G}_{ll} + \rho v^{2}, G_{lli} = \hat{G}_{lli} + \hat{G}_{ll} v_{i} + \hat{F}_{li} v_{l} + \hat{F}_{ll} v_{i} + \rho v^{2} v_{i}, H_{llmm} = \hat{H}_{llmm} + 4\hat{G}_{lli} v_{i} + 2\hat{G}_{ll} v^{2} + 4\hat{F}_{ij} v_{i} v_{j} + \rho v^{4},$$
(22)

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

$$\begin{array}{ll} \text{mass density:} & \rho = \int_{\mathbb{R}^3} \int_0^{+\infty} mf \, \varphi(I) \, dI dC = \int_{\mathbb{R}^3} \int_0^{+\infty} mf_E \, \varphi(I) \, dI dC, \\ \text{velocity:} & v_i = \frac{1}{\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} m\xi_i f \, \varphi(I) \, dI d\xi = \frac{1}{\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} m\xi_i f_E \, \varphi(I) \, dI d\xi, \\ \text{specific internal energy density:} & \varepsilon = \varepsilon^K + \varepsilon^I = \frac{1}{2\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} mC^2 f \, \varphi(I) \, dI dC, \\ \text{specific internal energy density:} & \varepsilon^I = \frac{1}{\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} mC^2 f \, \varphi(I) \, dI dC, \\ \text{specific internal energy density:} & \varepsilon^I = \frac{1}{\rho} \int_{\mathbb{R}^3} \int_0^{+\infty} mC^2 f \, \varphi(I) \, dI dC, \\ \text{specific internal energy density:} & \mathcal{P} = \frac{2}{3} \rho \varepsilon^K = \frac{1}{3} \int_{\mathbb{R}^3} \int_0^{+\infty} mC^2 f \, \varphi(I) \, dI dC, \\ \text{dynamic pressure:} & \Pi = \mathcal{P} - p = \frac{1}{3} \int_{\mathbb{R}^3} \int_0^{+\infty} mC^2 (f - f_E) \, \varphi(I) \, dI dC, \\ \text{shear stress:} & \sigma_{\langle ij \rangle} = - \int_{\mathbb{R}^3} \int_0^{+\infty} mC_{\langle i} C_{j \rangle} f \, \varphi(I) \, dI dC, \\ \text{heat flux:} & q_i = \frac{1}{2} \int_{\mathbb{R}^3} \int_0^{+\infty} (mC^2 + 2I) C_i f \, \varphi(I) \, dI dC, \end{array}$$

are related to the intrinsic moments as follows:

$$\hat{G}_{ll} = 2\rho\varepsilon = 2\rho(\varepsilon^{K} + \varepsilon^{I}), \quad \hat{F}_{ll} = 3\mathcal{P} = 3(p + \Pi), \quad \hat{F}_{\langle ij \rangle} = -\sigma_{\langle ij \rangle}, \quad \hat{G}_{lli} = 2q_{i}, \tag{24}$$

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

$$\varepsilon = \varepsilon_E(T). \tag{25}$$

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

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

where

$$y^I = \frac{\rho}{p} \varepsilon^I_E(T)$$

and  $\Delta$  is defined by

$$\Delta = \int_{\mathbb{R}^3} \int_0^{+\infty} \left( mC^2 + 4I \right) C^2 (f - f_E) \varphi(I) \, dI \, dC.$$
<sup>(26)</sup>

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

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

$$(27) \\ Q_{lli} &= 2v_l \hat{P}_{il} + \hat{Q}_{lli}, \\ R_{llmm} &= 4v_i v_j \hat{P}_{ij} + 4v_i \hat{Q}_{lli} + \hat{R}_{llmm}. \end{aligned}$$

The velocity dependences in (22) and (27) take the system (10) Galilean invariant in agreement with the general theorem on Galilean invariance for a generic system of balance laws (see [32]).

The constitutive quantities are now the following moments

$$\begin{split} \hat{F}_{ijk} &= \int_{\mathbb{R}^3} \int_0^{+\infty} mC_i C_j C_k f \varphi(I) \, dI \, dC, \\ \hat{G}_{llik} &= \int_{\mathbb{R}^3} \int_0^{+\infty} (mC^2 + 2I) C_i C_k f \varphi(I) \, dI \, dC, \\ \hat{H}_{llmmk} &= \int_{\mathbb{R}^3} \int_0^{+\infty} (mC^2 + 4I) C^2 C_k f \varphi(I) \, dI \, dC, \end{split}$$

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

# <sup>69</sup> 2.1.1. 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 with the principle, the most suitable distribution function f of the truncated system (10) is the one that maximize the entropy

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

under the constraints that the density moments F,  $F_i$ ,  $F_{ij}$ ,  $G_{ll}$ ,  $G_{lli}$ ,  $H_{llmm}$  are prescribed as in (20). Therefore the best approximated distribution function  $f_{15}$  is obtained as the solution of a variational problem of the following functional

$$\mathcal{L}(f) = -k_B \int_{\mathbb{R}^3} \int_0^{+\infty} f \log f \varphi(I) dI d\xi + \lambda \Big( F - \int_{\mathbb{R}^3} \int_0^{+\infty} mf \varphi(I) dI d\xi \Big) + \lambda_i \Big( F_i - \int_{\mathbb{R}^3} \int_0^{+\infty} m\xi_i f \varphi(I) dI d\xi \Big)$$
(28)  
$$+ \lambda_{ij} \Big( F_{ij} - \int_{\mathbb{R}^3} \int_0^{+\infty} m\xi_i \xi_j f \varphi(I) dI d\xi \Big) + \mu \Big( G_{ll} - \int_{\mathbb{R}^3} \int_0^{+\infty} \big( m\xi^2 + 2I \big) f \varphi(I) dI d\xi \Big) + \mu_i \Big( G_{lli} - \int_{\mathbb{R}^3} \int_0^{+\infty} \big( m\xi^2 + 2I \big) \xi_i f \varphi(I) dI d\xi \Big) + \zeta \Big( H_{llmm} - \int_{\mathbb{R}^3} \int_0^{+\infty} \big( m\xi^2 + 4I \big) \xi^2 f \varphi(I) dI d\xi \Big),$$

where  $\lambda$ ,  $\lambda_i$ ,  $\lambda_{ij}$ ,  $\mu$ ,  $\mu_i$ , and  $\zeta$  are the corresponding Lagrange multipliers of the constraints. As  $\mathcal{L}$  is a scalar independent of frame proceeding as in [32], we can evaluate the right side of (28) 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 [32]):

$$\lambda = \hat{\lambda} - \hat{\lambda}_{i}v_{i} + \hat{\lambda}_{ij}v_{i}v_{j} + \hat{\mu}v^{2} - \hat{\mu}_{i}v^{2}v_{i} + \hat{\zeta}v^{4},$$

$$\lambda_{i} = \hat{\lambda}_{i} - 2\hat{\lambda}_{ij}v_{j} - 2\hat{\mu}v_{i} + 3\hat{\mu}_{i}v^{2} - 4\hat{\zeta}v^{2}v_{i},$$

$$\lambda_{ij} = \hat{\lambda}_{ij} - 2\hat{\mu}_{i}v_{i} + 4\hat{\zeta}v_{i}v_{j},$$

$$\mu = \hat{\mu} - \hat{\mu}_{i}v_{i} + 2\hat{\zeta}v^{2},$$

$$\mu_{i} = \hat{\mu}_{i} - 4\hat{\zeta}v_{i},$$

$$\zeta = \hat{\zeta}.$$
(29)

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

$$f_{15} = \exp\left(-1 - \frac{m}{k_B}\chi\right), \quad \text{with}$$

$$\chi = \lambda + C_i\lambda_i + C_iC_j\lambda_{ij} + \left(C^2 + \frac{2I}{m}\right)\hat{\mu} + \left(C^2 + \frac{2I}{m}\right)C_i\hat{\mu}_i + \left(C^2 + \frac{4I}{m}\right)C^2\hat{\zeta}.$$
(30)

Taking into account that, in equilibrium,  $f_{15}$  coincides with the equilibrium distribution function (13), we can easily see that the equilibrium components of the Lagrange multipliers are given by

$$\lambda_E = \frac{1}{T} \left( -g + \frac{v^2}{2} \right), \quad \lambda_{i_E} = -\frac{v_i}{T}, \quad \lambda_{ll_E} = 0, \quad \lambda_{\langle ij \rangle_E} = 0, \quad \mu_E = \frac{1}{2T}, \quad \mu_{i_E} = 0, \quad \zeta_E = 0, \quad (31)$$

where  $g(=\varepsilon_E(T) + p/\rho - Ts)$  is the chemical potential. We remark that  $\lambda_E, \lambda_{i_E}, \mu_E$  in (31) are the Lagrange

multipliers of the Euler system, and those are the *main field* symmetrize the Euler system as was proved first by  $C_{1}$  =  $C_{1}$  =  $C_{2}$  =

# <sup>72</sup> Godunov (see [4,33]).

We observe that the highest power of peculiar velocity in  $\chi$  in  $(30)_2$  is even, i.e.,  $C^4$ . The highest power is same with the highest tensorial order of the system, and it is revealed in [19] that the highest tensorial order of the system obtained in the classical limit is always even, i.e., 2N. This fact indicates that, in principle, the moments can be integrable with the distribution function  $f_{15}$  (concerning the integrability of moments see [13]). Nevertheless, for the non-linear moment closure, there is the problematic that was noticed first by Junk [34] 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 this difficulties in the molecular extended thermodynamics approach, we consider, as usual, the processes near equilibrium. Then, we expand (30) around an equilibrium state in the following form:

$$f_{15} = f_E \left( 1 - \frac{m}{k_B} \tilde{\chi} \right),$$

$$\tilde{\chi} = \tilde{\lambda} + C_i \tilde{\lambda}_i + C_i C_j \tilde{\lambda}_{ij} + \left( C^2 + \frac{2I}{m} \right) \tilde{\mu} + \left( C^2 + \frac{2I}{m} \right) C_i \tilde{\mu}_i + \left( C^2 + \frac{4I}{m} \right) C^2 \tilde{\zeta},$$
(32)

where a tilde on a quantity indicates its nonequilibrium part. In the following, for simplicity, we use the notation  $f_4$  f instead of  $f_{15}$ . Although the expansion of the exponential (30) is truncated at the first order with respect to the

<sup>75</sup> nonequilibrium variables, there exists the possibility to construct RET theories wit high expansion as was presented

<sup>76</sup> first by Brini and Ruggeri in [35]. The high order expansion has the advantage to have a larger domain of hyperbolicity

<sup>77</sup> [36,37] and to reduce the magnitude of the sub-shock formation in the shock structure [38].

Inserting (32) into (23) and (26), we obtain the following algebraic relation for Lagrange multipliers:

$$\begin{split} \tilde{\lambda}\rho + \frac{1}{3}\tilde{\lambda}_{ll}\hat{F}_{ll}^{E} + \tilde{\mu}\hat{G}_{llj}^{E} + \tilde{\zeta}\hat{H}_{llmm}^{E} &= 0, \\ \tilde{\lambda}_{i}\hat{F}_{ij}^{E} + \tilde{\mu}_{i}\hat{G}_{llij}^{E} &= 0, \\ \tilde{\lambda}\hat{G}_{ll}^{E} + \frac{1}{3}\tilde{\lambda}_{ll}\hat{G}_{llmm}^{E} + \tilde{\mu}\hat{H}_{llmm}^{E} + \tilde{\zeta}\left(\hat{F}_{llmmn}^{E} + 3\hat{J}_{llmm}^{1|E} + 2\hat{J}_{ll}^{2|E}\right) &= 0, \\ \tilde{\lambda}\hat{G}_{ll}^{E} + \frac{1}{3}\tilde{\lambda}_{ll}\hat{G}_{llmm}^{E} + \tilde{\mu}\hat{G}_{llij}^{E} + \tilde{\zeta}\left(\hat{F}_{llmmij}^{E} + 2\hat{J}_{llij}^{1|E}\right) &= -\frac{k_{B}}{m}\left(\Pi\delta_{ij} - \sigma_{\langle ij\rangle}\right), \end{split}$$
(33)  
$$\tilde{\lambda}_{i}\hat{G}_{llij}^{E} + \tilde{\mu}_{i}\left(\hat{F}_{llmmij}^{E} + 2\hat{J}_{llij}^{E|1} + \hat{J}_{ij}^{E|2}\right) &= -2\frac{k_{B}}{m}q_{j}, \\ \tilde{\lambda}\left(\hat{F}_{llmm}^{E} + 2\hat{J}_{ll}^{E|1}\right) + \frac{1}{3}\tilde{\lambda}_{ll}\left(\hat{F}_{llmmn}^{E} + 2\hat{J}_{llmm}^{E|1}\right) + \tilde{\mu}\left(\hat{F}_{llmmn}^{E} + 3\hat{J}_{llmm}^{E|1} + 2\hat{J}_{ll}^{E|2}\right) + \tilde{\zeta}\left(\hat{F}_{kkllmmn}^{E} + 4\hat{J}_{llmmn}^{E|2}\right) &= -\frac{k_{B}}{m}\Delta, \end{split}$$

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

$$\hat{J}_{k_{1}k_{2}\cdots k_{s}}^{1|E} = \hat{G}_{llk_{1}k_{2}\cdots k_{s}}^{E} - \hat{F}_{llk_{1}k_{2}\cdots k_{s}}^{E} = \int_{\mathbb{R}^{3}} \int_{0}^{+\infty} 2C_{k_{1}}C_{k_{2}}\cdots C_{k_{s}}f_{E} I \varphi(I) dI dC$$
$$\hat{J}_{k_{1}k_{2}\cdots k_{t}}^{2|E} = \int_{\mathbb{R}^{3}} \int_{0}^{+\infty} mC_{k_{1}}C_{k_{2}}\cdots C_{k_{t}}f_{E} \left(\frac{2I}{m}\right)^{2} \varphi(I) dI dC.$$

Taking into account the moments of  $f_E^I$ , i.e., (18), (17) and (19), we obtain the following relation:

$$\begin{split} \hat{F}^{E}_{k_{1}k_{2}\cdots k_{r}} &= \hat{F}^{M}_{k_{1}k_{2}\cdots k_{r}}, \\ \hat{J}^{1|E}_{k_{1}k_{2}\cdots k_{s}} &= 2\frac{p}{\rho}y^{I}\hat{F}^{M}_{k_{1}k_{2}\cdots k_{s}}, \\ \hat{J}^{2|E}_{k_{1}k_{2}\cdots k_{t}} &= 4\frac{p}{\rho}\left(\hat{c}^{I}_{\nu} + y^{I^{2}}\right)\hat{F}^{M}_{k_{1}k_{2}\cdots k_{t}} \end{split}$$

where  $\hat{F}^{M}_{k_{1}k_{2}...k_{r}}$  is the equilibrium moments for monatomic gas defined by

$$\hat{F}^{M}_{k_{1}k_{2}\ldots k_{r}} = m \int_{\mathbb{R}^{3}} f^{K}_{E} C_{k_{1}} C_{k_{2}} \ldots C_{k_{r}} dC.$$
(34)

Since  $f_E^K$  is the Maxwell distribution (14)<sub>1</sub>,  $\hat{F}_{k_1k_2...k_r}^M$  are easily obtained, e.g.,

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

From (33), 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,  $\Pi, \sigma_{\langle ij \rangle}, q_i$  and  $\Delta$ . Instead of  $\Delta$ , it may be useful to introduce the following nonequilibrium field

$$\tilde{\Pi} = \frac{1}{3(4\hat{c}_{\nu}^{I} + 5)} \left\{ 12\Pi(y^{I} + 1) - \frac{\rho}{p} \Delta \right\}.$$
(35)

Then, we obtain as solution of (33):

$$\begin{split} \tilde{\lambda} &= \frac{3(\hat{c}_{\nu}^{l} - y^{l})}{2\hat{c}_{\nu}^{l}\rho T} \Pi + \frac{3(4y^{l} + 5)}{8\rho T} \tilde{\Pi}, \\ \tilde{\lambda}_{i} &= \frac{(2y^{l} + 5)p}{p^{2}T(2\hat{c}_{\nu}^{l} + 5)} q_{i}, \\ \tilde{\lambda}_{il} &= -\frac{3(2\hat{c}_{\nu}^{l} + 3)}{4\hat{c}_{\nu}^{l}pT} \Pi - \frac{3(y^{l} + 1)}{2pT} \tilde{\Pi}, \\ \tilde{\lambda}_{\langle ij \rangle} &= \frac{\sigma_{\langle ij \rangle}}{2pT}, \\ \tilde{\mu} &= \frac{3}{4\hat{c}_{\nu}^{l}pT} \Pi - \frac{3}{4pT} \tilde{\Pi}, \\ \tilde{\mu}_{i} &= -\frac{\rho}{p^{2}T(2\hat{c}_{\nu}^{l} + 5)} q_{i}, \\ \tilde{\zeta} &= \frac{\rho}{8p^{2}T} \tilde{\Pi}. \end{split}$$
(36)

Inserting (31) and (36) into (29), we can write down the explicit form of the Lagrange multipliers. As is well known, the multipliers coincide with the main field

$$\mathbf{u}' \equiv (\lambda, \lambda_i, \lambda_{ij}, \mu, \mu_i, \zeta) \tag{37}$$

<sup>78</sup> by which the system (10) becomes symmetric hyperbolic. Therefore we heave the well-posed Cauchy problem (local <sup>79</sup> in time) [13,39], and in some circumstances for small initial data, there exists global smooth solutions for all time

(see [4,5] and references therein).

# 81 2.2. Constitutive equations

By using the distribution function (32) with (36), we obtain the constitutive equations for the fluxes up to the first order with respect to the nonequilibrium variables as follows:

$$\hat{F}_{ijk} = \frac{2}{2\hat{c}_{\nu}^{I} + 5} (q_k \delta_{ij} + q_j \delta_{ik} + q_i \delta_{jk}),$$

$$\hat{G}_{llij} = (2y^I + 5) \frac{p^2}{\rho} \delta_{ij} + (2y^I + 7) \frac{p}{\rho} \Pi \delta_{ij} - (2\hat{c}_{\nu}^{I} + 5) \frac{p}{\rho} \tilde{\Pi} \delta_{ij} - (2y^I + 7) \frac{p}{\rho} \sigma_{\langle ij \rangle},$$

$$\hat{H}_{llmmk} = 20 \frac{p}{\rho} \frac{2y^I + 2\hat{c}_{\nu}^{I} + 7}{2\hat{c}_{\nu}^{I} + 5} q_k.$$
(38)

# 82 2.3. Nonequilibrium temperatures and generalized BGK model

## <sup>83</sup> 2.3.1. Nonequilibrium temperatures

We recall that  $\varepsilon^K$  and  $\varepsilon^I$  given in (23) are not equilibrium variables since these are the moments of the nonequilibrium distribution function (instead, the sum of the two is an equilibrium value). Then, we can define two nonequilibrium temperatures  $(\theta^K, \theta^I)$  such that, by inserting in the equilibrium state function instead of *T*, we obtain the non equilibrium internal energies  $(\varepsilon^K, \varepsilon^I)$ , i.e.:

$$\varepsilon^{K} = \varepsilon^{K}_{E}(\theta^{K}) = \frac{3}{2} \frac{k_{B}}{m} \theta^{K}, \qquad \varepsilon^{I} = \varepsilon^{I}_{E}(\theta^{I}).$$
(39)

Recalling  $2\rho \varepsilon^K = 3\mathcal{P}$  and (17) with (39)<sub>1</sub>, the total nonequilibrium pressure is expressed with  $\theta^K$  from (12)<sub>1</sub> as follows:

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

Since  $\mathcal{P} = p + \Pi$ , we have the following relations 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 (16) and (25) as follows:

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

<sup>84</sup> 2.3.2. 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  $\theta^K$ , explicit expression of which is shown below. However, the internal mode *I* remains, in general, in nonequilibrium. This process exists also 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 generalized BGK collision term [40,41] (see also [25,42,43]) which treats the translational relaxation and internal relaxation separately is as follows:

$$Q(f) = -\frac{1}{\tau_K} (f - f^K) - \frac{1}{\tau} (f - f_E),$$
(40)

where the distribution functions  $f^K$  is

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

with

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

#### 94 2.3.3. Production terms

From the generalized BGK model (40), the production terms given by (21) are evaluated as follows:

$$\hat{P}_{ll} = -\frac{3}{\tau}\Pi, \quad \hat{P}_{\langle ij\rangle} = \left(\frac{1}{\tau_K} + \frac{1}{\tau}\right)\sigma_{\langle ij\rangle}, \quad \hat{Q}_{lli} = -2\left(\frac{1}{\tau_K} + \frac{1}{\tau}\right)q_i,$$

$$\hat{R}_{llmm} = -\left(\frac{1}{\tau_K} + \frac{1}{\tau}\right)\Delta + \frac{1}{\tau_K}\frac{p}{\rho}\Pi\left(12y^I + 12 - 3\frac{\Pi}{p}\right).$$
(41)

Since we consider linear constitutive equations, we neglect the quadratic term in the last expression of (41):

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

# 95 2.4. 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}{\partial t} + \frac{\partial}{\partial x_{i}}\left\{ \left[ p + \Pi \right] \delta_{ij} - \sigma_{(ij)} + \rho_{Vi}v_{j} \right] = 0, \\ \frac{\partial}{\partial t} \left[ p(2y^{l} + 3) + \rho x^{2} \right] + \frac{\partial}{\partial x_{i}} \left\{ 2q_{i} + \left[ p(2y^{l} + 5) + 2\Pi \right] v_{i} - 2\sigma_{(ib)}v_{i} + \rho v^{2}v_{i} \right] = 0, \\ \frac{\partial}{\partial t} \left[ 3(p + \Pi) + \rho v^{2} \right] + \frac{\partial}{\partial x_{i}} \left\{ \frac{10}{2z_{v}^{l} + 5}q_{k} + 5(p + \Pi)v_{k} - 2\sigma_{(ib)}v_{i} + \rho v^{2}v_{k} \right\} = -\frac{3\Pi}{\tau}, \\ \frac{\partial}{\partial t} \left( -\sigma_{(ij)} + \rho v_{(i'j)} \right) + \frac{\partial}{\partial x_{k}} \left\{ \frac{2}{1 + \varepsilon_{v}}q_{(i}\delta_{jk} + 2[p + \Pi]v_{(i}\delta_{jk} - \sigma_{(ij)}v_{k} - 2\sigma_{(ki)}v_{j} + \rho v_{(i'j)}v_{k} \right\} = \left(\frac{1}{\tau_{K}} + \frac{1}{\tau}\right)\sigma_{(ij)}, \\ \frac{\partial}{\partial t} \left[ 2q_{i} + \left[ p(2y^{l} + 5) + 2\Pi \right]v_{i} - 2\sigma_{(ij)}v_{i} + \rho v^{2}v_{i} \right] + \\ &+ \frac{\partial}{\partial x_{k}} \left\{ (2y^{l} + 5) \frac{p^{2}}{\rho}\delta_{ik} + (2y^{l} + 7) \frac{p}{\rho}\Pi\delta_{ik} - \frac{p}{\rho} \frac{2\varepsilon_{v}^{l} + 5}{3(4\varepsilon_{v}^{l} + 5)} \left( 12\Pi(y^{l} + 1) - \frac{\rho}{\rho}\Delta \right)\delta_{ik} - (2y^{l} + 7) \frac{p}{\rho}\sigma_{(ik)} \\ &+ \frac{2}{2\varepsilon_{v}^{l} + 5}q_{i}v_{i}\delta_{ik} + 4\frac{\varepsilon_{v}^{l} + 3}{2\varepsilon_{v}^{l} + 5}(q_{i}v_{k} + q_{k}v_{i}) + (p + \Pi)v^{2}\delta_{ik} + \left[ (2y^{l} + 7)p + 4\Pi \right]v_{i}v_{k} \\ &- \sigma_{(ik)}v^{2} - 2\sigma_{(ik)}v_{i}v_{i} - 2v_{i}v_{k}\sigma_{(ij)} + \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_{(ij}v_{i} - 2\left(\frac{1}{\tau_{K}} + \frac{1}{\tau}\right)q_{i}, \\ \frac{\partial}{\partial t} \left\{ 3\frac{p^{2}}{\rho} \left( 4y^{l} + 5 \right) + \Delta + 8v_{i}q_{i} + 2v^{2} \left[ p(2y^{l} + 5) + 2\Pi \right] - 4v_{i}v_{j}\sigma_{(ij)} + \rho v^{4} \right\} + \\ &+ \frac{\partial}{\partial x_{k}} \left\{ \frac{20\rho}{\rho(2\varepsilon_{v}^{l} + 5)} \left( 2\varepsilon_{v}^{l} + 2y^{l} + 7 \right)q_{k} + 5\left( 4y^{l} + 7 \right)\frac{p^{2}}{\rho}v_{k} + 20\left(y^{l} + 2\right)\frac{p}{\rho}\Pi v_{k} - \frac{5p(4\varepsilon_{v}^{l} + 7)}{3\rho(4\varepsilon_{v}^{l} + 5)} \left[ 12\Pi(y^{l} + 1) - \frac{\rho}{\rho}\Delta \right]v_{k} \\ &- 4\left(2y^{l} + 7\right)\frac{p}{\rho}\sigma_{(ik)}v_{i} + \frac{4\left(2\varepsilon_{v}^{l} + 7}{2\varepsilon_{v}^{l} + 5} \left(q_{k}v^{2} + 2q_{i}v_{i}v_{k}\right) - 4\sigma_{(ij)}v^{2}v_{i} - 4\sigma_{(ij)}v_{i}v_{i}v_{i} + 2\left[ p(2y^{l} + 7) + 4\Pi \right]v^{2}v_{k} + \rho v^{4}v_{k} \right\} \\ &= -4v^{2}\frac{\Pi}{\tau} + 4\left(\frac{1}{\tau_{K}} + \frac{1}{\tau}\right)v_{i}v_{j}\sigma_{(ij)} + 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{1}{\tau_{K}}\frac{p}{\tau}\left(y^{l} + 1\right)\Pi. \end{aligned}$$

where, from (35),

$$\Delta = 3\frac{p}{\rho} \left\{ 4(y^{I}+1)\Pi - (4\hat{c}_{v}^{I}+5)\tilde{\Pi} \right\}.$$
(43)

In conclusion: *The system* (42) *formed by* 15 *equations in the* 15 *unknown is closed with the provided equilibrium* state function (12) and relaxation times  $\tau$  and  $\tau_K$ .

We remark that the field equations of  $\rho$ ,  $v_i$ , T,  $\Pi$  and  $\sigma_{\langle ij \rangle}$  are same with the ones of polyatomic 14 field theory and the presence of  $\Delta$  involves only the last two equations of (42).

100 2.5. 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  $\varphi_i$  is the non-convective entropy flux and  $\Sigma$  is the entropy production which are defined below.

By adopting (32) with (36), we obtain the entropy density within second order with respect to the nonequilibrium variables

$$h = \rho s - \frac{3(2\hat{c}_{\nu}^{I} + 3)}{8\hat{c}_{\nu}^{I}pT}\Pi^{2} - \frac{3(4\hat{c}_{\nu}^{I} + 5)}{16pT}\tilde{\Pi}^{2} - \frac{1}{4pT}\sigma_{\langle ij\rangle}\sigma_{\langle ij\rangle} - \frac{\rho}{(2\hat{c}_{\nu}^{I} + 5)p^{2}T}q_{i}q_{i}.$$
(44)

This means that the entropy density is convex (in the limit of the approximation), it reaches the maximum at equilibrium and the system (42) provides the symmetric form in the main field components. Similarly, the entropy flux is obtained as follows:

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

The entropy production  $\Sigma$  according with the symmetrization theorem [4,5,39] is obtained as scalar product between the main field given by (37) and the production vector given by (21). By taking into account (41) and (36), we have

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

<sup>102</sup> It is noteworthy that the entropy production is positive provided the relaxation times are together with  $\hat{c}_{\nu}^{I} \geq 0$ .

#### <sup>103</sup> 2.6. Characteristic velocities

The differential system (42) is particular case of a generic balance law system:

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

and it is well known that the characteristic velocity V associated with a hyperbolic system of equations can be obtained by using the operator chain rule (see [4]):

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

where  $n_i$  denotes the *i*-component of the unit normal to the wave front, **f** is the production terms and  $\delta$  is a differential operator.

Let us consider only one dimensional space-variable, and the system (42) 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 characteristic velocities evaluated in equilibrium:

$$V^{(1)} = v - U_E^{1\text{st}} \sqrt{\frac{k_B}{m}T}, \quad V^{(2)} = v - U_E^{2\text{nd}} \sqrt{\frac{k_B}{m}T},$$

$$V^{(3)} = V^{(4)} = V^{(5)} = v,$$

$$V^{(6)} = v + U_E^{2\text{nd}} \sqrt{\frac{k_B}{m}T}, \quad V^{(7)} = v + U_E^{1\text{st}} \sqrt{\frac{k_B}{m}T},$$
(45)

with

$$U_E^{1\text{st}} = \frac{1}{\sqrt{6(4\hat{c}_\nu - 1)(\hat{c}_\nu + 1)}} \sqrt{8\hat{c}_\nu(7\hat{c}_\nu + 11) - 13} + \sqrt{4\hat{c}_\nu\left\{64\hat{c}_\nu^2(\hat{c}_\nu + 16) + 897\hat{c}_\nu - 482\right\} + 349}, \quad (46)$$

$$U_E^{2\mathrm{nd}} = \frac{1}{\sqrt{6(4\hat{c}_\nu - 1)(\hat{c}_\nu + 1)}} \sqrt{8\hat{c}_\nu(7\hat{c}_\nu + 11) - 13 - \sqrt{4\hat{c}_\nu\left\{64\hat{c}_\nu^2(\hat{c}_\nu + 16) + 897\hat{c}_\nu - 482\right\} + 349}},$$
 (47)

where  $\hat{c}_v = 3/2 + \hat{c}_v^I$  is the dimensionless specific heat. It is easy to prove that  $U_E^{1\text{st}}$  given by (46) and  $U_E^{2\text{nd}}$  by (47) are real because  $\hat{c}_v \ge 3/2$ , and therefore the characteristic velocities (45) are all real in agreement that any symmetric systems are hyperbolic.

Note that the fastest velocity  $U_E^{1st} > U_E^{2nd}$  is larger than the corresponding one of the polyatomic ET<sub>14</sub> theory, 109 and this indicates that the subcharacteristic condition [44] is satisfied due to the convexity of entropy (44). In the limit 110 of monatomic gases ( $\hat{c}_v = 3/2$ ),  $U_E^{1\text{st}} \sim 2.27655$  and  $U_E^{2\text{nd}} \simeq 1.16218$ , which coincide with the ones of monatomic ET<sub>14</sub>. In the limit that  $\hat{c}_v \to \infty$ ,  $U_E^{1\text{st}} \to \sqrt{3}$  which is same with the one predicted by polyatomic ET<sub>14</sub> in this limit. 111 112 Recalling the general discussion of the dependence of the characteristic velocities on the degrees of freedom [26], 113 this is the value of the characteristic velocity of monatomic ET theory with 10 moments (ET<sub>10</sub>) in which  $(F, F_i, F_{ij})$ 114 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 ET<sub>14</sub> 115 but is same with the equilibrium sound velocity (the characteristic velocity of Euler system) of monatomic gases in 116 which  $(F, F_i, F_{ll})$  are the only independent fields. While,  $U_E^{2nd}$  of  $ET_{14}$  approaches to 1 which is the characteristic 117 velocity of ET theory with 4 moments (ET<sub>4</sub>) in which  $(F, F_i)$  are the only independent fields. 118

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



**Figure 1.** Dependence of the normalized characteristic velocities  $U_E^{1\text{st}}$  (left) and  $U_E^{2\text{nd}}$  (right) with respect to *D*. The solid and dashed lines are the normalized characteristic velocities of  $\text{ET}_{15}$  and polyatomic  $\text{ET}_{14}$ . The limit value of the normalized characteristic velocities of  $D \to 3$  and  $D \to \infty$  are indicated with dotted lines. In the limit that  $D \to 3$ ,  $U_E^{1\text{st}}$  and  $U_E^{2\text{nd}}$  of  $\text{ET}_{15}$  coincide with the monatomic  $\text{ET}_{14}$ . In the limit that  $D \to \infty$ , both of  $U_E^{1\text{st}}$  of  $\text{ET}_{15}$  and  $\text{ET}_{14}$  approach to the one of monatomic  $\text{ET}_{10}$ , and  $U_E^{2\text{nd}}$  of  $\text{ET}_{15}$  and  $\text{ET}_{14}$  approach, respectively, to monatomic Euler and  $\text{ET}_4$ .

#### 121 2.7. Maxwellian iteration and phenomenological coefficients

The NSF theory is obtained by carrying out the Maxwellian iteration [45] on (42) in which only the first order terms with respect to the relaxation times are retained. Then we obtain

$$\Pi = -p\tau \frac{4\hat{c}_{\nu}^{I}}{6\hat{c}_{\nu}^{I} + 9} \frac{\partial v_{k}}{\partial x_{k}}, \quad \sigma_{\langle ij \rangle} = 2p\tau_{\sigma} \frac{\partial v_{\langle i}}{\partial x_{j \rangle}}, \quad q_{i} = -p\tau_{q} \frac{2\hat{c}_{\nu}^{I} + 5}{2} \frac{k_{B}}{m} \frac{\partial T}{\partial x_{i}}, \tag{48}$$

and

$$\Delta = -\tau_{\Delta} \frac{16\hat{c}_{\nu}^{I}}{2\hat{c}_{\nu}^{I} + 3} \frac{p^{2}}{\rho} \left( y^{I} + 1 \right) \left( 1 + \frac{\tau}{\tau_{K}} \right) \frac{\partial v_{I}}{\partial x_{l}},\tag{49}$$

where

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

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

$$\Pi = -\nu \frac{\partial v_i}{\partial x_i}, \qquad \sigma_{\langle ij \rangle} = 2\mu \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}, \qquad q_i = -\kappa \frac{\partial T}{\partial x_i}, \tag{50}$$

we have from (48)

$$\nu = \frac{4\hat{c}_{\nu}^{I}}{6\hat{c}_{\nu}^{I} + 9}p\tau, \qquad \mu = p\tau_{\sigma}, \qquad \kappa = \frac{2\hat{c}_{\nu}^{I} + 5}{2}p\tau_{q}.$$
(51)

We note that  $\Delta$  and  $\hat{\Pi}$  is not present in the conservation laws of mass, momentum and energy. In particular, (49) indicates with (43)

 $\tilde{\Pi} = 0.$ 

This result seems similar to the case of monatomic  $ET_{14}$  in which the nonequilibrium scalar field is equal to 0 in the Maxwellian iteration [9].

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  $\tau$ ,  $\tau_{\sigma}$  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,  $\tau_{\Delta}$  and  $\tau_{K}$  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.

Summarizing we have the following result: *With the Maxwellian iteration procedure, the hyperbolic system* (42) converges (in similar way of the 14 fields theory) to the classical parabolic system of NFS formed by the first five equations of (42) with the constitutive equations (50) with bulk and shear viscosities and heat conductivity related to the relaxation times by (51).

#### 133 2.8. Principal subsystem

The concept of the principal subsystem for a general system of hyperbolic system of balance laws was introduced in [44]. 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 has 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 consequence, in the
 moments theory, the maximum characteristic velocity increases with the number of moments [13].

In the present case, the polyatomic  $\text{ET}_{14}$  is obtained as a principal subsystem of  $\text{ET}_{15}$  under the condition  $\zeta = 0$ , i.e., from (36)<sub>7</sub>,

$$\Pi = 0,$$

or, in other words,

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

 $_{140}$  and  $(42)_7$  is ignored.

#### 141 2.9. Monatomic gas limit

The monatomic gases are described in the limit  $\varepsilon^I \to 0$  ( $y^I \to 0$ ) and therefore  $\hat{c}_v^I \to 0$ . In the limit, the equation for  $\Pi$  obtained by subtracting (42)<sub>3</sub> from (42)<sub>4</sub> becomes

$$\frac{\partial \Pi}{\partial t} + v_k \frac{\partial \Pi}{\partial x_k} = -\left(\frac{1}{\tau_{\Pi}} + \frac{\partial v_k}{\partial x_k}\right) \Pi.$$
(52)

This is the first-order quasi-linear partial differential equation with respect to  $\Pi$ . As it has been studied in [23], the initial condition for (52) 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 Eq. (52) is given by

$$\Pi(t, \mathbf{x}) = 0 \quad \text{(for any } t\text{)}. \tag{53}$$

If we insert the solution (53) into (24) and (38) with  $y^I = 0$  and  $\hat{c}_v^I = 0$ , the velocity independent moments are expressed by the velocity independent moments of monatomic gas  $\hat{F}_{i_1i_2\cdots i_n}^M$  which are given in (34) as follows:

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

<sup>142</sup> 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, solutions of ET<sub>15</sub> converge to those of monatomic 14 theory by Kremer [9].

It may be remarkable that, from this coincidence, we can set the inessential phenomenological constants appear in monatomic ET<sub>14</sub> theory [9] as zero. Therefore, the molecular approach can determine the constitutive equations without arbitrariness except for the production terms, although the phenomenological approach can provide the theory for the gas with generic equations of state, e.g., the theory for degenerate Fermi and Bose gases [9].

#### **3. Dispersion Relation**

<sup>150</sup> The dependences of the phase velocity and the attenuation per wavelength on the frequency are studied.

### 151 3.1. Phase velocity and attenuation factor

Let us confine our study within one-dimensional problem, that is, a plane longitudinal wave propagating in *x*-direction. Therefore, considering the symmetry of the wave, we have the following form:

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

Moreover, we study a harmonic wave for the fields  $u = (\rho, v, T, \Pi, \sigma, q, \Delta)$  with the angular frequency  $\omega$  and the complex wave number k such that

$$u = w \mathrm{e}^{\mathrm{i}(\omega t - kx)},\tag{55}$$

where w is a constant amplitude vector. From Eq. (10) with (54) and (55), the dispersion relation  $k = k(\omega)$  is obtained by the standard way [3]. The phase velocity  $v_{ph}$  and the attenuation factor  $\alpha$  are calculated as the functions of the frequency  $\omega$  by using the following relations:

$$w_{ph} = \frac{\omega}{\mathcal{R}e(k)}, \quad \alpha = -\mathcal{I}m(k)$$

In addition, it is useful to introduce the attenuation per wavelength  $\alpha_{\lambda}$ :

$$\alpha_{\lambda}(\omega) = \alpha \lambda = \frac{2\pi v_{ph} \alpha}{\omega} = -2\pi \frac{Im(k)}{\mathcal{R}e(k)},$$

where  $\lambda$  is the wavelength.

Let us introduce the following dimensionless parameters:

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

<sup>153</sup> Then the dispersion relation depends on these parameters with dimensionless specific heat of internal mode  $\hat{c}_{v}^{l}$ .

We emphasize that  $k = k(\omega)$  does not depend on  $\rho$ , and its temperature dependence is determined through the dimensionless specific heat that can be determined from statistical mechanics or experimental data.

As an example, we adopt  $\hat{\tau}_K = 0.001$  which indicates the existence of the slow relaxation of internal mode [42,46,47]. We show the dependence of the phase velocity normalized by the equilibrium sound velocity  $c_0$ :

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

and the attenuation per wavelength on the dimensionless frequency in Fig. 2 in the case with  $\hat{c}_{\nu}^{I} = 2$ . Around

<sup>157</sup>  $\Omega \sim 10^0 (\omega \sim \tau^{-1})$ , we can observe a change of  $v_{ph}$  and a peak of  $\alpha_{\lambda}$ . Since this is due to the relaxation of internal <sup>158</sup> mode relating to  $\Pi$ , both of the predictions by ET<sub>14</sub> and ET<sub>15</sub> coincide each other. Around  $\Omega \sim 10^3 (= \hat{\tau}_{\kappa}^{-1})$ , we can

<sup>159</sup> 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

<sup>160</sup> between two theories emerges.



**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<sub>15</sub> and polyatomic ET<sub>14</sub> theories.

#### 161 4. Conclusions

According to the general results of Pennisi and Ruggeri [19], the classical limit of the relativistic theory of 162 moments provides more complex hierarchy than the F' and G' binary hierarchy. In this paper, we have studied the 163 case of N = 2 in which the classic limit dictates 15 fields for a non-polytropic polyatomic gas. We have obtained the 164 closure using the MEP. The closed field equations include the classical NSF theory as its parabolic limit and converge 165 to the monatomic ET<sub>14</sub> theory obtained by Kremer [9] in the monatomic singular limit. Moreover, we proved that the 166 polyatomic  $ET_{14}$  theory is a principal subsystem of the present one, and according to the general results, the spectrum 167 of characteristic velocities of  $ET_{15}$  includes the spectrum of eigenvalues of  $ET_{14}$ . Finally, we have evaluated the 168 dispersion relation proving that, in the low-frequency region, the predictions by  $ET_{14}$  and  $ET_{15}$  theories coincide with 169 each other, while, in the high-frequency region, the difference between two theories emerges due to the existence of 170 the additional higher order moment. 171

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 [42,43].

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