

Molecular Extended Thermodynamics of a Rarefied Polyatomic Gas



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Abstract Extended Thermodynamics can be considered as a theory of *continuum with structure* because there are new field variables with respect to the classical approach and they are dictated at mesoscopic level by the kinetic theory. In this survey I present some recent results on the so called *Molecular Extended Thermodynamics* (MET) in which the macroscopic fields are related to the moments of a distribution function that for polyatomic gas contains an extra variable taking into account the internal degrees of freedom of a molecule. The closure is obtained via the variational procedure of the *Maximum Entropy Principle* (MEP). Particular attention will be paid on the simple model of MET with six independent fields, i.e., the mass density, the velocity, the temperature and the dynamic pressure, without adopting near-equilibrium approximation. The model obtained is the simplest example of non-linear dissipative fluid after the ideal case of Euler. The system is symmetric hyperbolic with the convex entropy density and the K-condition is satisfied. Therefore, in contrast to the Euler case, there exist global smooth solutions provided that the initial data are sufficiently smooth.

1 Continuum and Kinetic Approaches of a Non-Equilibrium Gas

The study of nonequilibrium phenomena in gases is particularly important from a theoretical point of view and also from a viewpoint of many possible practical applications. We have two complementary approaches to study rarefied gases, namely the *continuum approach* and the *kinetic approach*.

The continuum model consists in the description of the system by means of macroscopic equations (e.g., fluid-dynamic equations) obtained on the basis of

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conservation laws and appropriate constitutive equations. A typical example is the *thermodynamics of irreversible processes* (TIP). The applicability of this classical macroscopic theory is, however, inherently restricted to a nonequilibrium state characterized by a small *Knudsen number* K_n , which is a measure to what extent the gas is rarefied:

$$K_n = \frac{\text{mean free path of molecule}}{\text{macroscopic characteristic length}}.$$

The approach based on the kinetic theory postulates that the state of a gas can be described by the velocity distribution function. The evolution of the distribution function is governed by the Boltzmann equation. The kinetic theory is applicable to a nonequilibrium state characterized by a large K_n , and the transport coefficients naturally emerge from the theory itself. Therefore the range of the applicability of the Boltzmann equation is limited to rarefied gases.

The Rational Extended Thermodynamics theory (RET) [1], which is a generalization of the TIP theory, also belongs to the continuum approach but is applicable to a nonequilibrium state with larger K_n . In a sense, RET is a sort of bridge between TIP and the kinetic theory. An interesting point to be noticed is that, in the case of rarefied gases, there exists a common applicability range of the RET theory and the kinetic theory. Therefore, in such a range, the results from the two theories should be consistent with each other. Because of this, we can expect that the kinetic-theoretical considerations can motivate us at mesoscopic level to establish the mathematical structure of the RET theory.

2 Extended Thermodynamics of Rarefied Monatomic Gases

The kinetic theory describes a state of a rarefied gas by using the phase density (velocity distribution function) $f(\mathbf{x}, t, \mathbf{c})$, where $f(\mathbf{x}, t, \mathbf{c})d\mathbf{c}$ is the number density of (monatomic) molecules at the point \mathbf{x} and time t that have velocities between \mathbf{c} and $\mathbf{c} + d\mathbf{c}$. Time-evolution of the phase density is governed by the Boltzmann equation:

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

where the right-hand side, the collision term, describes the effect of collisions between molecules. Here

$$\partial_t \equiv \frac{\partial}{\partial t} \quad \text{and} \quad \partial_i \equiv \frac{\partial}{\partial x_i},$$

and as usual we omit the symbol of sum over repeated italic indexes between 1 to 3. Most macroscopic thermodynamic quantities are identified as the moments of the phase density

$$F = \int_{\mathbb{R}^3} f d\mathbf{c}, \quad F_{k_1 k_2 \dots k_j} = \int_{\mathbb{R}^3} f c_{k_1} c_{k_2} \dots c_{k_j} d\mathbf{c}, \quad (j = 1, \dots) \quad (2)$$

and due to the Boltzmann equation (1), the moments satisfy an infinite hierarchy of balance laws in which the flux in one equation becomes the density in the next one:

$$\begin{aligned} \partial_t F + \partial_i F_i &= 0 \\ &\swarrow \\ \partial_t F_{k_1} + \partial_i F_{ik_1} &= 0 \\ &\swarrow \\ \partial_t F_{k_1 k_2} + \partial_i F_{ik_1 k_2} &= P_{<k_1 k_2>} \\ &\swarrow \\ \partial_t F_{k_1 k_2 k_3} + \partial_i F_{ik_1 k_2 k_3} &= P_{k_1 k_2 k_3} \\ &\vdots \\ \partial_t F_{k_1 k_2 \dots k_N} + \partial_i F_{ik_1 k_2 \dots k_N} &= P_{k_1 k_2 \dots k_N} \\ &\vdots \end{aligned} \quad (3)$$

where

$$P_{k_1 k_2 \dots k_j} = \int_{\mathbb{R}^3} Q c_{k_1} c_{k_2} \dots c_{k_j} d\mathbf{c}.$$

As $P_{kk} = 0$, we notice that the first five equations are exactly the conservation laws, and correspond to the conservation laws of mass, momentum and energy (except for the factor 2) of continuum thermomechanics. For this reason we have the expression, in particular, for the flux of (3)₂:

$$F_{ik} = \rho v_i v_k - t_{ik}, \quad (4)$$

where ρ is the mass density, v_i the velocity, and t_{ij} denotes the stress tensor:

$$t_{ik} = -p\delta_{ik} + \sigma_{ik}, \quad \sigma_{ik} = -\Pi\delta_{ik} + \sigma_{<ik>}$$

with p , Π , and $\sigma_{<ik>}$ being, respectively, the equilibrium pressure, the dynamical (non-equilibrium) pressure, and the shear viscous deviatoric tensor $\sigma_{<ik>}$. While the trace of the density in (3)₃ denotes, except for the factor 2, the total energy:

$$F_{ll} = 2\rho\varepsilon + \rho v^2, \quad (5)$$

where ε is the specific internal energy. As a consequence from the trace of (4) and (5), we have the relationship $3(p + \Pi) = 2\rho\varepsilon$. As Π is a nonequilibrium quantity that vanishes in equilibrium, we obtain

$$p = \frac{2}{3}\rho\varepsilon \quad \text{and} \quad \Pi \equiv 0. \quad (6)$$

Then the gas under consideration is indeed monatomic, and the dynamic pressure vanishes identically. This is a strong limitation on the kinetic theory. It is valid only for rarefied monatomic gases with viscous stress tensor σ_{ij} that must be deviatoric, i.e., traceless: $\Pi \equiv 0$.

When we cut the hierarchy at the density with tensor of rank N , we have the problem of closure because the last flux and the production terms are not in the list of the densities. The first idea of RET [1] was to view the truncated system as a phenomenological system of continuum mechanics and then we consider the new quantities as local constitutive functions of the densities:

$$\begin{aligned} F_{k_1 k_2 \dots k_N k_{N+1}} &\equiv F_{k_1 k_2 \dots k_N k_{N+1}}(F, F_{k_1}, F_{k_1 k_2}, \dots, F_{k_1 k_2 \dots k_N}), \\ P_{\langle k_1 k_2 \rangle} &\equiv P_{\langle k_1 k_2 \rangle}(F, F_{k_1}, F_{k_1 k_2}, \dots, F_{k_1 k_2 \dots k_N}), \\ P_{k_1 k_2 \dots k_j} &\equiv P_{k_1 k_2 \dots k_j}(F, F_{k_1}, F_{k_1 k_2}, \dots, F_{k_1 k_2 \dots k_N}), \quad 3 \leq j \leq N. \end{aligned} \quad (7)$$

According with the continuum theory, the restrictions on the constitutive equations come only from *universal principles*, i.e.: *Entropy principle*, *Objectivity Principle* and *Causality and Stability* (convexity of the entropy).

The most interesting physical cases was the 13 fields theory in classical framework [2] and the 14 fields in the context of relativistic fluids [3]. In both cases the previous universal principles are enough to determine completely the form of the constitutive equations (7) at least in a theory not so far from a equilibrium state (linear with respect the non-equilibrium variables).

3 Closure via the Maximum Entropy Principle and Molecular Extended Thermodynamics of Monatomic Gases

If the number of moments increases, it becomes to be too difficult to adopt the pure continuum approach for a system with such a large number of field variables. Therefore it is necessary to recall that the field variables are the moments of a distribution function. To obtain the closure of the balance equations of the moments truncated at some tensorial order N , we adopt the *maximum entropy principle* (MEP). This is the procedure of the so-called *molecular extended thermodynamics* (molecular RET) [4].

The principle of maximum entropy has its root in statistical mechanics. It is developed by Jaynes [5] in the context of the theory of information basing on the Shannon entropy. Nowadays the importance of MEP is recognized fully due to the numerous applications in many fields [6], for example, in the field of computer graphics. MEP states that the probability distribution that represents the current state of knowledge in the best way is the one with the largest entropy. Another way of stating this is as follows: take precisely stated prior data or testable information about a probability distribution function. Then consider the set of all trial probability distributions that would encode the prior data. Of those, one with maximal information entropy is the proper distribution, according to this principle.

Concerning the applicability of MEP in nonequilibrium thermodynamics, this was originally by the observation made by Kogan [7] that Grad's distribution [8] function maximizes the entropy. The MEP was proposed in RET for the first time by Dreyer [9]. In this way the 13-moment theory closure can be obtained in three different ways: phenomenological RET, Grad kinetic method, and MEP. A remarkable point is that all closures are equivalent to each other! The MEP procedure was then generalized by Müller and Ruggeri to the case of any number of moments in the first edition of their book proving that the closed system is symmetric hyperbolic [4]. In MET the complete equivalence between the closures via the entropy principle and via the MEP was finally proved by Boillat and Ruggeri in [10].

In the case of monatomic gases, we can define the moments (2) using a multi-index:

$$F_A = \begin{cases} F & \text{for } A = 0 \\ F_{k_1 k_2 \dots k_A} & \text{for } 1 \leq A \leq N, \end{cases}$$

and in this way the truncated system (3) at the tensorial order N can be rewritten in a simple form:

$$\partial_t F_A + \partial_i F_{iA} = P_A, \quad A = 0, \dots, N \quad (8)$$

with

$$F_A = m \int_{\mathbb{R}^3} c_A f \, d\mathbf{c}, \quad F_{iA} = m \int_{\mathbb{R}^3} c_i c_A f \, d\mathbf{c}, \quad P_A = m \int_{\mathbb{R}^3} c_A Q \, d\mathbf{c} \quad (9)$$

and

$$c_A = \begin{cases} 1 & \text{for } A = 0 \\ c_{k_1} c_{k_2} \dots c_{k_A} & \text{for } 1 \leq A \leq N. \end{cases}$$

The variational problem, from which the distribution function f render the entropy

$$h = -k_B \int_{\mathbb{R}^3} f \log f \, d\mathbf{c}$$

(k_B is the Boltzmann constant) maximum for the prescribed moments, is obtained through the functional (we omit the symbol of sum from 0 to N in the repeated capital indexes A, B, \dots):

$$\mathcal{L}_N(f) = -k_B \int_{\mathbb{R}^3} f \log f \, d\mathbf{c} + u'_A \left(F_A - m \int_{\mathbb{R}^3} c_A f \, d\mathbf{c} \right),$$

where u'_A are the Lagrange multipliers:

$$u'_A = \begin{cases} u' & \text{for } A = 0 \\ u'_{k_1 k_2 \dots k_A} & \text{for } 1 \leq A \leq N. \end{cases}$$

The distribution function f_N which maximizes the functional \mathcal{L}_N is given by [1, 4, 11, 12]:

$$f_N = \exp \left(-1 - \frac{m}{k} \chi_N \right), \quad \chi_N = u'_A c_A. \quad (10)$$

In an equilibrium state, (10) reduces to the Maxwellian distribution function $f^{(M)}$. Then, the system may be rewritten as follows:

$$J_{AB} \partial_t u'_B + J_{iAB} \partial_i u'_B = P_A(u'_C), \quad A = 0, \dots, N \quad (11)$$

where

$$J_{AB}(u'_C) = -\frac{m^2}{k_B} \int_{\mathbb{R}^3} f_N c_A c_B \, d\mathbf{c}, \quad J_{iAB}(u'_C) = -\frac{m^2}{k_B} \int_{\mathbb{R}^3} f_N c_i c_A c_B \, d\mathbf{c}.$$

Because of the fact that the matrices J_{AB}, J_{iAB} are symmetric with respect to the multi-index A, B and J_{AB} is definite negative, the system (11) is symmetric hyperbolic [1, 4, 11] and the Lagrange multipliers coincide with the *main field* according with the general theory of systems of balance laws with a convex entropy density [13–17]. We observe that f_N is not a solution of the Boltzmann equation. But we have the conjecture (open problem) that, for $N \rightarrow \infty$, f_N tends to a solution of the Boltzmann equation.

4 Convergence Problem and Approximation Near an Equilibrium State

All results explained above are valid also for a case far from equilibrium provided that the integrals in (9) are convergent. The problem of the convergence of the moments is one of the main questions in a far-from-equilibrium case. In particular

the index of truncation N must be even [11, 18]. This implies, in particular, that a theory with 13 moments is not allowed when far from equilibrium! Moreover, if the conjecture that the distribution function f_N , when $N \rightarrow \infty$, tends to the distribution function f that satisfies the Boltzmann equation is true, we need another convergence requirement for χ given in (11). These problems were studied by Boillat and Ruggeri [11].

To bypass the question of convergence of integrals, the distribution function obtained as the solution of the variational problem is considered only in the neighborhood of a local equilibrium state, and we formally expand the distribution function (10) as the perturbation of the Maxwellian distribution $f^{(M)}$:

$$f_N \approx f^{(M)} \left(1 - \frac{m}{k_B} \tilde{u}'_A c_A \right), \quad \tilde{u}'_A = u'_A - u'^E_A, \quad (12)$$

where u'^E_A are the main field components evaluated in the local equilibrium state. More high expansion was considered in the paper [19].

This is a big limitation of the theory because the theory is valid only near equilibrium and hyperbolicity exists only in some small domain of the configuration space near equilibrium. Notice that f_N given by (12) is not always positive!

5 ET Beyond the Monatomic Gas: Polyatomic Gas

The previous ET theory, being strictly connected with the kinetic theory, suffers from nearly the same limitations as the Boltzmann equation.

In the case of polyatomic gases, on the other hand, the rotational and vibrational degrees of freedom of a molecule, which are not present in monatomic gases, come into play [20], and in the case of dense gases, as the average distance between the constituent molecules is finite, the interaction between the molecules cannot be neglected. From a mathematical standpoint, these effects are responsible for intrinsic changes in the structure of the system of field equations. Single hierarchy of field equations as in the case of monatomic gases is no longer valid. In particular, the internal specific energy is no longer related to the pressure in a simple way.

After several tentative theories, a satisfactory *14-field* ET theory for dense gases and for rarefied polyatomic ones, was recently developed by Arima, Taniguchi, Ruggeri and Sugiyama [21]. This theory adopts two parallel hierarchies (binary hierarchy) for the independent fields: the mass density, the velocity, the internal energy, the shear stress, the dynamic pressure and the heat flux. One hierarchy consists of balance equations for the mass density, the momentum density and the

momentum flux (*momentum-like* hierarchy), and the other one consists of balance equations for the energy density and the energy flux (*energy-like* hierarchy):

$$\begin{aligned}
 \partial_t F + \partial_i F_i &= 0, \\
 \partial_t F_{k_1} + \partial_i F_{ik_1} &= 0, \\
 \partial_t F_{k_1 k_2} + \partial_i F_{ik_1 k_2} &= P_{k_1 k_2}, \quad \partial_t G_{kk} + \partial_i G_{ikk} = 0, \\
 \partial_t G_{kkk_1} + \partial_i G_{kiki_1} &= Q_{kkk_1}.
 \end{aligned} \tag{13}$$

These hierarchies cannot merge with each other in contrast to the case of rarefied monatomic gases because the specific internal energy (the intrinsic part of the energy density) is no longer related to the pressure (one of the intrinsic parts of the momentum flux).

By means of the closure procedure of the ET theory, the constitutive equations are determined explicitly by the thermal and caloric equations of state. For example, let us consider the particular case of rarefied polyatomic gases with the thermal and caloric equations of state given by (polytropic gas)

$$p = \frac{k_B}{m} \rho T \quad \text{and} \quad \varepsilon = \frac{D}{2} \frac{k_B}{m} T, \quad (D = 3 + f^i) \tag{14}$$

where m is the atomic mass, T the absolute temperature, and the constant D is related to the degrees of freedom of a molecule given by the sum of the space dimension 3 for the translational motion and the contribution from the internal degrees of freedom $f^i (\geq 0)$. For monatomic gases, $D = 3$ (see (6)₁).

Concerning the kinetic counterpart, a crucial step towards the development of the theory of rarefied polyatomic gases was made by Borgnakke and Larsen [22]. The distribution function is assumed to depend on an additional continuous variable representing the energy of the internal modes of a molecule in order to take into account the exchange of energy (other than translational one) in binary collisions. This model was initially used for Monte Carlo simulations of polyatomic gases, and later it was applied to the derivation of the generalized Boltzmann equation by Bourgat, Desvillettes, Le Tallec and Perthame [23].

As a consequence of the introduction of one additional parameter I , the velocity distribution function $f(t, \mathbf{x}, \mathbf{c}, I)$ is defined on the extended domain $[0, \infty) \times R^3 \times R^3 \times [0, \infty)$. Its rate of change is determined by the Boltzmann equation which has the same form as the one of monatomic gases (1) but the collision integral $Q(f)$ takes into account the influence of the internal degrees of freedom through the collisional cross section.

Pavić, Ruggeri and Simić proved [24]¹ that, by means of the MEP, the kinetic model for rarefied polyatomic gases presented in [22] and [23] yields appropriate macroscopic balance laws. This is a natural generalization of the classical procedure

¹There are some typos in the paper [24] that were corrected in the Chapter 12 of the book [12].

of MEP from monatomic gases to polyatomic gases. They considered the case of 14 moments, and showed the complete agreement with the binary hierarchy (21). The moments are defined by

$$\begin{aligned} \begin{pmatrix} F \\ F_{i1} \\ F_{i_1 i_2} \end{pmatrix} &= \int_{\mathbb{R}^3} \int_0^\infty m \begin{pmatrix} 1 \\ c_{i_1} \\ c_{i_1} c_{i_2} \end{pmatrix} f(t, \mathbf{x}, \mathbf{c}, I) \varphi(I) dI d\mathbf{c}, \\ \begin{pmatrix} G_{pp} \\ G_{ppk_1} \end{pmatrix} &= \int_{\mathbb{R}^3} \int_0^\infty m \begin{pmatrix} c^2 + 2\frac{I}{m} \\ (c^2 + 2\frac{I}{m}) c_{k_1} \end{pmatrix} f(t, \mathbf{x}, \mathbf{c}, I) \varphi(I) dI d\mathbf{c}, \\ \begin{pmatrix} P_{k_1 k_2} \\ Q_{kkj} \end{pmatrix} &= \int_{\mathbb{R}^3} \int_0^\infty m \begin{pmatrix} c_{k_1} c_{k_2} \\ (c^2 + 2\frac{I}{m}) c_{k_1} \end{pmatrix} Q \varphi(I) dI d\mathbf{c}. \end{aligned}$$

The weighting function $\varphi(I)$ is determined in such a way that it recovers the caloric equation of state in equilibrium for polyatomic gases. It can be shown that $\varphi(I) = I^\alpha$ leads to an appropriate caloric equation for polytropic gas (14) provided that

$$\alpha = \frac{D-5}{2}. \quad (15)$$

Therefore, also for rarefied polyatomic gases, the three closure procedures (ET, MEP and Grad) give the same result as in the monatomic case!

5.1 ET of Polyatomic Rarefied Gases with Many Moments

In the case of many moments, by using similar notations as in (8)

$$\begin{aligned} F_A &= \begin{cases} F & \text{for } A = 0 \\ F_{k_1 k_2 \dots k_A} & \text{for } 1 \leq A \leq N, \end{cases} & G_{llA'} &= \begin{cases} G_{ll} & \text{for } A' = 0 \\ G_{llk_1 k_2 \dots k_{A'}} & \text{for } 1 \leq A' \leq M, \end{cases} \\ P_A &= \begin{cases} 0 & \text{for } A = 0, 1 \\ P_{k_1 k_2 \dots k_A} & \text{for } 2 \leq A \leq N, \end{cases} & Q_{llA'} &= \begin{cases} 0 & \text{for } A' = 0 \\ Q_{llk_1 k_2 \dots k_{A'}} & \text{for } 1 \leq A' \leq M, \end{cases} \end{aligned}$$

the system of moments can be rewritten in the form of a binary hierarchy:

$$\begin{aligned} \partial_t F_A + \partial_i F_{iA} &= P_A, & (A = 0, \dots, N), \\ \partial_t G_{llA'} + \partial_i G_{illA'} &= Q_{llA'}, & (A' = 0, \dots, M), \end{aligned}$$

with

$$F_A = m \int_{\mathbb{R}^3} \int_0^\infty c_A f \varphi(I) dI d\mathbf{c}, \quad F_{iA} = m \int_{\mathbb{R}^3} \int_0^\infty c_i c_A f \varphi(I) dI d\mathbf{c},$$

$$P_A = m \int_{\mathbb{R}^3} \int_0^\infty c_A Q \varphi(I) dI d\mathbf{c},$$

$$G_{IIA'} = m \int_{\mathbb{R}^3} \int_0^\infty \left(c^2 + \frac{2I}{m} \right) c_{A'} f \varphi(I) dI d\mathbf{c},$$

$$G_{IiA'} = m \int_{\mathbb{R}^3} \int_0^\infty \left(c^2 + \frac{2I}{m} \right) c_i c_{A'} f \varphi(I) dI d\mathbf{c},$$

$$Q_{IIA'} = m \int_{\mathbb{R}^3} \int_0^\infty \left(c^2 + \frac{2I}{m} \right) c_{A'} Q \varphi(I) dI d\mathbf{c},$$

$$c_A = \begin{cases} 1 & \text{for } A = 0 \\ c_{k_1} c_{k_2} \cdots c_{k_A} & \text{for } 1 \leq A \leq N, \end{cases} \quad c_{A'} = \begin{cases} 1 & \text{for } A' = 0 \\ c_{k_1} c_{k_2} \cdots c_{k_{A'}} & \text{for } 1 \leq A' \leq M. \end{cases}$$

The variational problem, from which the distribution function $f_{(N,M)}$ maximizes the entropy

$$h = -k_B \int_{\mathbb{R}^3} \int_0^\infty f \log f \varphi(I) dI d\mathbf{c}, \tag{16}$$

is connected to the functional:

$$\begin{aligned} \mathcal{L}_{(N,M)}(f) = & -k_B \int_{\mathbb{R}^3} \int_0^\infty f \log f \varphi(I) dI d\mathbf{c} \\ & + u'_A \left(F_A - m \int_{\mathbb{R}^3} \int_0^\infty c_A f \varphi(I) dI d\mathbf{c} \right) + \\ & + v'_{A'} \left(G_{IIA'} - m \int_{\mathbb{R}^3} \int_0^\infty \left(c^2 + \frac{2I}{m} \right) c_{A'} f \varphi(I) dI d\mathbf{c} \right), \end{aligned}$$

where u'_A and $v'_{A'}$ are the Lagrange multipliers:

$$u'_A = \begin{cases} u' & \text{for } A = 0 \\ u'_{k_1 k_2 \dots k_A} & \text{for } 1 \leq A \leq N, \end{cases}, \quad v'_{A'} = \begin{cases} v' & \text{for } A' = 0 \\ v'_{k_1 k_2 \dots k_{A'}} & \text{for } 1 \leq A' \leq M. \end{cases}$$

The distribution function $f_{(N,M)}$ which maximizes the functional $\mathcal{L}_{(N,M)}$ is given by

$$f_{(N,M)} = \exp \left(-1 - \frac{m}{k} \chi_{(N,M)} \right), \quad \chi_{(N,M)} = u'_A c_A + \left(c^2 + \frac{2I}{m} \right) v'_{A'} c_{A'}.$$

Then, the system may be rewritten as follows:

$$\begin{pmatrix} J_{AB}^0 & J_{AB'}^1 \\ J_{A'B}^1 & J_{A'B'}^2 \end{pmatrix} \partial_t \begin{pmatrix} u'_B \\ v'_{B'} \end{pmatrix} + \begin{pmatrix} J_{iAB}^0 & J_{iAB'}^1 \\ J_{iA'B}^1 & J_{iA'B'}^2 \end{pmatrix} \partial_i \begin{pmatrix} u'_B \\ v'_{B'} \end{pmatrix} = \begin{pmatrix} P_A \\ Q_{iIA'} \end{pmatrix}, \tag{17}$$

where

$$\begin{aligned} J_{AB}^0 &= -\frac{m^2}{k} \int_{\mathbb{R}^3} \int_0^\infty f c_A c_B \varphi(I) dI d\mathbf{c}, \\ J_{iAB}^0 &= -\frac{m^2}{k} \int_{\mathbb{R}^3} \int_0^\infty f c_i c_A c_B \varphi(I) dI d\mathbf{c}, \\ J_{AB'}^1 &= -\frac{m^2}{k} \int_{\mathbb{R}^3} \int_0^\infty f c_A c_{B'} \left(c^2 + \frac{2I}{m} \right) \varphi(I) dI d\mathbf{c}, \\ J_{iAB'}^1 &= -\frac{m^2}{k} \int_{\mathbb{R}^3} \int_0^\infty f c_i c_A c_{B'} \left(c^2 + \frac{2I}{m} \right) \varphi(I) dI d\mathbf{c}, \\ J_{iA'B'}^2 &= -\frac{m^2}{k} \int_{\mathbb{R}^3} \int_0^\infty f c_i c_{A'} c_{B'} \left(c^2 + \frac{2I}{m} \right)^2 \varphi(I) dI d\mathbf{c}. \end{aligned}$$

Also in this case the closed system is symmetric hyperbolic [12, 25], and the theory of monatomic gases is a singular limit of the theory of polyatomic gases [26].

In the present case we have in principle two index of truncation M and N . In the paper [25], the following two theorems are proved:

Theorem 1 *The differential system is Galilean invariant if and only if $M \leq N - 1$.*

Theorem 2 *If $M < N - 1$, all characteristic velocities are independent of the internal degrees of freedom D and coincide with the ones of F -hierarchy of monatomic gases with the truncation order N .*

The requirement that the system is Galilean invariant and the characteristic velocities are functions of D leads to the relationship $M = N - 1$. According with this result, the most interesting cases are the Euler system $N = 1, M = 0$ and the system with 14 fields that describes the ET of dissipative fluids in the presence of viscosity and heat conduction $N = 2, M = 1$.

Also in the case of polyatomic gases, we have the same problematic concerning the convergence of the integrals. In particular, not only the Grad theory of monatomic gases but also the theory with 14 moments are invalid in the case far from equilibrium!

Therefore as in the monatomic gas case, the distribution function obtained as a solution of the variational problem is expanded in the neighborhood of a local equilibrium state:

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

where $u_A'^E$ and $v_A'^E$ are the main field components evaluated in the local equilibrium state. The equilibrium distribution function is given by [12, 24]

$$f^{(E)} = \frac{\rho}{m A(T)} \left(\frac{m}{2\pi k_B T} \right)^{3/2} \exp \left\{ -\frac{1}{k_B T} \left(\frac{1}{2} m C^2 + I \right) \right\}, \quad (18)$$

where

$$A(T) = \int_0^\infty \exp \left(-\frac{I}{k_B T} \right) \varphi(I) dI. \quad (19)$$

This generalizes the Maxwellian distribution function in the case of polyatomic gases, which was obtained first with different arguments in [23]. In the polytropic case, (19) becomes

$$A(T) = (k_B T)^{1+\alpha} \Gamma(1 + \alpha),$$

with α related with D through (15), and Γ denotes the Gamma function.

As an example we write down the differential closed system of 14 fields [12, 21]:

$$\begin{aligned} \dot{\rho} + \rho \frac{\partial v_k}{\partial x_k} &= 0, \\ \rho \dot{v}_i + \frac{\partial p}{\partial x_i} + \frac{\partial \Pi}{\partial x_i} - \frac{\partial \sigma_{(ij)}}{\partial x_j} &= 0, \\ \dot{T} + \frac{2}{D \frac{k_B}{m} \rho} (p + \Pi) \frac{\partial v_k}{\partial x_k} - \frac{2}{D \frac{k_B}{m} \rho} \frac{\partial v_i}{\partial x_k} \sigma_{(ik)} + \frac{2}{D \frac{k_B}{m} \rho} \frac{\partial q_k}{\partial x_k} &= 0, \\ \dot{\sigma}_{(ij)} + \sigma_{(ij)} \frac{\partial v_k}{\partial x_k} - 2\Pi \frac{\partial v_{(i}}{\partial x_{j)}} + 2 \frac{\partial v_{(i}}{\partial x_k} \sigma_{(j)k)} - \frac{4}{D+2} \frac{\partial q_{(i}}{\partial x_{j)}} - 2p \frac{\partial v_{(i}}{\partial x_{j)}} &= -\frac{1}{\tau_\sigma} \sigma_{(ij)}, \\ \dot{\Pi} + \frac{5D-6}{3D} \Pi \frac{\partial v_k}{\partial x_k} - \frac{2(D-3)}{3D} \frac{\partial v_{(i}}{\partial x_{k)}} \sigma_{(ik)} + \frac{4(D-3)}{3D(D+2)} \frac{\partial q_k}{\partial x_k} + \frac{2(D-3)}{3D} p \frac{\partial v_k}{\partial x_k} &= -\frac{1}{\tau_\Pi} \Pi, \\ \dot{q}_i + \frac{D+4}{D+2} q_i \frac{\partial v_k}{\partial x_k} + \frac{2}{D+2} q_k \frac{\partial v_k}{\partial x_i} + \frac{D+4}{D+2} q_k \frac{\partial v_i}{\partial x_k} & \\ + \frac{k_B}{m} T \frac{\partial \Pi}{\partial x_i} - \frac{k_B}{m} T \frac{\partial \sigma_{(ik)}}{\partial x_k} + \Pi \left[-\frac{k_B}{m} T \frac{\partial \rho}{\partial x_i} + \frac{D+2}{2} \frac{k_B}{m} \frac{\partial T}{\partial x_i} - \frac{1}{\rho} \frac{\partial \Pi}{\partial x_i} + \frac{1}{\rho} \frac{\partial \sigma_{(ik)}}{\partial x_k} \right] & \\ - \sigma_{(ik)} \left[-\frac{k_B}{m} T \frac{\partial \rho}{\partial x_k} + \frac{D+2}{2} \frac{k_B}{m} \frac{\partial T}{\partial x_k} - \frac{1}{\rho} \frac{\partial \Pi}{\partial x_k} + \frac{1}{\rho} \frac{\partial \sigma_{(pk)}}{\partial x_p} \right] + \frac{D+2}{2} \left(\frac{k_B}{m} \right)^2 \rho T \frac{\partial T}{\partial x_i} & \\ = -\frac{1}{\tau_q} q_i. & \end{aligned} \quad (20)$$

where τ_σ , τ_Π and τ_q are relaxation times. In the present case the thermal and caloric equations of state are given by (14) and the dot indicate the material derivative:

$$\dot{} = \frac{\partial}{\partial t} + v_i \frac{\partial}{\partial x_i}.$$

If we apply the so-called *Maxwellian iteration* [27] (a sort of Chapman-Enskog formal expansion with respect the relaxation times) then (20)_{3,4} converges to the Navier-Stokes constitutive equations, while (20)₅ reduces to the Fourier law [12]. For this reason the relaxations times τ_σ , τ_Π , and τ_q are connected, respectively, with the shear viscosity, bulk viscosity, and heat conductivity. We conclude that the Navier-Stokes-Fourier parabolic system of TIP is an approximation of the previous hyperbolic system when the relaxation times are small. The reader who is interested in how the usual constitutive equations (Navier-Stokes', Fourier's, Fick's, Darcy's) are approximated from the hyperbolic balance laws when some relaxation times are negligible can read the paper [28].

A relativistic theory with 14 fields was recently given by Pennisi and Ruggeri [29].

6 The 6-Moment Case and Non-Linear Closure

The 14-field theory gives us a complete phenomenological model but its differential system is rather complex and the closure is in any way limited within near equilibrium. Let us consider now a simplified theory (ET₆) with 6 independent field-variables (ρ , v_i , T , Π). This simplified theory preserves the main physical properties of the more complex theory of 14 variables, in particular, when the bulk viscosity plays more important role than the shear viscosity and the heat conductivity. ET₆ has another advantage to offer us a more affordable hyperbolic partial differential system. In fact, it is the simplest system that takes into account a dissipation mechanism after the Euler system of perfect fluids. In the present case we have

$$\begin{aligned} \frac{\partial F}{\partial t} + \frac{\partial F_i}{\partial x_i} &= 0, \\ \frac{\partial F_j}{\partial t} + \frac{\partial F_{ji}}{\partial x_i} &= 0, \\ \frac{\partial F_{ll}}{\partial t} + \frac{\partial F_{lli}}{\partial x_i} &= P_{ll}, \quad \frac{\partial G_{ll}}{\partial t} + \frac{\partial G_{lli}}{\partial x_i} = 0, \end{aligned} \tag{21}$$

where (21)_{1,2,4} represent the conservation laws of mass, momentum and energy provided that $F = \rho$, $F_i = \rho v_i$, $F_{ij} = \rho v_i v_j + (p + \Pi)\delta_{ij}$, $G_{ll} = \rho v_l v_l + 2\rho\varepsilon$, and $G_{lli} = (\rho v_l v_l + 2\rho\varepsilon + 2p + 2\Pi)v_i$ with p and ε being, respectively, the

pressure and the specific internal energy. The phenomenological ET₆ was studied in the papers [12, 30, 31].

In the molecular approach we have

$$\begin{pmatrix} F \\ F_i \\ F_{ll} \end{pmatrix} = \begin{pmatrix} \rho \\ \rho v_i \\ \rho v^2 + 3(p + \Pi) \end{pmatrix} = \int_{\mathbb{R}^3} \int_0^\infty m \begin{pmatrix} 1 \\ c_i \\ c^2 \end{pmatrix} f \varphi(I) dI d\mathbf{c} \quad (22)$$

and

$$G_{ll} = \rho v^2 + 2\rho\varepsilon = \int_{\mathbb{R}^3} \int_0^\infty m(c^2 + 2I/m) f \varphi(I) dI d\mathbf{c}, \quad (23)$$

while the production term is given by

$$P_{ll} = m \int_{\mathbb{R}^3} \int_0^\infty c^2 Q \varphi(I) dI d\mathbf{c}. \quad (24)$$

Note that the internal energy density can be divided into the translational part ε_K and the part of the internal degrees of freedom ε_I :

$$\begin{aligned} \rho\varepsilon_K &= \int_{\mathbb{R}^3} \int_0^\infty \frac{1}{2} m C^2 f(t, \mathbf{x}, \mathbf{C}, I) \varphi(I) dI d\mathbf{C}, \\ \rho\varepsilon_I &= \int_{\mathbb{R}^3} \int_0^\infty I f(t, \mathbf{x}, \mathbf{C}, I) \varphi(I) dI d\mathbf{C}, \end{aligned} \quad (25)$$

where we have introduced the peculiar velocity:

$$\mathbf{C} \equiv (C_i), \quad C_i = c_i - v_i. \quad (26)$$

6.1 Molecular ET₆ for a Polytopic Gas

The MEP in the nonlinear polytopic ET₆ gives the following distribution function f that maximizes the entropy (16) under the constraints (22), (23)

$$\begin{aligned} f_{\text{Poly}} &= \frac{\rho}{m (k_B T)^{1+\alpha} \Gamma(1+\alpha)} \left(\frac{m}{2\pi k_B T} \frac{1}{1 + \frac{\Pi}{p}} \right)^{3/2} \left(\frac{1}{1 - \frac{3}{2(1+\alpha)} \frac{\Pi}{p}} \right)^{1+\alpha} \\ &\times \exp \left\{ -\frac{1}{k_B T} \left(\frac{1}{2} m C^2 \left(\frac{1}{1 + \frac{\Pi}{p}} \right) + I \left(\frac{1}{1 - \frac{3}{2(1+\alpha)} \frac{\Pi}{p}} \right) \right) \right\}. \end{aligned}$$

The proof was given in the paper [32]. It is important to remark that the distribution function is non-linear in the dynamical pressure in contrast to the usual closure of moment theory in which the non-equilibrium distribution function is a linear perturbation of the equilibrium one. The closed system and the non-equilibrium entropy thus obtained [32] are exactly the same as the ones obtained by the phenomenological approach [12, 31].

6.2 Molecular ET_6 for a Non-Polytropic Gas

In the case of ideal non-polytropic gases the specific heat $c_v = d\varepsilon(T)/dT$ is, in general, a nonlinear function of the temperature and the caloric and thermal equations of state read:

$$\varepsilon \equiv \varepsilon(T), \quad p = \frac{k_B}{m} \rho T. \quad (27)$$

As c_v can be measured by experiments as a function of the temperature T we can obtain the specific internal energy ε as

$$\varepsilon(T) = \frac{k_B}{m} \int_{T_0}^T \hat{c}_v(T') dT', \quad (28)$$

where $\hat{c}_v = (m/k_B)c_v$ is the dimensionless specific heat and T_0 is an inessential reference temperature.

From (25), inserting the equilibrium distribution (18) and taking into account (19), we obtain the internal energy at equilibrium due to the internal motion:

$$\varepsilon_I(T) = \frac{k_B}{m} T^2 \frac{d \log A(T)}{dT}, \quad \varepsilon_I = \varepsilon - \varepsilon_K, \quad (29)$$

with ε_K given by

$$\varepsilon_K = \frac{3}{2} \frac{k_B}{m} T.$$

Therefore if we know the caloric equation of state (28) we know from (29)₂ ε_I and therefore from (29)₁ we can obtain $A(T)$:

$$A(T) = A_0 \exp \left(\frac{m}{k_B} \int_{T_0}^T \frac{\varepsilon_I(T')}{T'^2} dT' \right), \quad (30)$$

where A_0 and T_0 are inessential constants. As was observed in [33], the function A is, according to (19), the Laplace transform of φ :

$$A(T) = \mathcal{L}_u [\varphi(I)](s), \quad s = \frac{1}{k_B T},$$

and then we can obtain the weighting function φ as the inverse Laplace transform of A :

$$\varphi(I) = \mathcal{L}_u^{-1} [A(T)](I), \quad T = \frac{1}{k_B s}.$$

Bisi, Ruggeri and Spiga [34] proved the following theorem about the nonequilibrium distribution function:

Theorem 3 *The distribution function that maximizes the entropy (16) under the constraints (22) and (23) has the form:*

$$f_{\text{Non-Poly}} = \frac{\rho}{mA(\Theta)} \left(\frac{m}{2\pi k_B T} \frac{1}{1 + \frac{\Pi}{p}} \right)^{3/2} \exp \left\{ -\frac{1}{k_B T} \left(\frac{1}{2} m C^2 \left(\frac{1}{1 + \frac{\Pi}{p}} \right) + I \frac{T}{\Theta} \right) \right\}, \tag{31}$$

where the nonequilibrium temperature Θ is related to the dynamical pressure Π and the temperature T through the relation:

$$\frac{\varepsilon_I(T) - \varepsilon_I(\Theta)}{\varepsilon_K(T)} = \frac{\Pi}{p},$$

and $A(\Theta)$ is the function (30) evaluated at the temperature Θ :

$$A(\Theta) = A_0 \exp \left(\frac{m}{k_B} \int_{T_0}^{\Theta} \frac{\varepsilon_I(T')}{T'^2} dT' \right).$$

All the moments are convergent and the bounded solutions satisfy the inequalities:

$$-1 < \frac{\Pi}{p} < \frac{\varepsilon_I(T)}{\varepsilon_K(T)}. \tag{32}$$

The distribution function is non-linear in the dynamical pressure and is positive.

The proof of this theorem is given in [34]. In the polytropic case the non-equilibrium distribution function (31) reduces to the expression (26).

6.3 Closure and Field Equations

Substituting (31) into the fluxes we obtain the closed system of ET₆:

$$\begin{aligned}
 \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho v_i) &= 0, \\
 \frac{\partial(\rho v_j)}{\partial t} + \frac{\partial}{\partial x_i} [(p + \Pi)\delta_{ij} + \rho v_i v_j] &= 0, \\
 \frac{\partial}{\partial t}(2\rho\varepsilon + \rho v^2) + \frac{\partial}{\partial x_i} \left\{ \left[2(p + \Pi) + 2\rho\varepsilon + \rho v^2 \right] v_i \right\} &= 0, \\
 \frac{\partial}{\partial t} [3(p + \Pi) - 2\rho\varepsilon] + \frac{\partial}{\partial x_i} \{ [3(p + \Pi) - 2\rho\varepsilon] v_i \} &= P_{ll}.
 \end{aligned} \tag{33}$$

Concerning the production term P_{ll} , the main problem is that, in order to have explicit expression of the production (see (24)), we need a model for the collision term, which is, in general, not easy to obtain in the case of polyatomic gases. In the case of a BGK model we have:

$$P_{ll} = -3\frac{\Pi}{\tau}.$$

The system (33) with the thermal and caloric equations of state (27) is a closed system for the 6 unknowns (ρ, v_i, T, Π) , provided that we know the collision term in (33)₄. These results are in perfect agreement with the results derived from the phenomenological theory [31]. The differential system is symmetric hyperbolic for any possible field and the bounded solutions satisfy automatically the inequalities (32).

6.4 Entropy Density and Main Field

Concerning the entropy density (16) it is possible to obtain the following explicit expression [34]:

$$\begin{aligned}
 k &= \frac{h - h^{\text{eq}}}{\rho} = \int_T^\Theta \frac{\varepsilon_I(T')}{T'^2} dT' + \frac{3k_B}{2m} \log(1 + Z) + \frac{\varepsilon_I(\Theta)}{\Theta} - \frac{\varepsilon_I(T)}{T} \\
 Z &= \frac{\Pi}{p} = \frac{\varepsilon_I(T) - \varepsilon_I(\Theta)}{\varepsilon_K(T)},
 \end{aligned} \tag{34}$$

where h^{eq} is the equilibrium entropy solution of the equilibrium Gibbs equation:

$$Td\left(\frac{h^{\text{eq}}}{\rho}\right) = d\varepsilon - \frac{p}{\rho^2}d\rho.$$

The function k is a convex function and have a global maximum at the equilibrium state. It is also interesting to see that expressions (34) coincide with those obtained by the phenomenological ET approach [31].

By using the results given in [34] with some algebra, it is possible to prove that the Lagrange multipliers have the following expressions:

$$\begin{aligned}\lambda &= -\frac{g}{T} + \int_T^\Theta \frac{\varepsilon_I(u)}{u^2} du - \frac{3k_B}{2m} \ln(1+Z) + \frac{v^2}{2T} \frac{1}{1+Z}, \\ \lambda_i &= -\frac{v_i}{T} \frac{1}{1+Z}, \\ \mu_{II} &= \frac{1}{2\Theta}, \\ \lambda_{II} &= -\frac{1}{2T} \left(\frac{1}{1+Z} - \frac{T}{\Theta} \right).\end{aligned}\tag{35}$$

According with the general theory, the Lagrange multipliers (35) coincide with the components of the main field for which the system (33) becomes to be symmetric hyperbolic in the form (17) [11, 12]. Notice that, in equilibrium where $\Pi = 0$ we have $Z = 0$ and $\Theta = T$ (see (34)₂), then the first five components of the main field (36) coincide with those obtained by Godunov for the Euler fluid [13]:

$$\lambda|_E = -\frac{1}{T} \left(g - \frac{v^2}{2} \right), \quad \lambda_i|_E = -\frac{v_i}{T}, \quad \mu_{II}|_E = \frac{1}{2T},$$

while $\lambda_{II}|_E = 0$ according to the fact that the Euler fluid is a *principal subsystem* of the 6-moment system. In the polytropic case,

$$\varepsilon_I(u) = \frac{D-3}{2} \frac{k_B}{m} u$$

and the expression (34) become the ones obtained in [32]:

$$k = \frac{k_B \rho}{2m} \ln \left((1+Z)^3 \left(1 - \frac{3}{D-3} Z \right)^{D-3} \right), \quad Z = \frac{\Pi}{p},$$

and the main field reduces to

$$\begin{aligned}\lambda &= -\frac{g}{T} + k + \frac{v^2}{2T} \frac{1}{1+Z}, \quad \lambda_i = -\frac{v_i}{T} \frac{1}{1+Z}, \quad \mu_{II} = \frac{1}{2T} \left(1 - \frac{3}{D-3} Z \right)^{-1}, \\ \lambda_{II} &= -\frac{1}{2T} \frac{D}{D-3} Z (1+Z)^{-1} \left(1 - \frac{3}{D-3} Z \right)^{-1}.\end{aligned}\tag{36}$$

7 Comparison Between the ET6 Theory and Meixner's Theory

The field equations (33) with the linear production can be rewritten by using the material derivative in the following simple form [12]:

$$\begin{aligned}
 \dot{\rho} + \rho \operatorname{div} \mathbf{v} &= 0, \\
 \rho \dot{v}_i + \frac{\partial}{\partial x_i} (p + \Pi) &= 0, \\
 \rho \dot{\varepsilon} + (p + \Pi) \operatorname{div} \mathbf{v} &= 0, \\
 \tau \dot{\Pi} + \left(\nu + \tau \frac{5D - 6}{3D} \Pi \right) \operatorname{div} \mathbf{v} &= -\Pi,
 \end{aligned} \tag{37}$$

where the bulk viscosity $\nu \propto D - 3$. When $D \rightarrow 3$ (monatomic gas) the previous system has the same solution as that of the Euler fluid provided $\Pi(\mathbf{x}, 0) = 0$ [12]. In [12, 30, 31] it was proved that the system (37) coincides with the well-known Meixner theory with one internal variable [35, 36] and the hidden variable is strictly related to the dynamical pressure Π .

Finally we note that, in the parabolic limit case where $\tau \rightarrow 0$, the system (37) reduces to a simplified version of Navier-Stokes system for compressible fluids:

$$\begin{aligned}
 \dot{\rho} + \rho \operatorname{div} \mathbf{v} &= 0, \\
 \rho \dot{v}_i + \frac{\partial}{\partial x_i} (p + \Pi) &= 0, \\
 \rho \dot{\varepsilon} + (p + \Pi) \operatorname{div} \mathbf{v} &= 0, \\
 \nu \operatorname{div} \mathbf{v} &= -\Pi,
 \end{aligned}$$

and the qualitative analysis of this parabolic system was studied in same papers, e.g. in [37, 38].

8 Qualitative Analysis

In the general theory of hyperbolic conservation laws and hyperbolic-parabolic conservation laws, the existence of a strictly convex entropy function, which is a generalization of the physical entropy, is a basic condition for the well-posedness. However, in the general case, and even for arbitrarily small and smooth initial data, there is no global continuation for these smooth solutions, which may develop singularities, shocks, or blow up in finite time, see for instance [39].

On the other hand, in many physical examples, thanks to the interplay between the dissipation due to the source term and the hyperbolicity there exist global smooth solutions for a suitable set of initial data.

In physical dissipative case, the hyperbolic systems are of mixed type, some equations are conservation laws and other ones are real balance laws, i.e., we are in the case in which

$$\mathbf{u}_t + \partial_i \mathbf{F}^i(\mathbf{u}) = \mathbf{F}(\mathbf{u})$$

with

$$\mathbf{F}(\mathbf{u}) \equiv \begin{pmatrix} 0 \\ \mathbf{g}(\mathbf{u}) \end{pmatrix}; \quad \mathbf{g} \in \mathbb{R}^{N-M}.$$

In this case the coupling condition, which is discovered for the first time by Kawashima and Shizuta (K-condition) [40] such that the dissipation in the second block has an effect also on the first block of equation, plays a very important role in this case for the global existence of smooth solutions.

In fact, if the system of balance law is endowed with a convex entropy law, and it is dissipative, then the K-condition becomes a sufficient condition for the existence of global smooth solutions provided that the initial data are sufficiently smooth (Hanouzet and Natalini [41], Wen-An Yong [42], Bianchini, Hanouzet and Natalini [43]):

Theorem 4 (Global Existence) *Assume that the system of balance laws is strictly dissipative and the K-condition is satisfied. Then there exists $\delta > 0$, such that, if $\|\mathbf{u}(x, 0)\|_2 \leq \delta$, there is a unique global smooth solution, which verifies*

$$\mathbf{u} \in C^0([0, \infty); H^2(\mathbb{R}) \cap C^1([0, \infty); H^1(\mathbb{R})).$$

Moreover Ruggeri and Serre [44] proved in the one-dimensional case that the constant states are stable:

Theorem 5 (Stability of Constant State) *Under natural hypotheses of strongly convex entropy, strict dissipativeness, genuine coupling and “zero mass” initial for the perturbation of the equilibrium variables, the constant solution stabilizes*

$$\|\mathbf{u}(t)\|_2 = O(t^{-1/2}).$$

Lou and Ruggeri [45] observed that the weaker K-condition in which we require the K-condition only for the right eigenvectors corresponding to genuine nonlinear is a necessary (but not sufficient) condition for the global existence of smooth solutions. In [12, 32, 46] it was proved that ET theories satisfy the hypothesis of the previous theorems and therefore there exist global solutions provided initial data are sufficiently smooth.

9 Shock Wave Structure in a Rarefied Polyatomic Gas

As an application of the previous thermodynamic models, let us consider a shock wave propagating in a polyatomic gas. The shock wave structure in a rarefied polyatomic gas is, under some conditions, quite different from the shock wave structure in a rarefied monatomic gas due to the presence of the microscopic internal modes in a polyatomic molecule such as the rotational and vibrational modes. For examples: (1) The shock wave thickness in a rarefied monatomic gas is of the order of the mean free path. On the other hand, owing to the slow relaxation process involving the internal modes, the thickness of a shock wave in a rarefied polyatomic gas is several orders larger than the mean free path. (2) As the Mach number increases from unity, the profile of the shock wave structure in a polyatomic rarefied gas changes from the nearly symmetric profile (Type A) to the asymmetric profile (Type B), and then changes further to the profile composed of thin and thick layers (Type C)

Schematic profiles of the mass density are shown in Fig. 1. Such change of the shock wave profile with the Mach number cannot be observed in a monatomic gas. In order to explain the shock wave structure in a rarefied polyatomic gas, there have been two well-known approaches. One was proposed by Bethe and Teller and the other is proposed by Gilbarg and Paolucci. Although the Bethe-Teller theory can describe qualitatively the shock wave structure of Type C, its theoretical basis is not clear enough. The Gilbarg-Paolucci theory, on the other hand, cannot explain asymmetric shock wave structure (Type B) nor thin layer (Type C).

Recently it was shown that the ET_{14} [47] and also ET_6 [48] theories can describe the shock wave structure of all Types A to C in a rarefied polyatomic gas. This new result indicates clearly the usefulness of the ET theory for the analysis of shock wave phenomena.

Other interesting and successful applications of RET in polyatomic gas show good agreement with experiments concerning the dispersion relation in the high frequency limit, and in the light scattering problem (see [12] and reference therein).

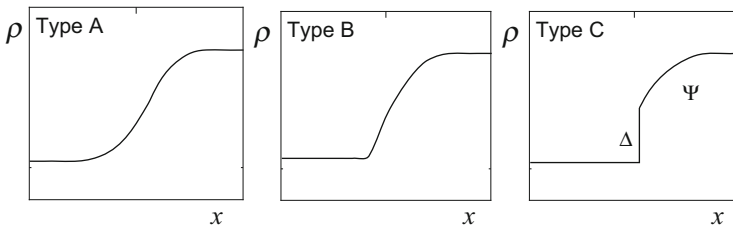


Fig. 1 Schematic representation of three types of the shock wave structure in a rarefied polyatomic gas, where ρ and x are the mass density and the position, respectively. As the Mach number increases from unity, the profile of the shock wave structure changes from Type A to Type B, and then to Type C that consists of the thin layer Φ and the thick layer Ψ

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