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# Mesoscopic approach to inviscid gas dynamics with thermal lag

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A phenomenological model for thermal relaxation and wave propagation in ideal polyatomic gases is developed by introducing a dynamical non-equilibrium temperature. The system of equations governing the evolution of the gas is derived and the speeds of propagation of thermo-mechanical disturbances together with the Rankine-Hugoniot jump conditions for shock waves are calculated. The hyperbolic theories of heat propagation in incompressible fluids and rigid solids are recovered as particular cases. For rigid solids, the well posedness of the Cauchy problem is proved by a classical method.

## 1 Introduction

The field equations of the inviscid gas dynamics are derived under the assumption that the heat flux is zero. Thus, wave propagation through the fluid may occur. Relaxing this hypothesis by the Fourier constitutive equation, waves are damped and the theory becomes parabolic. On the other hand, for several systems as, for instance, ideal polyatomic gases, a time lag in the temperature, due to the adjustment of the internal degrees of freedom, is expected [1]. Several different proposals for modeling this memory effect may be found in the literature [2]. Among them, the most celebrated one is the Maxwell-Cattaneo-Vernotte (MCV) equation [3]

$$\tau \dot{q}_i + q_i = -\kappa \vartheta_{,i}, \quad (1)$$

where  $\tau$  is a suitable relaxation time,  $\kappa$  is the heat conductivity,  $q_i$  are the components of the heat flux, and  $\vartheta$  is the absolute temperature.

In gas dynamics, the equation above is needed to achieve a satisfactory analysis of shock wave profile within the frame of the Navier-Stokes models with strong anisotropy in the temperature, which predict a shock width greater than expected [4]. Thus, additional dissipation is required. Eq. (1) is capable to provide such a dissipation and, meantime, allows the description to re-

main at a macroscopic level, with recourse neither to higher-order expansions of the fluxes nor to more complex methods of solution of the Boltzmann equation [4]. The results agree with non equilibrium molecular dynamics simulations in the ideal gas regime, that goes beyond Navier-Stokes and improves the prediction of the shockwave thickness [4].

In earlier and recent works [6–12], heat conduction with finite speed has been modeled by introducing a dynamical temperature as internal variable, related to the absolute temperature by a suitable evolution equation. The material functions relative to the model are determined through second sound measurements [7, 8]. Two different experiments allowing to measure this dynamical temperature and to compare it with the classical absolute temperature, have been designed and proposed in [9, 12]. Indeed, the temperature represents a basic concept in thermodynamics, and it is the topic of several discussions, since its definition and measurement in non-equilibrium situations is not yet fully understood. In steady states it is different from the local-equilibrium temperature  $\vartheta$  and, in ideal gases, it corresponds to the kinetic temperature in the directions perpendicular to the heat flux [13, 14]. The reason for introducing a non-equilibrium temperature is that the local-equilibrium temperature loses its validity in situations where the deviation from equilibrium ensemble is not negligible. Therefore, for a better understanding of temperature in non-equilibrium states, the exploration of the consequences of the introduction of dynamical temperatures in heat transport may be very useful. Let's refer the reader to Refs. [13, 14] for an extensive analysis of the concept of temperature in non-equilibrium situations.

The present paper is concerned with the thermodynamic modeling of ideal polyatomic gases, with special attention to the heat conduction phenomenon with

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finite thermal wave speed. For the sake of simplicity, we suppose that the mechanical relaxation effects are negligible, limiting ourselves to take into account only the thermal ones.

In Sec. 2, a non-equilibrium temperature is defined by phenomenological considerations on the motion of the molecules constituting the gas. A differential equation governing its evolution is derived as well. That way, we obtain a mapping between the material parameters entering the kinetic theory of gases and those entering the macroscopic Cattaneo theory. In this paper we will be content to this connection, although more sophisticated relations between different theories may be established. For a detailed discussion of the connections between Peierls kinetic theory of phonons, Cattaneo-like extensions of the Fourier theory, Fourier theory, and the equilibrium theory, let's refer the reader to Ref. [15].

At a first sight our approach could appear unusual, since classical kinetic theory expansions [5] or phenomenological methods [2] give rather similar results in the framework of a uniform approach. However, the first ones, although rigorous, are not immediately intuitive, and require complex mathematical tools. The second ones, instead, although more close to the experimental evidence, often disregard the mechanism of heat conduction at a molecular level. Thus, the present approach aims to analyze the problem from a mesoscopic point of view, giving a deeper insight at the molecular level but still obtaining manageable model equations at the macroscopic level.

In Sec. 3, a constitutive theory is developed in the framework of weakly nonlocal thermodynamics. The response functions are permitted to depend on the gradients of the unknown fields [16]. As result, we show that the free energy can be decoupled in the sum of a classical equilibrium part, which represents the free energy in the absence of heat flux, and a nonequilibrium one, which depends on the heat flux too. The same decomposition is true for entropy, stress and internal energy.

In Sec. 4, the complete set of field equations governing the evolution of mass density, gas velocity and non-equilibrium temperature is carried out. To engage our equations to the experimental data, we use typical fitting curves modeling the specific heat of polyatomic gases at constant pressure.

In Sec. 5, the propagation of thermo-mechanical disturbances is studied. It is proved that the theory is hyperbolic for arbitrary values of the temperature. The Rankine-Hugoniot jump conditions on a shock front are

derived as well and the fields behind the shock are obtained as functions of those ahead the shock.

In Sec. 6, heat wave propagation in a fluid at rest is analyzed. The theory of rigid heat conductors is recovered as a particular case and the well posedness of the Cauchy problem is proved by a classical method, which consists in proving that the system of governing equations can be put in symmetric hyperbolic form.

In Sec. 7 we append some concluding remarks on the results obtained and on the possible developments of the present theory.

## 2 Dynamical non-equilibrium temperature

In this section, in order to define a non equilibrium dynamical temperature, we apply the method introduced by Cattaneo [3] for the analysis of the heat flux in gases. Thus, following the path paved in [3], let us consider a moving gas not in thermodynamic equilibrium and let  $Q$  the kinetic energy carried by each molecule of the gas and  $G$  the average of  $Q$  in a point  $P$  of the gas. For the sake of simplicity, let us assume  $G$  constant with respect to its spatial variables on each of the planes which are orthogonal to a given direction  $x$ . Hence

$$G = G(x, t).$$

Finally, we explicitly suppose that the thermodynamic state of the gas is not far from the equilibrium.

Let  $dN_c$  mean the number of molecules per unit of volume passing in the time interval  $dt$  across the unit area  $\omega$  of the plane  $x = x_0$ , whose velocity is in the interval  $[c, c + dc]$ . Moreover, let us denote by  $dn_{c\Theta}$  the fraction of  $dN_c$  of molecules moving along a given direction  $r$  forming with  $x$  a solid angle  $\Theta$ . It is easily seen that these molecules are contained in an oblique cylinder having base  $\omega$ , inclination  $\Theta$  and length  $c dt$ , so that

$$dn_{c\Theta} = \frac{c}{2} \sin\Theta \cos\Theta \, d\Theta \, dt \, dN_c. \quad (2)$$

Let us focus our attention on a single molecule running a free path of length  $\ell$  under an angle  $\Theta$  with respect to  $x$  and crossing  $\omega$  at the instant  $t' \in [t, t + dt]$ , with velocity  $v \in [c, c + dc]$ . The function  $G^+(x, t)$ , where the up-script + means that the molecule runs along the positive direction of  $x$ , can be expressed as a power series of  $x - x_0$  and

$t - t'$ . Up to the second-order approximation we have

$$\begin{aligned}
 G^+(x, t) = & G(x_0, t') + \frac{\partial G}{\partial x}(x_0, t')(x - x_0) \\
 & + \frac{\partial G}{\partial t}(x_0, t')(t - t') + v \frac{\partial G}{\partial x}(x_0, t')(t - t') \\
 & + \frac{1}{2} \frac{\partial^2 G}{\partial x^2}(x_0, t')(x - x_0)^2 + \frac{1}{2} \frac{\partial^2 G}{\partial t^2}(x_0, t')(t - t')^2 \\
 & + \frac{\partial^2 G}{\partial x \partial t}(x_0, t')(x - x_0)(t - t') \\
 & + v \frac{\partial^2 G}{\partial x^2}(x_0, t')(t - t')(x - x_0) \\
 & + \frac{\partial v}{\partial x} \frac{\partial G}{\partial x}(x_0, t')(t - t')(x - x_0) \\
 & + v \frac{\partial^2 G}{\partial x \partial t}(x_0, t')(t - t')^2 + \frac{\partial v}{\partial t} \frac{\partial G}{\partial x}(x_0, t')(t - t')^2 \\
 & + v^2 \frac{\partial^2 G}{\partial x^2}(x_0, t')(t - t')^2. \quad (3)
 \end{aligned}$$

A similar expression may be obtained for  $G^-(x, t)$ , once we take into account that, in this case, the spatial derivatives of  $G$  and  $v$  change their sign. Thus we get

$$\begin{aligned}
 G^-(x, t) = & G(x_0, t') - \frac{\partial G}{\partial x}(x_0, t')(x - x_0) \\
 & + \frac{\partial G}{\partial t}(x_0, t')(t - t') - v \frac{\partial G}{\partial x}(x_0, t')(t - t') \\
 & + \frac{1}{2} \frac{\partial^2 G}{\partial x^2}(x_0, t')(x - x_0)^2 + \frac{1}{2} \frac{\partial^2 G}{\partial t^2}(x_0, t')(t - t')^2 \\
 & - \frac{\partial^2 G}{\partial x \partial t}(x_0, t')(x - x_0)(t - t') \\
 & + v \frac{\partial^2 G}{\partial x^2}(x_0, t')(t - t')(x - x_0) \\
 & + \frac{\partial v}{\partial x} \frac{\partial G}{\partial x}(x_0, t')(t - t')(x - x_0) \\
 & - v \frac{\partial^2 G}{\partial x \partial t}(x_0, t')(t - t')^2 - \frac{\partial v}{\partial t} \frac{\partial G}{\partial x}(x_0, t')(t - t')^2 \\
 & + v^2 \frac{\partial^2 G}{\partial x^2}(x_0, t')(t - t')^2. \quad (4)
 \end{aligned}$$

In order to obtain meaningful expressions for the relations above, one should take into account that for the molecules running in the positive direction the last collision has taken place on the plane

$$x = x_0 - \ell \cos \Theta - v \frac{\ell}{c},$$

at the time

$$t = t' - \frac{\ell}{c},$$

while the molecules running along the negative direction undergo the last collision at the same time but on the plane

$$x = x_0 + \ell \cos \Theta - v \frac{\ell}{c}.$$

Then we get

$$\begin{aligned}
 G^+(x, t) = & G(x_0, t') - \frac{\partial G}{\partial x}(x_0, t') \left( \ell \cos \Theta + v \frac{\ell}{c} \right) \\
 & - \frac{\partial G}{\partial t}(x_0, t') \frac{\ell}{c} - v \frac{\partial G}{\partial x}(x_0, t') \frac{\ell}{c} \\
 & + \frac{1}{2} \frac{\partial^2 G}{\partial x^2}(x_0, t') \left( \ell \cos \Theta + v \frac{\ell}{c} \right)^2 \\
 & + \frac{1}{2} \frac{\partial^2 G}{\partial t^2}(x_0, t') \left( \frac{\ell}{c} \right)^2 \\
 & + \frac{\partial^2 G}{\partial x \partial t}(x_0, t') \left( \frac{\ell^2 \cos \Theta}{c^2} + v \frac{\ell^2}{c^2} \right) \\
 & + v \frac{\partial^2 G}{\partial x^2}(x_0, t') \left( \frac{\ell^2 \cos \Theta}{c^2} + v \frac{\ell^2}{c^2} \right) \\
 & + \frac{\partial v}{\partial x} \frac{\partial G}{\partial x}(x_0, t') \left( \frac{\ell^2 \cos \Theta}{c^2} + v \frac{\ell^2}{c^2} \right) \\
 & + v \frac{\partial^2 G}{\partial x \partial t}(x_0, t') \left( \frac{\ell}{c} \right)^2 + \frac{\partial v}{\partial t} \frac{\partial G}{\partial x}(x_0, t') \left( \frac{\ell}{c} \right)^2 \\
 & + v^2 \frac{\partial^2 G}{\partial x^2}(x_0, t') \left( \frac{\ell}{c} \right)^2, \quad (5)
 \end{aligned}$$

$$\begin{aligned}
 G^-(x, t) = & G(x_0, t') - \frac{\partial G}{\partial x}(x_0, t') \left( \ell \cos \Theta - v \frac{\ell}{c} \right) \\
 & - \frac{\partial G}{\partial t}(x_0, t') \frac{\ell}{c} - v \frac{\partial G}{\partial x}(x_0, t') \frac{\ell}{c} \\
 & + \frac{1}{2} \frac{\partial^2 G}{\partial x^2}(x_0, t') \left( \ell \cos \Theta - v \frac{\ell}{c} \right)^2 \\
 & + \frac{1}{2} \frac{\partial^2 G}{\partial t^2}(x_0, t') \left( \frac{\ell}{c} \right)^2 \\
 & + \frac{\partial^2 G}{\partial x \partial t}(x_0, t') \left( - \frac{\ell^2 \cos \Theta}{c^2} + v \frac{\ell^2}{c^2} \right) \\
 & + v \frac{\partial^2 G}{\partial x^2}(x_0, t') \left( - \frac{\ell^2 \cos \Theta}{c^2} + v \frac{\ell^2}{c^2} \right) \\
 & + \frac{\partial v}{\partial x} \frac{\partial G}{\partial x}(x_0, t') \left( - \frac{\ell^2 \cos \Theta}{c^2} + v \frac{\ell^2}{c^2} \right) \\
 & + v \frac{\partial^2 G}{\partial x \partial t}(x_0, t') \left( \frac{\ell}{c} \right)^2 + \frac{\partial v}{\partial t} \frac{\partial G}{\partial x}(x_0, t') \left( \frac{\ell}{c} \right)^2 \\
 & + v^2 \frac{\partial^2 G}{\partial x^2}(x_0, t') \left( \frac{\ell}{c} \right)^2. \quad (6)
 \end{aligned}$$

The net amount of  $G$  carried by all the molecules of the type considered is given by the difference

$\sum' G^+(x, t) - \sum' G^-(x, t)$ , where the prime indicates that the sum is extended to the molecules of the type considered above, only. To calculate such a sum we use a result by Boltzmann [17], namely  $\sum' \ell \approx \lambda_c dn_{c\Theta}$  and  $\sum' \ell^2 \approx \ell_c^2 dn_{c\Theta}$ , where  $\lambda_c$  and  $\ell_c^2$  are the mean free path and the squared mean free path of the molecules, respectively. Finally, we obtain

$$\begin{aligned} & \sum' G^+(x, t) - \sum' G^-(x, t) \\ &= \left[ 2 \frac{\partial G}{\partial x}(x_0, t') \lambda_c \cos \Theta + \frac{\partial^2 G}{\partial x \partial t}(x_0, t') \left( \frac{\ell^2}{c} \right) \cos \Theta \right. \\ & \quad + 2 \nu_c \frac{\partial^2 G}{\partial x^2}(x_0, t') \left( \frac{\ell^2}{c} \right) \cos \Theta + 2 \nu_c \frac{\partial^2 G}{\partial x \partial t}(x_0, t') \left( \frac{\ell}{c} \right)^2 \\ & \quad \left. + 2 \frac{\partial \nu_c}{\partial t} \frac{\partial G}{\partial x}(x_0, t') \left( \frac{\ell}{c} \right)^2 + 2 \nu_c^2 \frac{\partial^2 G}{\partial x^2}(x_0, t') \left( \frac{\ell}{c} \right)^2 \right] dn_{c\Theta}, \end{aligned} \quad (7)$$

where  $\nu_c$  denotes the mean speed of the molecules having velocity in the interval  $[c, c + dc]$ .

In order to derive from (7) the flux of  $Q$  across  $\omega$ , let call it  $dq_c$ , we must divide Eq. (7) by  $dt$  and then integrate the obtained expression on the interval  $[0, \frac{\pi}{2}]$ . It is immediately seen that the last three terms in (7) do not contribute to  $dq_c$ , due to the form (1) of  $dn_{c\Theta}$ . The first three terms, instead, may be easily integrated and yield

$$dq_c = \left[ \left( -c \frac{\lambda_c}{3} \right) \frac{\partial G}{\partial x} + \left( \frac{\ell_c^2}{3} \right) \frac{\partial^2 G}{\partial x \partial t} + \left( \nu_c \frac{\ell_c^2}{3} \right) \frac{\partial^2 G}{\partial x^2} \right] dN_c. \quad (8)$$

Let us observe that, being  $(x_0, t')$  arbitrary, we have omitted such a dependency in (8). Integration of (8) in the interval  $[c = 0, c = \infty]$  yields the total flux of  $Q$  across  $\omega$  as

$$q = -\kappa \frac{\partial \vartheta}{\partial x} + \sigma \frac{\partial^2 \vartheta}{\partial x \partial t} + \nu \sigma \frac{\partial^2 \vartheta}{\partial x^2}, \quad (9)$$

with  $G = \frac{3}{2} k_B \vartheta$ ,

$$\kappa = \int_0^\infty \frac{\lambda_c c k_B}{2} dN_c, \quad (10)$$

$$\sigma = \int_0^\infty \frac{\ell_c^2 k_B}{2} dN_c, \quad (11)$$

and  $\nu$  as the mean speed of all the molecules passing across the plane  $x$  at the time  $t$ , which may be identified with the velocity of the fluid in the point  $(x, t)$ .

Eq. (9) may be also written as

$$q = -\kappa \frac{\partial}{\partial x} \left( \vartheta - \frac{\sigma}{\kappa} \dot{\vartheta} \right), \quad (12)$$

where  $\dot{\vartheta} = \frac{\partial \vartheta}{\partial t} + \nu \frac{\partial \vartheta}{\partial x}$  denotes the convective time derivative. Thus, if we define a dynamical temperature  $\beta$  as

$$\beta = \vartheta - \frac{\sigma}{\kappa} \dot{\vartheta}, \quad (13)$$

Eq. (12) takes the Fourier's form

$$q = -\kappa \frac{\partial \beta}{\partial x}. \quad (14)$$

The second term in the RHS of Eq. (13) is a viscous term due to the Van der Waals forces between the molecules. It results in a delay in the propagation of temperature disturbances, allowing for finite speed. To prove that, let's observe that the combination of (12) with its time derivative yields

$$\tau \dot{\beta} + \beta = \vartheta - \tau^2 \ddot{\vartheta}, \quad (15)$$

with  $\tau = \frac{\sigma}{\kappa}$ . In order to evaluate the last term in the RHS of (15), let's recall that;

- the gas is in quasi-equilibrium;
- as first recognized by Cattaneo [3],  $\tau$  is very small.

From the mathematical point of view, both the circumstances above may be expressed by admitting that, if  $f$  is a physical quantity related to the heat conduction, the ratio  $|\tau \dot{f}/f|$  is a first-order quantity and the second-order quantities are negligible [3]. Under the previous hypothesis, we may compare the order of magnitude of  $\tau^2 \ddot{\vartheta}$  with that of  $\vartheta$  by observing that [3]

$$|\tau^2 \ddot{\vartheta}/\vartheta| = |\tau \ddot{\vartheta}/\dot{\vartheta}| |\tau \dot{\vartheta}/\vartheta|,$$

which proves that  $\tau^2 \ddot{\vartheta}$  is a second-order quantity. Neglecting it, the evolution of  $\beta$  is governed by the linear differential equation

$$\tau \dot{\beta} + \beta = \vartheta, \quad (16)$$

where  $\tau$  may be interpreted as a relaxation time. For vanishing  $\tau$  the dynamical temperature reduces to the absolute one. Taking the spatial derivative of Eq. (16), and multiplying it by  $-\kappa$ , one obtains the following evolution equation for the heat flux

$$\tau \dot{q} + q \left( 1 + \tau \frac{\partial \nu}{\partial x} \right) = -\kappa \frac{\partial \vartheta}{\partial x}. \quad (17)$$

It reduces to the classical Cattaneo's equation (1) for fluids at rest.

### 3 Constitutive theory

Let  $\mathcal{B}$  be a continuous body occupying a compact and simply connected region  $\mathcal{C}$  of a Euclidean point space  $E^3$ .  $\mathcal{B}$  will be supposed to be endowed with some internal properties, described by a scalar  $\beta \in \mathbb{R}$  whose evolution is governed by the differential equation (16).

Beside Eq. (16), we need to consider the equations governing the balance of mass, linear momentum and energy, namely

$$\dot{\rho} + \rho \operatorname{div} \mathbf{v} = 0, \quad (18)$$

$$\rho \dot{\mathbf{v}} - \operatorname{div} \mathbf{T} = 0, \quad (19)$$

$$\rho \dot{\varepsilon} - \mathbf{T} : \mathbf{L} + \operatorname{div} \mathbf{q} = 0, \quad (20)$$

where  $\rho$  is the mass density,  $\varepsilon$  is the specific internal energy,  $\mathbf{T}$  the Cauchy stress,  $\mathbf{L} = \operatorname{grad} \mathbf{v}$  and  $\mathbf{q}$  the heat flux. Moreover, hereafter, a double dot between two tensors denotes the full saturation, giving a scalar as result. For the sake of simplicity, we have assumed that body force and heat supply are zero. The entropy inequality is postulated in the form

$$\rho \dot{s} + \operatorname{div} \frac{\mathbf{q}}{\vartheta} \geq 0, \quad (21)$$

where  $s$  denotes the specific entropy. Note that the entropy flux has been taken in the classical form postulated in rational thermodynamics [18], namely  $\frac{\mathbf{q}}{\vartheta}$ . Although more general expressions for the entropy flux are possible in nonlocal theories [2, 16], we will show that this simple constitutive hypothesis allows to obtain a satisfactory modeling of thermal relaxation.

By the Legendre transformation

$$\psi = \varepsilon - \vartheta s, \quad (22)$$

with  $\psi$  as the Helmholtz free energy, once the balance of energy (20) has been taken into account, the inequality (21) can be rearranged as follows

$$-\rho \dot{\psi} - \rho s \dot{\vartheta} + \mathbf{T} : \mathbf{L} - \frac{1}{\vartheta} \mathbf{q} \cdot \operatorname{grad} \vartheta \geq 0. \quad (23)$$

Second Law of Thermodynamics demands that the inequality above is satisfied along arbitrary thermodynamic processes [19, 20]. To exploit this unilateral differential constraint, we have to define the state space. To this end let us recall that we are modelling a rarefied

gas, where the mechanical relaxation effects are negligible but not the thermal ones. Hence, since both viscous and nonlocal mechanical effects are negligible, it is not necessary that the gradients of the mass density and of the fluid velocity enter the state space. On the other hand, the results in Sec. 2 show that the nonlocal thermal effects are important and that the vectorial internal variable  $\operatorname{grad} \beta$  is suitable to represent them. Thus, we postulate the following state space

$$\mathcal{Z} = \{\rho, \vartheta, \operatorname{grad} \beta\}. \quad (24)$$

It is worth observing that the substitution of  $\operatorname{grad} \vartheta$  by a vectorial internal variable proportional to the heat flux is very common in hyperbolic heat conduction theory [2]. The difference of this approach with respect to the other ones is that we provide a physical interpretation of this new variable, as the gradient of the non equilibrium temperature. The relation between this non equilibrium temperature and the classical absolute temperature has been pointed out in [10], while two experiments which could allow to measure the difference between absolute and dynamical temperature have been proposed in [9, 12]. In order to engage our model to the experiments, in the present paper we will limit to consider the simpler case in which only  $\vartheta$  enters the state space. In fact, as it will be shown in the next section, the experimental data for the transport coefficients are all expressed as functions of  $\vartheta$ . It is worth noticing that a state space spanned by the dynamical temperature and a renormalized flux variable has been studied in Ref. [12], with the scope of designing an experiment for the comparison of the dynamical temperature with the absolute one. On the other hand, if  $\mathcal{Z}$  would contain  $\operatorname{grad} \vartheta$  too, then the theory of representation of isotropic vector functions depending on scalars and vectors [21], would lead to the following constitutive equation for the heat flux

$$\mathbf{q} = -\kappa_1 \operatorname{grad} \beta - \kappa_2 \operatorname{grad} \vartheta, \quad (25)$$

with  $\kappa_1$  and  $\kappa_2$  depending on  $\rho$ ,  $\vartheta$ , and on the modulus of both gradients. The consequences of Eq. (25) have been studied in [22], where it is showed that the model would be still parabolic. The system (16) and (18)–(20) may be closed by assigning suitable constitutive equations for  $\varepsilon$ ,  $\mathbf{T}$  and  $\mathbf{q}$ , as functions of the elements of  $\mathcal{Z}$ . Moreover, an additional constitutive equation for  $\psi$  is necessary to carry out the consequences of the entropy inequality



(23). In this way, Eq. (23) reads

$$-\rho \left( \frac{\partial \psi}{\partial \vartheta} + s \right) \dot{\vartheta} - \rho \frac{\partial \psi}{\partial \rho} \dot{\rho} - \rho \frac{\partial \psi}{\partial \text{grad} \beta} \cdot \overline{\text{grad} \beta} + \mathbf{T} : \mathbf{L} - \frac{1}{\vartheta} \mathbf{q} \cdot \text{grad} \vartheta \geq 0. \quad (26)$$

The inequality above, often referred to as Clausius-Duhem inequality [23], will be exploited by a generalization of the classical Coleman-Noll procedure, which has been proposed by Cimmelli and co-workers in recent papers [24, 25]. This technique for the exploitation of the Entropy Principle is based on the observation that the less restrictive conditions ensuring the fulfillment of Second Law of Thermodynamics are obtained when the number of equations constraining the entropy inequality and that of the independent variables entering the state space coincide [26]. The technique can be applied by substituting into the entropy inequality the field equations and the equations governing the evolution of the spatial gradients entering the state space, hereafter called *extended balance equations*. That way, one obtains an *extended Coleman-Noll inequality*, which is linear in the time derivatives which can not be expressed as functions of the elements of the state space and in the gradients which are two orders higher than the gradients in the state space. These time and space derivatives are called *highest derivatives*.

Note that, in deriving (26), the local balance of energy has been already taken into account, so that we must only consider the local balance of mass and the governing equation of  $\text{grad} \beta$ , which reads

$$\overline{\text{grad} \beta} = \frac{1}{\tau} \text{grad} \vartheta - \frac{1}{\tau} \text{grad} \beta - \text{grad} \beta \mathbf{L}. \quad (27)$$

Such an equation may be inserted into Eq. (26), so that the gradient of  $\vartheta$  therein can be eliminated.

Thus, if we use the constitutive equation

$$\mathbf{q} = -\kappa \text{grad} \beta, \quad (28)$$

proved in Sec. 2, once the Eqs. (18) and (27) have been taken into account, the Clausius-Duhem inequality takes the form

$$-\rho \left( \frac{\partial \psi}{\partial \vartheta} + s \right) \dot{\vartheta} + \left( \rho^2 \frac{\partial \psi}{\partial \rho} \mathbf{I} + \frac{\kappa \tau}{\vartheta} \text{grad} \beta \otimes \text{grad} \beta + \mathbf{T} \right) : \mathbf{L} - \left( \rho \frac{\partial \psi}{\partial \text{grad} \beta} - \frac{\kappa \tau}{\vartheta} \text{grad} \beta \right) \cdot \overline{\text{grad} \beta} + \frac{\kappa}{\vartheta} \text{grad} \beta^2 \geq 0. \quad (29)$$

The expression above is linear in the highest derivatives  $\{\dot{\vartheta}, \mathbf{L}, \overline{\text{grad} \beta}\}$ . These quantities are independent of their coefficients which, instead, depend on the elements of the state space only. Moreover, they may assume arbitrary and uncontrollable values. Hence, their coefficients must vanish, otherwise the inequality could be easily violated. Thus, we are led to the following set of thermodynamic restrictions

$$s = -\frac{\partial \psi}{\partial \vartheta}, \quad (30)$$

$$\mathbf{T} = -\rho^2 \frac{\partial \psi}{\partial \rho} \mathbf{I} - \frac{\kappa \tau}{\vartheta} \text{grad} \beta \otimes \text{grad} \beta, \quad (31)$$

$$\frac{\partial \psi}{\partial \text{grad} \beta} = \frac{\kappa \tau}{\rho \vartheta} \text{grad} \beta, \quad (32)$$

$$\frac{\kappa}{\vartheta} \text{grad} \beta^2 \geq 0. \quad (33)$$

Since for perfect gases the heat conduction coefficient depends on the temperature only, from the relationship (32) we get

$$\psi = \psi_0(\rho, \vartheta) + \frac{\tau}{2\rho\kappa\vartheta} \mathbf{q} \cdot \mathbf{q}. \quad (34)$$

Eq. (34) shows that the free energy can be decoupled in the sum of a classical equilibrium part, namely  $\psi_0(\rho, \vartheta)$ , which represents the free energy in the absence of heat flux, and a nonequilibrium one, which depends on the heat flux too. The same decomposition is true for entropy, stress and internal energy, since the relationships (30), (31), and (22) yield

$$s = -\frac{\partial \psi_0}{\partial \vartheta} + \left( \frac{\tau}{2\rho\kappa\vartheta^2} + \frac{\frac{d\kappa}{d\vartheta}\tau}{2\rho\kappa^2\vartheta} \right) \mathbf{q} \cdot \mathbf{q}, \quad (35)$$

$$\mathbf{T} = -\rho^2 \frac{\partial \psi}{\partial \rho} \mathbf{I} - \frac{\tau}{\kappa\vartheta} \mathbf{q} \otimes \mathbf{q}, \quad (36)$$

$$\varepsilon = \varepsilon_0(\rho, \vartheta) + \frac{1}{2} \varepsilon_1(\rho, \vartheta) \mathbf{q} \cdot \mathbf{q}, \quad (37)$$

with

$$\varepsilon_0 = \psi_0 - \theta \frac{\partial \psi_0}{\partial \theta}, \quad (38)$$

and

$$\varepsilon_1 = \frac{2\tau}{\rho\kappa\vartheta} + \frac{\frac{d\kappa}{d\vartheta}\tau}{\rho\kappa^2}. \quad (39)$$

## 4 Governing equations

The present section is devoted to derive the field equations governing the evolution of a moving gas in the presence of heat conduction. For the sake of simplicity, let us assume that the gas is polyatomic [27]. Experiments at pressure below 2 atm. show a marked dependence of the specific heat on temperature [27]. Typical fitting curves yield the specific heat at constant pressure  $c_p$  in the form

$$c_p = Rc_0 + 2b\vartheta + 3c\vartheta^2, \quad (40)$$

with  $R$  as the universal constant of gases and  $c_0$ ,  $b$ ,  $c$  as positive material constants, with  $c_0 > 1$  [27]. From Meyer's equation  $c_v = c_p - R$  with  $c_v$  as the specific heat at a constant volume, we get

$$c_v = a + 2b\vartheta + 3c\vartheta^2, \quad (41)$$

with  $a = R(c_0 - 1)$ .

Since the specific heat is measured in quasi-static situations, we may suppose that in such a situation the heat flux is zero while the internal energy reduces to its equilibrium part  $\varepsilon_0 = \psi_0 - \vartheta \frac{\partial \psi_0}{\partial \vartheta}$ . Then, from the relation  $c_v = \frac{\partial \varepsilon_0}{\partial \vartheta}$  we get

$$\varepsilon_0 = a\vartheta + b\vartheta^2 + c\vartheta^3 + \varepsilon_0(\rho), \quad (42)$$

where  $\varepsilon_0(\rho)$  can be put equal to zero by imposing that the equilibrium internal energy vanishes at 0 K<sup>0</sup>. This constitutive equation has nontrivial consequences on the form of the free energy. To see that, let us observe that the first term in Eq. (36) is the spherical part of the stress tensor with  $\rho^2 \frac{\partial \psi_0}{\partial \rho}$  as the equilibrium pressure  $p_0(\rho, \vartheta)$ . If we assume for  $p_0$  the Clapeyron's constitutive equation

$$p_0 = \alpha\rho\vartheta, \quad (43)$$

with  $\alpha = R/m$ , and  $m$  molecular weight, we are led to the differential equation

$$\frac{\partial \psi_0}{\partial \rho} = \frac{\alpha\vartheta}{\rho}, \quad (44)$$

which yields

$$\psi_0(\rho, \vartheta) = \alpha\vartheta \log \rho + \varphi_0(\vartheta). \quad (45)$$

Finally, by (22), (42) and (45) it follows

$$\varphi_0 - \vartheta \frac{d\varphi_0}{d\vartheta} = a\vartheta + b\vartheta^2 + c\vartheta^3, \quad (46)$$

so that

$$\varphi_0 = -a\vartheta \log \vartheta - b\vartheta^2 - \frac{1}{2}c\vartheta^3. \quad (47)$$

Thus, owing to the results in Eqs. (28), (36) and (37), the balances of linear momentum and energy take the form

$$\begin{aligned} \rho \dot{\mathbf{v}} + \alpha \vartheta \operatorname{grad} \rho + \alpha \rho \operatorname{grad} \vartheta - \lambda' \tau (\operatorname{grad} \beta)^2 \operatorname{grad} \vartheta \\ + 2\lambda \tau \operatorname{grad} \beta \cdot \operatorname{grad}^2 \beta \\ + 2\lambda' \tau (\operatorname{grad} \vartheta \cdot \operatorname{grad} \beta) \operatorname{grad} \beta = 0, \end{aligned} \quad (48)$$

$$\begin{aligned} \rho c_v \dot{\vartheta} + \frac{1}{2} \rho \frac{\partial \varepsilon_1}{\partial \rho} \dot{\rho} (\operatorname{grad} \beta)^2 + \frac{1}{2} \rho \frac{\partial \varepsilon_1}{\partial \vartheta} \dot{\vartheta} (\operatorname{grad} \beta)^2 \\ + \rho \varepsilon_1 \operatorname{grad} \beta \cdot \overline{\operatorname{grad} \beta} - \kappa' \operatorname{grad} \vartheta \cdot \operatorname{grad} \beta - \kappa \Delta \beta \\ + \alpha \rho \vartheta \operatorname{div} \mathbf{v} - \lambda \tau (\operatorname{grad} \beta)^2 \operatorname{div} \mathbf{v} \\ + 2\lambda \tau (\operatorname{grad} \beta \otimes \operatorname{grad} \beta) : \operatorname{grad} \mathbf{v} = 0, \end{aligned} \quad (49)$$

wherein  $c_v$  takes the form (41),  $\varepsilon_1$  is given by (39),  $\lambda = \frac{\kappa}{2\vartheta}$ , and a prime denotes the derivative with respect to  $\vartheta$ .

The quantities  $\{\vartheta, \dot{\vartheta}, \operatorname{grad} \vartheta\}$  in the equations above can be eliminated owing to Eqs. (16) and (27). Then the system of Eqs. (18), (48) and (49) allows to determine, in principle, the unknown fields  $\rho$ ,  $\mathbf{v}$  and  $\beta$ . Finally, the absolute temperature  $\vartheta$  may be determined by Eq. (16). Alternatively, one can use Eqs. (27) and (28) to obtain an evolution equation for the heat flux and to express in the system above  $\operatorname{grad} \beta$  and its time and space derivatives as functions of the heat flux and its temporal and spatial derivatives. That way, one obtains a system of governing equations for the four interacting fields  $\rho$ ,  $\mathbf{v}$ ,  $\vartheta$ , and  $\mathbf{q}$ , expressing the perturbations of mass-momentum and temperature-heat flux densities.

## 5 Wave propagation

In continuum physics the systems of governing equations may be put in the first-order quasi-linear form

$$\mathbf{A}_0(\mathbf{u}) \frac{\partial \mathbf{u}}{\partial t} + \mathbf{A}_i(\mathbf{u}) \frac{\partial \mathbf{u}}{\partial x_i} = \mathbf{f}(\mathbf{u}), \quad (50)$$

with the unknown N-column vector  $\mathbf{u}(\mathbf{x}, t) = (u_1, u_2, \dots, u_N)^T$ , where  $\mathbf{A}_0$  and  $\mathbf{A}_i$  are real  $N \times N$  matrices and  $\mathbf{f}$  is a N-column vector too. The most important consequence of nonlinearity is that non regular solutions may occur and propagate through the medium as waves.



A wave is a moving surface  $\Sigma$  represented mathematically by the equation

$$\Phi(x_i, t) = 0, \quad (51)$$

which defines the wave front. The unit normal  $\mathbf{n}$  on  $\Sigma$  and the normal speed  $V$  of  $\Sigma$ , are given by

$$\mathbf{n} = \frac{\text{grad} \Phi}{|\text{grad} \Phi|}, \quad V = -\frac{\frac{\partial \Phi}{\partial t}}{|\text{grad} \Phi|}. \quad (52)$$

Weak waves have a continuous velocity across the front but a jump of the acceleration. Meantime, the unknown fields  $u_\alpha$ ,  $\alpha = 1, \dots, N$ , are continuous across the front but their gradients are discontinuous, with the jump pointing in the normal direction. The symbols  $F^+$  and  $F^-$  will denote the limits of  $F$  on the side of  $\Sigma$  with positive and negative normal, respectively. The quantities  $\Pi_\alpha = \left[ \frac{\partial u_\alpha}{\partial x_i} \right] n_i$ , where  $[F] = F^+ - F^-$  is the jump of  $F$  along the normal, are called amplitudes of the acceleration wave, and their evolution is ruled by a Bernoulli equation. The wave speeds and the amplitudes of the acceleration waves are given, respectively, by the eigenvalues  $\lambda$  and the eigenvectors  $\mathbf{r}$  of the following eigenvalue problem

$$(\mathbf{A}_i n_i - \lambda \mathbf{A}_0) \mathbf{r} = \mathbf{0}. \quad (53)$$

The system (50) is said hyperbolic if  $\det \mathbf{A}_0 \neq 0$ , and the problem (53) has only real eigenvalues (characteristic speeds) and  $N$  independent eigenvectors. The system (50) is said symmetric if  $\mathbf{A}_0$  is positive definite and  $\mathbf{A}_i = \mathbf{A}_i^T$ . Any symmetric system is hyperbolic.

A remarkable consequence of the symmetry is the well-posedness of the Cauchy problem under very general conditions. In fact, for any symmetric system, the Cauchy problem with initial data in a Sobolev space  $W^{p,2}$  with  $p \geq 4$ , has a unique solution  $\mathbf{u} \in W^{p,2}$  in the neighborhood of the initial manifold [28].

For the sake of simplicity, let us evaluate the system (18), (48), (49) and (27) in the one-dimensional case, under the hypothesis that the heat conductivity can be approximated by a constant. Experimental results for some of the most common polyatomic gases show that such an hypothesis is allowed on a wide range of temperatures [29, 30].

It reads

$$\rho_t + v\rho_x + \rho v_x = 0, \quad (54)$$

$$\rho v_t + \alpha \vartheta \rho_x + \rho v v_x + \alpha \rho \vartheta_x - \frac{\tau q^2}{2\kappa \vartheta^2} \vartheta_x + \frac{\tau q}{\kappa \vartheta} q_x = 0, \quad (55)$$

$$\begin{aligned} & \rho c_v \vartheta_t + \rho c_v v \vartheta_x + \rho \varepsilon_1 q q_t + \rho \varepsilon_1 q v q_x + \frac{1}{2} \rho \frac{\partial \varepsilon_1}{\partial \vartheta} q^2 \vartheta_t \\ & + \frac{1}{2} \rho \frac{\partial \varepsilon_1}{\partial \vartheta} q^2 v \vartheta_x + \frac{1}{2} \rho \frac{\partial \varepsilon_1}{\partial \rho} q^2 \rho_t + \frac{1}{2} \rho \frac{\partial \varepsilon_1}{\partial \rho} q^2 v \rho_x \\ & + \left( \frac{3\tau q^2}{2\vartheta \kappa} + \alpha \rho \vartheta \right) v_x + q_x = 0, \end{aligned} \quad (56)$$

$$\tau q_t + \tau q v_x + \kappa \vartheta_x + \tau v q_x = -q. \quad (57)$$

In the equations above the coordinate  $x$  denotes the position of the points of the gas. Moreover, the symbols  $F_x$  and  $F_t$  denote the partial derivatives of  $F$  with respect to  $x$  and  $t$ , respectively.

The system (54)–(57) can be re-arranged in the form (50), with  $\mathbf{u} = (\rho, v, \vartheta, q)^T$ ,  $\mathbf{f} = (0, 0, 0, -q)^T$  and

$$\mathbf{A}_0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \rho & 0 & 0 \\ \frac{1}{2} \rho \frac{\partial \varepsilon_1}{\partial \rho} q^2 & 0 & \left( \rho c_v + \frac{1}{2} \rho \frac{\partial \varepsilon_1}{\partial \vartheta} q^2 \right) & \rho \varepsilon_1 q \\ 0 & 0 & 0 & \tau \end{bmatrix},$$

$$\mathbf{A}_1 = \begin{bmatrix} v & \rho & 0 & 0 \\ \alpha \vartheta & \rho v & \left( \alpha \rho - \frac{\tau q^2}{2\kappa \vartheta^2} \right) & \frac{\tau q}{\kappa \vartheta} \\ \frac{1}{2} \rho \frac{\partial \varepsilon_1}{\partial \rho} q^2 v & \left( \frac{3\tau q^2}{\kappa \vartheta} + \alpha \rho \vartheta \right) & \left( \rho c_v v + \frac{1}{2} \rho \frac{\partial \varepsilon_1}{\partial \vartheta} q^2 v \right) & \left( \rho \varepsilon_1 q v + 1 \right) \\ 0 & \tau q & \kappa & \tau v \end{bmatrix}.$$

The characteristic speeds  $\Lambda$  are given by the solutions of the following fourth-grade algebraic equation

$$\det \begin{bmatrix} v - \Lambda & \rho & 0 & 0 \\ \alpha \vartheta & \rho(v - \Lambda) & \left(\alpha \rho - \frac{\tau q^2}{2\kappa \vartheta^2}\right) & \frac{\tau q}{\kappa \vartheta} \\ \frac{1}{2} \rho \frac{\partial \varepsilon_1}{\partial \rho} q^2 (v - \Lambda) & \left(\frac{3\tau q^2}{2\kappa \vartheta} + \alpha \rho \vartheta\right) & \left(\rho c_v + \frac{1}{2} \rho \frac{\partial \varepsilon_1}{\partial \vartheta} q^2\right) (v - \Lambda) & \rho \varepsilon_1 q (v - \Lambda) + 1 \\ 0 & \tau q & \kappa & \tau (v - \Lambda) \end{bmatrix} = 0.$$

For the sake of simplicity, let us restrict to the case  $\varepsilon_1 = 0$  and a wave traveling into a thermally unperturbed state, i.e. with  $q = 0$ . By straightforward calculations we obtain the characteristic equation

$$\rho^2 \tau c_v (v - \Lambda)^4 - (\alpha \rho^2 c_v \tau \vartheta + \rho \kappa) (v - \Lambda)^2 + \alpha \rho \vartheta \kappa = 0. \quad (58)$$

Eq. (58) admits four real solutions, given by

$$v - \Lambda = \pm \sqrt{U}, \quad (59)$$

with

$$U = \frac{(\alpha \rho^2 c_v \tau \vartheta + \rho \kappa) \pm (\alpha \rho^2 c_v \tau \vartheta - \rho \kappa)}{2 \rho^2 \tau c_v}. \quad (60)$$

It is easily seen that by Eq. (60) it follows that the theory is hyperbolic whatever the temperature is.

Moreover, by the combination of Eqs. (59) and (60) with Eq. (43), it follows that the minimum and maximum characteristic speeds take the form

$$\Lambda_{\min} = v - \sqrt{\frac{p_0}{\rho}}, \quad (61)$$

$$\Lambda_{\max} = v + \sqrt{\frac{p_0}{\rho}}, \quad (62)$$

while two further waves propagate with intermediate speeds

$$\Lambda_2 = v - \sqrt{\frac{\kappa}{\rho \tau c_v}}, \quad (63)$$

$$\Lambda_3 = v + \sqrt{\frac{\kappa}{\rho \tau c_v}}. \quad (64)$$

The relations above give the speeds of propagation of four thermo-mechanical disturbances (as the number of unknown fields) generated by the interactions of the thermal field with mass and momentum transfer. The fastest and slowest speeds  $\Lambda_{\max}$  and  $\Lambda_{\min}$  are the velocities of propagation of two pressure waves, due to perturbations of mass-momentum density, and their form is the same of that arising in isentropic gas dynamics, with the sole difference that  $p_0$  depends now on the temperature too, as expected, being the fluid not in thermodynamic equilibrium. The two intermediate speeds  $\Lambda_2$  and

$\Lambda_3$ , instead, are the velocities of two heat waves, due to perturbations in the temperature-heat flux density, depending on the classical parameters which characterize hyperbolic heat conduction, i.e. heat conductivity, specific heat and relaxation time. For constant temperature  $\Lambda_{\max}$  and  $\Lambda_{\min}$  reproduce exactly the pressure waves of isentropic gas dynamics, while for a fluid at rest, and constant thermo-physical quantities,  $\Lambda_2$  and  $\Lambda_3$  yield the classical thermal wave speeds calculated by Cattaneo in his pioneering paper [3].

Shock waves have discontinuous velocity across the wavefront. Meantime, the unknown fields  $u_\alpha$ ,  $\alpha = 1, \dots, N$ , are discontinuous, too. If we still consider a one-dimensional system and shocks propagating into an unperturbed state, ( $v^+ = q^+ = 0$ ), then the system (54)–(57) leads to the following set of Rankine-Hugoniot jump conditions across the shock

$$\rho^+ S = \rho^- (S - v^-), \quad (65)$$

$$-\rho^- (S - v^-) v^- = -\alpha \rho^+ \vartheta^+ + \alpha \rho^- \vartheta^- + \frac{\tau q^{-2}}{2\kappa \theta^-}, \quad (66)$$

$$\begin{aligned} \rho^+ \varepsilon_0^+ S - \rho^- (S - v^-) \left( \varepsilon_0^- + \frac{\varepsilon_1^- q^{-2}}{2} + \frac{1}{2} v^{-2} \right) \\ = - \left( \alpha \rho^- \vartheta^- + \frac{\tau q^{-2}}{2\kappa \theta^-} \right) v^- + q^-, \end{aligned} \quad (67)$$

$$q^- (S - v^-) = \frac{\kappa}{\tau} (\vartheta^+ - \vartheta^-), \quad (68)$$

where  $S$  denotes the shock velocity. We can eliminate it from the previous expressions, getting so

$$\begin{aligned} \frac{-\rho^- v^-}{\rho^+ - \rho^-} &= \frac{\alpha \rho^+ \vartheta^+ - \alpha \rho^- \vartheta^- - \frac{\tau q^{-2}}{2\kappa \theta^-}}{\rho^+ v^-} \\ &= \frac{-v^- \left( \alpha \rho^- \vartheta^- + \frac{\tau q^{-2}}{2\kappa \theta^-} \right) - q^-}{\rho^+ \left( \varepsilon_0^+ - \varepsilon_0^- - \frac{\varepsilon_1^- q^{-2}}{2} \right) - \frac{\rho^+ v^{-2}}{2}} \\ &= \frac{\kappa (\vartheta^+ - \vartheta^-) + q^- v^-}{q^-}. \end{aligned} \quad (69)$$

In this way, the field  $\mathbf{u}^- = (\rho^-, v^-, \vartheta^-, q^-)$  ahead the shock may be determined, provided that the field  $\mathbf{u}^+ = (\rho^+, 0, \vartheta^+, 0)$  behind the shock is known. For shocks traveling through an unperturbed state along the positive direction,  $S$  is proved to satisfy the inequalities [31]

$$v - \sqrt{\frac{p_0}{\rho}} \leq S \leq v + \sqrt{\frac{p_0}{\rho}}, \quad (70)$$

referred to as "Lax conditions". It is known that the Lax conditions for a fluid imply the growth of the entropy production across the shock [31]. This is the reason why they are known in the literature as "entropy growth conditions". In practice, the constraints (70) select the physical shocks among the solutions of the Rankine-Hugoniot equations (65)–(68).

## 6 Incompressible fluids

In the previous section, under the hypothesis  $q = 0$  and  $\varepsilon \simeq \varepsilon_0$ , we have calculated the speeds of propagation of thermo-mechanical disturbances. It turns out that the theory is hyperbolic, whatever is the value of the temperature.

Let's now remove the hypotheses  $q = 0$  and  $\varepsilon \simeq \varepsilon_0$ , and assume that the fluid is at rest, namely  $v = 0$ . The system (54)–(57) gets now

$$\rho_t = 0, \quad (71)$$

$$\left( \alpha \rho \vartheta + \frac{\tau q^2}{2\kappa\theta} \right)_x = 0, \quad (72)$$

$$\rho c_v \vartheta_t + \rho \varepsilon_1 q q_t + \frac{1}{2} \rho \frac{\partial \varepsilon_1}{\partial \vartheta} q^2 \vartheta_t + q_x = 0, \quad (73)$$

$$\tau q_t + \kappa \vartheta_x = -q. \quad (74)$$

Eq. (71) proves that the fluid is now incompressible, while Eq. (72), which represents the condition of mechanical equilibrium, shows that the total pressure is uniform. Eqs. (73)–(74) instead, govern the evolution of the unknown fields  $\vartheta$  and  $q$ . They can be put in the form (50), with  $\mathbf{u} = (\vartheta, q)^T$ ,  $\mathbf{f} = (0, -q)^T$  and

$$\mathbf{A}_0 = \begin{bmatrix} \left( \rho c_v + \frac{1}{2} \rho \frac{\partial \varepsilon_1}{\partial \vartheta} q^2 \right) & \rho \varepsilon_1 q \\ 0 & \tau \end{bmatrix}, \quad \mathbf{A}_1 = \begin{bmatrix} 0 & 1 \\ \kappa & 0 \end{bmatrix}.$$

Once the expression of  $\varepsilon_1$  in Eq. (38) is taken into account, we get the characteristic speeds

$$U = \frac{-\frac{\tau q}{\vartheta} \pm \sqrt{\kappa \rho \tau c_v}}{\rho \tau c_v - \frac{\tau^2 q^2}{\kappa \vartheta^2}}. \quad (75)$$

Thus, also in this case the theory is hyperbolic for arbitrary values of  $q$ . For  $q = 0$  Eq. (75) yields

$$U = \pm \sqrt{\frac{\kappa}{\rho \tau c_v}}, \quad (76)$$

which represent the well-known second sound speeds in solids [3, 7, 8].

Further important properties of the system may be derived under the additional hypotheses  $c_v = a$ , and  $\varepsilon_1 = 0$ . Then, Eqs. (73) and (74) read

$$\rho a \vartheta_t + q_x = 0, \quad (77)$$

$$\tau q_t + \kappa \vartheta_x = -q, \quad (78)$$

while the matrices  $\mathbf{A}_0$  and  $\mathbf{A}_1$  become

$$\mathbf{A}_0 = \begin{bmatrix} \rho a & 0 \\ 0 & \tau \end{bmatrix}, \quad \mathbf{A}_1 = \begin{bmatrix} 0 & 1 \\ \kappa & 0 \end{bmatrix}.$$

The system above is representative of the linear hyperbolic heat conduction in solids at low temperatures, with the free energy and the entropy depending on temperature and heat flux, and the internal energy which, according to the experimental observations, depends on the temperature only. It is easily seen that the vectors

$$\mathbf{w} = (\vartheta, q)^T, \quad \mathbf{F} = (\rho a \vartheta, \tau q), \quad \mathbf{G} = (\kappa q, \vartheta), \quad (79)$$

are such that

$$\mathbf{A}_0 = \frac{\partial \mathbf{F}}{\partial \mathbf{w}}, \quad \mathbf{A}_1 = \frac{\partial \mathbf{G}}{\partial \mathbf{w}}. \quad (80)$$

That way, the system (77)–(78) may be put in the conservative form [32]

$$\frac{\partial \mathbf{F}}{\partial t} + \frac{\partial \mathbf{G}}{\partial x} = \mathbf{f}. \quad (81)$$

Thus, by introducing the new field  $\mathbf{u} = \mathbf{F} = (u_1, u_2)$ , with  $u_1 = \rho a \vartheta$  and  $u_2 = \tau q$ , from Eq. (81) we get

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \tilde{\mathbf{G}}(\mathbf{u})}{\partial x} = \tilde{\mathbf{f}}, \quad (82)$$

with

$$\tilde{\mathbf{G}}(\mathbf{u}) = (\kappa u_2 / \tau, u_1 / \rho a), \quad \tilde{\mathbf{f}}(\mathbf{u}) = (0, u_2 / \tau)^T. \quad (83)$$

Moreover, the specific entropy takes the form

$$s = -\alpha \log \rho + a \log u_1 - a \log(\rho a) + \frac{\rho a^2}{2k} \frac{u_2^2}{u_1^2}. \quad (84)$$

By straightforward calculations, it is easily proved that the condition

$$|u_2| \leq \sqrt{\frac{2k}{3\rho a}} u_1, \quad (85)$$

is necessary and sufficient to ensure that  $s(u_1, u_2)$  is concave. Such a property, which allows to satisfy the principle of maximum entropy at the equilibrium, has important consequences from the mathematical point of view. First of all, it ensures that the function  $h^0(u_1, u_2) = -\rho s(u_1, u_2)$  is convex. Moreover, making use of the entropy balance (21), and taking into account the thermodynamic restrictions (30)–(33), one attains the following additional balance law

$$h_t^0 + h_x^1 = g(u_1, u_2), \quad (86)$$

with

$$h^1(u_1, u_2) = -\frac{\rho a u_2}{\tau u_1}, \quad g(u_1, u_2) = -\frac{\rho a u_2^2}{\tau^2 u_1^2} \leq 0. \quad (87)$$

The conditions above ensure that there exists a  $2 \times 2$  matrix  $\mathbf{H}(\mathbf{u})$  such that the system

$$\mathbf{H}(\mathbf{u}) \left( \frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \tilde{\mathbf{G}}(\mathbf{u})}{\partial x} - \tilde{\mathbf{f}} \right) = \mathbf{0}, \quad (88)$$

is symmetric [32, 33]. Then, by the results referred in Sec. 5 for symmetric systems, we infer that the Cauchy problem for the system (77)–(78) is well posed.

## 7 Concluding remarks

In the present paper we have proposed a mesoscopic model of ideal polyatomic gases, with thermal lag and finite thermal wave speed. To account for the thermal relaxation effect, we have defined a non-equilibrium dynamical temperature starting by phenomenological considerations on the motion of the molecules constituting the gas. That way, we have built a bridge between the kinetic theory of gases and the macroscopic Cattaneo theory. Although classical kinetic theory expansions [5] or phenomenological methods [2] give rather similar results, in the present paper we have analyzed the problem from a mesoscopic point of view, giving a more deep insight at the molecular level but still obtaining manageable model equations at the macroscopic level. Our

main hypothesis was a Fourier's type constitutive equation for the heat flux, where the absolute temperature has been substituted by the dynamical one. By design, at the equilibrium the dynamical temperature coincides with the classical absolute temperature, otherwise it follows the absolute temperature after a certain delay, controlled by a small parameter, playing the role of relaxation time. This delay introduces propagation with finite speed and, if chosen small, controls the passage to the diffusive regime.

The constitutive theory was developed by allowing the response functions to depend on the gradients of the unknown fields [16]. As result, entropy, free energy, internal energy and Cauchy stress can be decoupled in the sum of a classical equilibrium part and a nonequilibrium one, which depends on the heat flux too.

The system of field equations governing the evolution of mass density, gas velocity and non-equilibrium temperature has been engaged to the experimental data by the use of typical fitting curves modeling the specific heat of polyatomic gases at constant pressure.

The propagation of thermo-mechanical disturbances has been studied as well. In the case of one dimensional system we obtained four thermo-mechanical disturbances (as the number of unknown fields), generated by the interactions of the thermal field with mass and momentum transfer. The fastest and slowest speeds are the velocities of propagation of two pressure waves, while the two intermediate speeds are the velocities of two heat waves, due to perturbations in the temperature-heat flux density. The Rankine-Hugoniot jump conditions on a shock front are derived as well and the fields behind the shock are obtained as functions of those ahead the shock.

In the case of a fluid at rest, the theory of rigid heat conductors is recovered as a particular case. It is proved that the system of governing equations can be put in symmetric hyperbolic form, so that the well posedness of the Cauchy problem is ensured [32].

The proposed model could be easily validated by measurements of the speeds of propagation of thermo-mechanical disturbances in some of the most common polyatomic gases. The calculated wave speeds could be obtained by the results in Sec. 5, with the experimental values of specific heat, thermal conductivity and transport coefficients taken by [27, 29, 30, 34, 35]. As further development of the theory, we plan to extend the results of Sec. 5 to the case of temperature dependent heat conductivity and thermal relaxation. Moreover, we aim to calculate the interval of temperatures in which the unilateral constraints in Eq. (70) are satisfied, in order to determine the range of temperature in which physical

shocks may occur. Finally, from the mathematical point of view, the methodology applied in Sec. 6 could be used to study the well posedness of the Cauchy problem for moving gases.

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**Key words.** Weakly nonlocal thermodynamics, dynamical non-equilibrium temperature, exploitation of Second Law, extended Coleman–Noll procedure, heat waves.

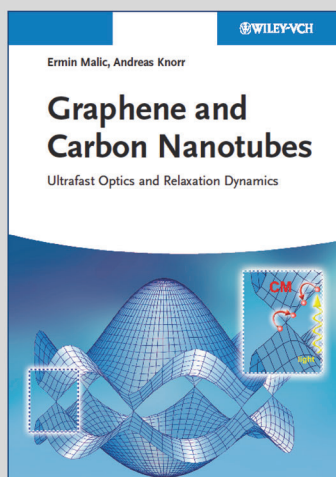
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