### **Research Article**

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# Two Temperature Extension of Phonon Hydrodynamics

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**Abstract:** Phonon hydrodynamics uses the fields of the total energy and the heat flux as state variables. We extend it by promoting the microscopic internal energy field into the status of an extra independent state variable. The governing equations of both the phonon and the extended (two temperature) phonon hydrodynamics are formulated as particular realizations of the abstract GENERIC equation. Such unified formulation makes both theories manifestly compatible with mechanics and thermodynamics. Also differences and similarities (in the physical content, in the mathematical structure, and in qualitative properties of solutions) between the two heat transfer theories, as well as their mutual compatibility, become manifestly displayed.

Keywords: heat transport, thermodynamics, GENERIC

# **1** Introduction

Disagreement of results of experimental observations of heat transfer with theoretical predictions [1–14] have led from the Fourier theory to the Cattaneo–Vernotte theory [15], [16] and then to its viscoelastic extension [17]. The physical basis of both extensions is the inclusion of inertia. In the case of the Cattaneo–Vernotte theory the extension is made by adopting the heat flux as an extra state variable and in [17] by adopting the flux of the heat flux (i. e., a heat deformation tensor) as an extra state variable. In the context of the classical hydrodynamics, the first extension leads to the Euler–Navier–Stokes type hydrodynamics (this analogy gives the Cattaneo–Vernotte theory the name phonon hydrodynamics) and the extension in [17] leads to rheology (hydrodynamics of viscoelastic fluids).

Following still the analogy with classical hydrodynamics, we recall (see, e. g., [18]) that the extra state variables introduced in extensions do not have to be always fluxes, but they can also be some types of characterizations of the internal structure of the fluids under investigation (as is the case for instance in extensions needed in investigations of polymeric fluids). The extension of the Fourier heat transfer theory that we are making in this paper is inspired by the following three types of previous heat transfer investigations. First, it is the thermomass extension [19–26] of the Fourier theory. The internal energy is seen as mass (via the Einstein mass–energy relation) and the scalar field of thermal mass is adopted as a new state variable. Another, independent, motivation comes from an attempt to introduce a Lagrangian formulation of the Cattaneo–Vernotte phonon hydrodynamics [27]. The internal energy of the heat fluid particles (called caloric particles in [27]) then plays a role that is analogous to the role of mass that the fluid particles play in the Lagrangian formulation of Euler–Navier–Stokes–Fourier hydrodynamics. Still another, also independent, source of motivation comes from investigating Grad hierarchies [28–30]. The velocity moments of the one particle distribution function are equipped in [28–30], with an additional structure. They are divided into two classes: F-moments (mass-like moments) and G-moments (energy-like moments) in [29], [30] and Grad moments and entropic

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moments in [28]. The Grad hierarchy becomes a double hierarchy, F-hierarchy governing the time evolution of F-moments, and G-hierarchy governing the time evolution of G-moments. The G-hierarchy, or alternatively the hierarchy of entropic moments, is then our motivation.

Our objective in this paper is to formulate both the phonon hydrodynamics and its extensions as particular realizations of the GENERIC time evolution equation. The unified (and manifestly compatible with mechanics, thermodynamics, and each other) formulation allows us to see clearly differences and similarities in physical and mathematical aspects of both heat transfer theories. In Section 2 we recall the GENERIC equation, in Section 3 we discuss the phonon hydrodynamics, and in Section 4 we discuss its two temperature extension.

# 2 GENERIC

What is the mathematical structure of the time evolution equations that (i) guarantees compatibility of its solutions with mechanics and thermodynamics and (ii) is identified as a common structure of well-established (i. e., well-tested with experimental observations) mesoscopic dynamical theories like the Boltzmann kinetic theory and Navier–Stokes–Fourier hydrodynamics? It has been suggested that the GENERIC structure answers both questions. A detailed formulation of GENERIC, its history, its consequences, and many illustrations can be found in [18]. Both the phonon and the two temperature hydrodynamics are presented below as particular realizations of the GENERIC structure. We therefore begin by briefly recalling GENERIC.

Let *x* denote the state variable and

$$E = E(x),$$
  

$$S = S(x)$$
(1)

the fundamental thermodynamic relation, where E(x), a real valued function of x, is the energy and S(x), a real valued and concave function of x, is the entropy.

The Hamiltonian time evolution is generated by the energy E(x) and the energy E(x) is preserved in it. The Hamiltonian part of the GENERIC time evolution is also generated by E(x), the energy is also preserved in it, and in addition, another potential, called entropy S(x), is required to be preserved in it. From the physical point of view, the Hamiltonian time evolution expresses mechanics. The Hamiltonian part of the GENERIC time evolution expresses an incomplete mechanics. The mechanics is incomplete because some of the state variables that are needed to follow all the details are missing. Due to the incompleteness, the Hamiltonian part of the time evolution is supplemented in GENERIC by another, non-Hamiltonian part, which expresses the influence of the missing data. The extra part still preserves the energy E(x) but increases the entropy S(x). Due to the latter consequence the non-Hamiltonian part of the GENERIC time evolution is called a dissipative part. In this section we present first the Hamiltonian part and then the dissipative part.

The vector field generating the Hamiltonian time evolution of *x* is a gradient  $E_x$  of energy E(x) (i. e., a co-vector) transformed into a vector by a Poisson structure *L*,

$$\dot{\kappa} = LE_{\chi}.$$
(2)

We use hereafter the notation  $E_x = \frac{\partial E}{\partial x}$ . In the case when *x* is an element of an infinite dimensional space (as is the case for example in hydrodynamics) the partial derivative is an appropriate functional derivative (see, e. g., the Appendix in [18]). From the physical point of view, the gradient  $E_x$  of the energy E(x) is the driving force of the time evolution and the Poisson structure *L* expresses kinematics of the state variable *x*. The general properties required from *L* are conveniently expressed with the help of the Poisson bracket

$$\{A, B\} = \langle A_x, LB_x \rangle, \tag{3}$$

where *A* and *B* are sufficiently regular real valued functions of *x* and <, > is the inner product. We say that  $\{A, B\}$  is a Poisson bracket if (i)  $\{A, B\} = -\{B, A\}$ , (ii)  $\{A, B\}$  is linear in  $A_x$  and  $B_x$ , and (iii) the Jacobi identity

 ${A, {B, C}} + {B, {C, A}} + {C, {A, B}} = 0$  holds (for details, see [18]). Using the Poisson bracket, the time evolution (2) can be written in the form

$$\dot{A} = \{A, E\}, \forall A. \tag{4}$$

The energy E(x) is automatically preserved in the Hamiltonian time evolution (2) since  $\dot{E} = \{E, E\} = 0$ . The physical requirement of energy conservation thus does not restrict in any way the freedom of choice of the energy E(x). If x is a mesoscopic state variable (i. e., x is not ( $\mathbf{r}_1, ..., \mathbf{r}_n, \mathbf{u}_1, ..., \mathbf{u}_n$ ) or the n-particle distribution function  $f_n(\mathbf{r}_1, ..., \mathbf{r}_n, \mathbf{u}_1, ..., \mathbf{u}_n)$ , where  $n \sim 10^{23}$  is the number of particles composing the macroscopic system under investigation and ( $\mathbf{r}_1, \mathbf{u}_i$ ); i = 1, ..., n, are their position vectors and momenta), then (2) represents only a part of the mesoscopic time evolution. An extra term on its right hand side has to be added and an extra requirement has to be placed on the first term on the right hand side of (2). The extra requirement is that in addition to the energy E(x), also another potential, namely, the entropy S(x), is preserved. The extra term on the right hand side of (2), generated by the entropy S(x), is presented in the next paragraph. The conservation of S(x) in the Hamiltonian time evolution generated by (2) can be achieved by making the Poisson structure L degenerate. A function C(x) is called a Casimir of the Poisson bracket  $\{A, B\}$  if  $\{A, C\} = 0, \forall A$ . A degenerate Poisson structure is often referred to as a Poisson structure. The physical requirement of the conservation of the entropy in the Hamiltonian part of the mesoscopic time evolution of macroscopic systems is thus mathematically formulated as

$$\{A,S\} = 0, \forall A,\tag{5}$$

or in other words, the entropy S(x) is a Casimir of the Poisson bracket  $\{A, B\}$ .

Now we proceed to the dissipation part of the time evolution. If x represents a complete microscopic characterization of macroscopic systems (i.e., x includes all position vectors and momenta of all n particles composing the macroscopic system or alternatively x is the *n*-particle distribution function  $f_n$ , then (2) is a complete time evolution equation. If however x is a mesoscopic state variable characterizing only some overall important features, then the right hand side of the time evolution equation (2) has to be supplemented with an extra term expressing the influence of the ignored details. The extra term is generated by the entropy S(x), makes the entropy increase, and leaves the energy E(x) unchanged. As argued in [18], [31], the general mathematical formulation of the extra term is  $[\Xi(x, x^*)_{x^*}]_{x^*=S_y}$ . The quantity  $\Xi(x, x^*)$  is a real valued function (*x*, *x*<sup>\*</sup>), called a dissipation potential, satisfying the following four properties: (i)  $\Xi(x, 0) = 0$ , (ii)  $\Xi(x, x^*)$ , as a function of  $x^*$ , reaches its minimum at  $x^* = 0$ , (iii)  $\Xi(x, x^*)$  is a convex function of  $x^*$  in a neighborhood of  $x^* = 0$ , and (iv)  $\langle E_x, [\Xi(x, x^*)_{x^*}]_{x^*=S_x} \geq 0$ . It is easy to verify (see details in [18]) that solutions to  $\dot{x} = [\Xi(x, x^*)_{x^*}]_{x^*=S_u}$  satisfy  $\dot{E} = 0$  and  $\dot{S} > 0$ . In the Boltzmann kinetic equation, the details ignored in the time evolution are details of the gas particle trajectories during their collisions. The right hand side of the Boltzmann kinetic equation consists of two terms; the first one is the right hand side of (2) expressing physically the influence of the free flow of the gas particles and the second one is the Boltzmann collision term expressing the influence of binary collisions.

The abstract formulation of a mesoscopic time evolution equation (called GENERIC equation – for its complete formulation and its provenance see [18]) is

$$\dot{x} = LE_{x} + \left[\Xi(x, x^{*})_{x^{*}}\right]_{x^{*} = S_{y}}.$$
(6)

In the absence of the Hamiltonian term, the time evolution governed by

$$\dot{\mathbf{x}} = \left[\Xi(\mathbf{x}, \mathbf{x}^*)_{\mathbf{x}^*}\right]_{\mathbf{x}^* = \mathbf{S}_{\mathbf{x}}} \tag{7}$$

is called a generalized gradient time evolution. With the choice  $\Xi(x, x^*) = \langle x^*, \Lambda(x)x^* \rangle$ , where  $\Lambda$  is a symmetric positive operator satisfying  $\Lambda E_x = 0$ , the time evolution governed by

$$\dot{x} = \Lambda S_{x} \tag{8}$$

is called a gradient time evolution.

In the course of the time evolution generated by (6), (7), and (8), the energy E(x) is conserved and the entropy S(x) increases, i. e.,

$$\dot{E} = 0,$$
  
$$\dot{S} > 0.$$
 (9)

As the time  $t \to \infty$ , the state variable  $x \to x_{\infty}$  and the fundamental thermodynamic relation (1) transforms into the fundamental thermodynamic equilibrium relation  $S^{(eq)} = S^{(eq)}(E^{(eq)})$ , where  $E^{(eq)} = E(x_{\infty})$  is the equilibrium energy,  $S^{(eq)} = S(x_{\infty})$  is the equilibrium entropy, and  $x_{\infty}$  is the equilibrium state reached as  $t \to \infty$ . From the physical point of view, the GENERIC equation (6) is a mathematical formulation of mechanics with incomplete data. The influence of the missing data is taken into account in the second term on the right hand side of (6). The GENERIC equation (6) expresses a common mathematical structure of a very large class of well-established (i. e., well tested with experimental observations) mesoscopic time evolution equations (see more in [18]).

## **3** Phonon hydrodynamics

We recall first the Fourier theory and then its Cattaneo–Vernotte extension. Both theories are required to be compatible with mechanics and thermodynamics and thus both theories are presented as particular realizations of (6).

### 3.1 Fourier

In the Fourier theory of heat transfer the energy field

$$\boldsymbol{x}^{(F)} = \boldsymbol{e}(\boldsymbol{r}) \tag{10}$$

serves as the only state variable. The fundamental thermodynamic relation (1) is

$$E = \int d\mathbf{r} e(\mathbf{r}),$$
  

$$S = \int d\mathbf{r} s(\mathbf{r}),$$
(11)

where the local entropy  $s(\mathbf{r})$  is a function of  $e(\mathbf{r})$ :

$$s(\mathbf{r}) = s(e; \mathbf{r}). \tag{12}$$

We require that  $s_e > 0$  so that there is a one-to-one transformation ( $e(\mathbf{r}) \leftrightarrows s(\mathbf{r})$ ). Following the terminology established in [32], we call the formulation in which  $e(\mathbf{r})$  serves as the state variable and  $s(\mathbf{r})$  is given by the fundamental thermodynamic relation an entropy representation and the inverse an energy representation.

The time evolution in the Fourier theory is governed by (7). The Hamiltonian part is absent. With the dissipation potential

$$\Xi^{(F)}(e,e^*) = \frac{1}{2} \int d\mathbf{r} \partial_i e^* \Lambda^{(F)} \partial_i e^*, \qquad (13)$$

eq. (7) becomes the classical Fourier equation

$$\frac{\partial e}{\partial t} = -\partial_i \left( \Lambda^{(F)} \partial_i \left( s_e \right) \right). \tag{14}$$

We use hereafter the summation convention,  $\partial_i = \frac{\partial}{\partial r_i}$ , and  $\Lambda^{(F)}$  is a positive definite operator. Since we are restricting ourselves in this paper to externally unforced macroscopic systems, the boundary conditions associated with (14), as well as with all time evolution equations introduced later in this paper, are such that all the integrals over boundaries arising in investigations of their solutions equal zero (e. g., periodic boundary conditions).

Since (14) is a particular realization of (6), its solutions imply (9), which, together with the existence of readily available walls  $W^{(e)}$  (called thermodynamic walls), which either prevent passing ( $W^{(e;closed)}$ ) or freely allow passing ( $W^{(e;open)}$ ) of the energy *e*, provide the basis for observing the heat transfer experimentally. The essential element of the experimental observations is the measurement of temperature by a thermometer. A thermometer is a macroscopic system surrounded by  $W^{(e;open)}$ . If we put the thermometer in contact with the macroscopic system under investigation at position *r* and surround both the system and the thermometer by the wall  $W^{(e;closed)}$ , then, due to (9), the system and the thermometer reach, as  $t \to \infty$ , an equilibrium at which ( $s_{e(r)}$ )<sub>system</sub> = ( $s_e$ )<sub>thermometer</sub>. Using the standard terminology

$$s_{e(r)} = \frac{1}{T(\mathbf{r})},\tag{15}$$

where  $T(\mathbf{r})$  is the local absolute temperature, the temperature of the system at position  $\mathbf{r}$  becomes at equilibrium the same as the temperature of the thermometer. What remains is to make  $[T]_{\text{thermometer}}$  visible in the thermometer. This is done by identifying a state variable of the thermometer that can be made visible and for which its dependence on the temperature is known (e. g., volume).

In passing from the entropy to the energy representation  $S_{e(r)} = \frac{1}{T(\mathbf{r})}$  changes into  $E_{s(r)} = T(\mathbf{r})$ .

### 3.2 Cattaneo–Vernotte

The Cattaneo–Vernotte extension of (14) consists in introducing inertia into the heat transfer. The right hand side of (14) is written as  $-\partial_i q_i$  and the heat flux  $\boldsymbol{q}$  is adopted as an independent state variable for which a new time evolution equation is introduced. This is like in mechanics where the time derivative of the position vector  $\boldsymbol{r}$  equals velocity  $\boldsymbol{v}$  and Newtonian mechanics introduces a new time evolution equation for the velocity. In the Hamiltonian formulation of the Newton mechanics it becomes clear that the newly adopted state variable is not in fact the velocity but the momentum (i. e., the variable that is conjugate to the velocity). We therefore anticipate that the newly adopted state variable in the heat transfer will not be exactly the heat flux  $\boldsymbol{q}(\boldsymbol{r})$  but a vector field (we denote it by the symbol  $\boldsymbol{w}(\boldsymbol{r})$ ) related to it. We shall call the field  $\boldsymbol{w}(\boldsymbol{r})$  a phonon momentum. Its relation to the heat flux  $\boldsymbol{q}$  will be revealed in the time evolution equations (see (21)).

The state variables of the Cattaneo-Vernotte theory are thus

$$x^{(CV)} = (e(\mathbf{r}), \mathbf{w}(\mathbf{r})). \tag{16}$$

The fundamental thermodynamic relation (11) remains the same but the local entropy  $s(\mathbf{r})$ ,

$$s(\mathbf{r}) = s(e, \mathbf{w}; \mathbf{r}), \tag{17}$$

depends now also on the field  $w(\mathbf{r})$  since  $w(\mathbf{r})$  is one of the state variables. As in (12), we require that  $s_e > 0$  so that we can use both the entropy and the energy representations. We recall that the derivatives transform in the passage from one representation to another as follows:  $E_s = \frac{1}{S_e}$ ;  $E_{w_i} = -\frac{S_{w_i}}{S_e}$ . Moreover, we choose (17) in such a way that w = 0 at equilibrium, i. e., we require that equation to  $s_w = 0$  is w = 0. In most papers devoted to the Cattaneo–Vernotte theory [33] the function  $s(e, w; \mathbf{r})$  is chosen as  $s(e, w; \mathbf{r}) = s(e; \mathbf{r}) - \frac{1}{2}aw^2$ , where a > 0 is a constant.

#### 3.2.1 Hamiltonian time evolution

Having chosen the state variables (16), our next task is to find their kinematics, i.e., the Poisson bracket  $\{A, B\}^{(CV)}$  expressing it mathematically. In order to guarantee the required degeneracy of the Poisson structure, we change the representation. Instead of using the entropy representation, we pass to the energy representation in which the entropy field *s*(*r*) serves as the state variable.

What is the Poisson bracket expressing kinematics of  $(s(\mathbf{r}), \mathbf{w}(\mathbf{r}))$ ? Inspired by the mass-like view of heat transfer suggested in [27], it has been conjectured in [34–36] that the kinematics of  $(s(\mathbf{r}), \mathbf{w}(\mathbf{r}))$  is the same as the kinematics of  $(s(\mathbf{r}), \mathbf{u}(\mathbf{r}))$ , where  $\mathbf{u}$  is the mass momentum, i. e.,

$$\{A, B\}^{(CV)} = \int d\mathbf{r} \left[ s[\partial_j(A_s)B_{w_j} - \partial_j(B_s)A_{w_j}] + w_j[\partial_i(A_{w_j})B_{w_j} - \partial_i(B_{w_j})A_{w_j}] \right].$$
(18)

There are several ways to derive (18) with  $\boldsymbol{w}$  replaced by the momentum  $\boldsymbol{u}$  (see [18]). We briefly recall one of them. From the mathematical point of view, motion of continuum (i. e., of a region in  $\mathbb{R}^3$ ) is a sequence of mappings  $\mathbb{R}^3 \to \mathbb{R}^3$ . These mappings form a Lie group. A part of the general theory of Lie groups is the following result. The dual of the Lie algebra associated with a Lie group is equipped with a Poisson structure (see [18] for references and details). In the case of the Lie group of transformations  $\mathbb{R}^3 \to \mathbb{R}^3$ , the field  $\boldsymbol{u}(\boldsymbol{r})$  is an element of the dual of its Lie algebra. The second line in (18) is the Poisson bracket expressing mathematically its Poisson structure. The remaining one line in (18) represents a contribution to the Poisson bracket due to the passive advection of the scalar field  $\boldsymbol{s}(\boldsymbol{r})$  by the motion the continuum (see references and details in [18]).

The Hamiltonian time evolution equation (4) corresponding to the Poisson bracket (18) becomes

$$\frac{\partial S}{\partial t} = -\partial_j (SE_{w_j}),$$

$$\frac{\partial e}{\partial t} = -\partial_j (E_{w_j}(e + \pi)),$$

$$\frac{\partial w_i}{\partial t} = -\partial_j (w_i E_{w_j} + \pi \delta_{ij}),$$
(19)

$$\pi = -e + sE_s + w_i E_{w_i},\tag{20}$$

where the energy *E* is given in (11),  $e(\mathbf{r}) = e(s, \mathbf{w}; \mathbf{r})$  is the fundamental thermodynamic relation (17), and  $\pi(\mathbf{r})$  is the local phonon pressure.

The required degeneracy of the Poisson bracket (18) (i. e., conservation of the total entropy *S* in the time evolution governed by (2)) is clearly satisfied (the first equation in (19) has the form of the local conservation law). Moreover, the energy *E* is, of course, also conserved during the time evolution since (19) are Hamilton's equations. Both *E* and *S* are defined in (11). In addition, also the total phonon momentum  $\mathbf{W} = \int d\mathbf{r}\mathbf{w}(\mathbf{r})$  remains unchanged during the Hamiltonian time evolution because the right of the third equation in (19) has the form of the local conservation law. From the second equation in (19) we also see that the heat flux  $\mathbf{q}$  is related to  $\mathbf{w}$  by

$$q_i = (e + \pi)E_{w_i}.\tag{21}$$

#### 3.2.2 Gradient time evolution

We turn now to the dissipative (gradient) part of the time evolution (i. e., to the second term on the right hand side of (7)). In order to satisfy the required degeneracy (i. e., the requirement that the energy is conserved), it is convenient to pass to the entropy representation (i. e., (e(r), w(r)) serve as state variables). The dissipation potential with which (6) becomes the Cattaneo–Vernotte equation is

$$\Xi^{(CV)}(\boldsymbol{e}, \boldsymbol{w}; \boldsymbol{w}^*) = \frac{1}{2} \int d\boldsymbol{r} w_i^* \Lambda^{(CV)} w_i^*, \qquad (22)$$

where  $\Lambda^{(CV)}$  is a positive definite operator. With the dissipative term  $\Xi_{w^*}^{(CV)}|_{w^*=S_w}$ , eqs. (19) take the form

$$\frac{\partial s}{\partial t} = -\partial_j (sE_{w_j}) + \sigma, 
\frac{\partial e}{\partial t} = -\partial_j ((e + \pi)E_{w_j}), 
\frac{\partial w_i}{\partial t} = -\partial_j (w_i E_{w_j} + \pi \delta_{ij}) - \frac{\Lambda^{(CV)}}{E_s} E_{w_i},$$
(23)

where

$$\sigma = \frac{E_{w_i}}{E_s} \Lambda^{(CV)} \frac{E_{w_i}}{E_s} > 0$$
(24)

is the entropy production.

The equations in (23) become the Guyer–Krumhansl equations [37], [38] if the Guyer–Krumhansl dissipation potential (22) is supplemented with another term,

$$\Xi^{(GK)} = \int d\mathbf{r} \frac{1}{2} \left( \partial_i \left( \frac{w_j^*}{e^*} \right) + \partial_j \left( \frac{w_i^*}{e^*} \right) \right) \Lambda^{(GK)} \frac{1}{2} \left( \partial_i \left( \frac{w_j^*}{e^*} \right) + \partial_j \left( \frac{w_i^*}{e^*} \right) \right), \tag{25}$$

that is analogical to the Navier–Stokes term in the classical hydrodynamics. The quantity  $\Lambda^{(GK)}$  is related to the phonon viscosity coefficient (see details in [18]).

Solutions to (23) imply (9) since they are a particular realization of (6). As discussed in Section 3.1, these two properties, together with the existence of thermodynamic walls  $W^{(e)}$ , provide again a basis for measuring the local temperature (15). Since the entropy depends in this section also on w, the local temperature depends also on w. What we measure with thermometers depends on the nature of the thermodynamic walls W. In principle, we can think of several different types of walls: *Type 1 walls* that allow to pass freely or block completely the passing of the total energy e, *Type 2 walls* that block the passing of the part of the energy that arises due to the heat flux, and *Type 3 walls* that allow to pass freely both types of energies (i. e., the internal energy and the energy that arises due to the heat flux) but with different relaxation times. Only with the Type 1 walls the measured temperatures will be the same as those in Section 3.1. In order to investigate the remaining two types of walls, we need an extended heat transfer theory. One such theory is introduced in Section 4.

#### 3.2.3 Compatibility with mechanics, thermodynamics, and the Fourier theory

The Hamiltonian nature of the nondissipative part of the equations in (23) and the conservation of the total energy  $E = \int d\mathbf{r} e(\mathbf{r})$  in the time evolution governed by (23) demonstrate the compatibility of (23) with mechanics. The positivity of the entropy production (24) demonstrates the compatibility of (23) with thermodynamics. Moreover, (23) is also compatible with the Fourier equation (14) (see [18], [36], [39]). Here we only briefly recall the essential idea of the demonstration. We assume that  $\mathbf{w}$  relaxes to equilibrium faster than eand s and that we are already close to the equilibrium (i. e.,  $\mathbf{w}$  is small). If we neglect in the second and third equations in (23) the quadratic and higher order terms in  $\mathbf{w}$  we obtain

$$\frac{\partial e}{\partial t} = -\partial_j ((e+\pi)E_{w_j}),$$

$$\frac{\partial w_i}{\partial t} = -\partial_i \pi - \frac{\Lambda^{(CV)}}{E_s}E_{w_i}.$$
(26)

Assuming that  $\Lambda^{(CV)}$  is a positive constant and that **w** already reached its stationary value, we see that (26) implies

$$\frac{\partial e}{\partial t} - \partial_i \left( \left( \frac{(e+\pi)T}{\Lambda^{(CV)}} \right) \partial_i \pi \right), \tag{27}$$

which, when we use e = Ts, becomes (14) with  $\Lambda^{(F)} = \frac{((e+\pi)T)^2}{\Lambda^{(CV)}}$ .

## 4 Two temperature hydrodynamics

Disagreements of results of experimental observations of the propagation of heat pulses with predictions of the Cattaneo–Vernotte theory [17] call for extensions of the phonon hydrodynamics. One such extension is made in [17]. The right hand side of the third equation in (23) is written as  $-\partial_j Q_{ij}$  and the tensor field  $Q_{ij}(\mathbf{r})$  (the flux of the heat flux) is adopted as an independent state variable. The phonon hydrodynamics becomes a phonon viscoelastic hydrodynamics. GENERIC formulation of this extra-inertia modification of the Cattaneo–Vernotte equation can be found in [36].

The two temperature hydrodynamics that we are going to develop below is still another modification of the governing equations in (23) of the Cattaneo–Vernotte phonon hydrodynamics. More details are not introduced into the fluxes but into the energy. We distinguish the part of the energy associated with the heat flux and the remaining part, which we call microscopic internal energy. The latter, denoted  $\varepsilon(\mathbf{r})$ , is a scalar field that we adopt as an independent state variable. The state variables

$$\boldsymbol{x}^{(2th)} = (\boldsymbol{e}(\boldsymbol{r}), \boldsymbol{\varepsilon}(\boldsymbol{r}), \boldsymbol{w}(\boldsymbol{r}))$$
(28)

thus include two energies: the total energy field  $e(\mathbf{r})$  and the microscopic internal energy field  $\varepsilon(\mathbf{r})$ . The fundamental thermodynamic relation corresponding to the state variables (28) is again (11) but with

$$s(\mathbf{r}) = s(e, \varepsilon, \mathbf{w}; \mathbf{r}). \tag{29}$$

As we did in the Fourier and Cattaneo–Vernotte theories, we assume that  $s_e > 0$  so that there is a one-toone transformation between the state variables  $(e(\mathbf{r}), \varepsilon(\mathbf{r}), \mathbf{w}(\mathbf{r}))$  and  $(s(\mathbf{r}), \varepsilon(\mathbf{r}), \mathbf{w}(\mathbf{r}))$  and we can use always both the energy and the entropy representations. We shall moreover assume that the function  $s(e, \varepsilon, \mathbf{w}; \mathbf{r})$  is concave and that  $s_{\mathbf{w}} = 0$  implies  $\mathbf{w} = 0$ . Having two energy fields, namely, the total energy field  $e(\mathbf{r})$  and the internal energy field  $\varepsilon(\mathbf{r})$ , we also have two temperatures, namely,

$$s_{e(r)} = \frac{1}{T(\mathbf{r})},$$
  

$$s_{\varepsilon(r)} = \frac{1}{\vartheta(\mathbf{r})},$$
(30)

where  $T(\mathbf{r})$  is the local temperature (the same as in (15)) and  $\vartheta(\mathbf{r})$  is the local internal temperature. The presence of two temperatures in our extension is the reason why we call it a two temperature extension. We recall that mesoscopic theories with more energies and thus with more than one temperature have been introduced before (see for example the investigations in [40] with the translational, rotational, and vibrational temperatures).

The physics that is behind the two temperature hydrodynamics can come from several sources. The first one is the thermomass hydrodynamics introduced in [19–26]. The internal energy is regarded in [19–26] as mass via the Einstein mass–energy relation. Since the mass field serves as an independent state variable in the classical hydrodynamics, it is natural to adopt the internal energy as an independent state variable. The second source is an attempt [27] to formulate a Lagrangian version of the Cattaneo–Vernotte hydrodynamics (i. e., to formulate (23) as the time evolution of phonon fluid – called in [27] caloric – particles). The third motivation comes from investigations [29], [30] of the Grad hierarchy. Velocity moments of the one particle distribution function are equipped in [29], [30] with an extra structure. They are divided into two groups, F-moments (called mass or mass-momentum moments) and G-moments (called energy moments). The part of the hierarchy governing the time evolution of G-moments (called G-hierarchy) represents then an extended Cattaneo–Vernotte hydrodynamics that motivates our two temperature extension.

Two other physical considerations support the two temperature extension. The first begins with the microscopic viewpoint in which macroscopic systems are seen as being composed of  $n \sim 10^{23}$  atoms. The state variable is  $x^{(\text{Micro})}$  (for instance the *n*-particle distribution function). The time evolution of  $x^{(\text{Micro})}$  is governed by Hamilton's equations with the energy  $E^{(\text{Micro})}(x^{(\text{Micro})})$ . Collection of their solutions for a family of initial conditions and a family of energies  $E^{(\text{Micro})}(x^{(\text{Micro})})$  is called a microscopic phase portrait  $\mathcal{P}^{(M)}$ . In order to gain

an insight into the overall mesoscopic behavior we have to recognize in  $\mathcal{P}^{(M)}$  a pattern  $\mathcal{P}^{(m)}$  that can then be regarded as a mesoscopic phase portrait  $\mathcal{P}^{(m)}$  corresponding to the mesoscopic time evolution of mesoscopic state variables  $x^{(\text{meso})} = \Pi^{(Mm)}(x^{(\text{Micro})})$ , where  $\Pi^{(Mm)}$  is a projection. The first step made on this route is the phonon viewpoint of heat, mathematically formulated in the phonon kinetic equation [41]. The next step can then be, following [29], [30], a passage to mesoscopic phonons with an internal structure characterized by the microscopic internal energy  $\varepsilon(\mathbf{r})$ . The remaining part of the total energy (kinetic and potential energies) comes from the overall motion (characterized by the heat flux) of the mesoscopic phonons. Extrapolating results obtained in investigations of the time evolution of gases with long range interactions [42], [43], we can anticipate that the mesoscopic phonons can also experience a turbulent motion. This could then be another type of energy arising in the heat transfer.

The second type of physical considerations supporting the two temperature hydrodynamics stays inside the continuum viewpoint. Taking inspiration from fluid mechanics, in particular from the fluid mechanics of complex fluids (for example polymeric fluids, see, e. g., [18]), extensions are made not only by adopting the fluxes as new state variables but also by entering deeper into the microscopic nature of the fluids and adopting some characterizations of their internal structure as extra state variables. This type of considerations represents another route to the two temperature hydrodynamics. The internal energy becomes the new state variable characterizing the internal structure. Following the analogy between mass and heat transfer, the two temperature extension of the heat transfer becomes analogous to two component extension in the mass transfer in which more detailed observations reveal that the fluid under investigation is in fact a two component fluid. The two energy fields in the two temperature theory (one being the overall energy  $e(\mathbf{r})$  and the other the microscopic internal energy  $\varepsilon(\mathbf{r})$ ) play the role that the total mass density and the mass density of one of the two components play in the two component hydrodynamics.

The above considerations lead us to the more specific fundamental thermodynamic relation (29). In the entropy representation, we assume that

$$E = E^{(\text{micint})} + E^{(\text{mesint})}, \tag{31}$$

where the microscopic internal energy  $E^{(\text{micint})}$  is the energy of the atoms generating their microscopic motion and the mesoscopic internal energy  $E^{(\text{mesint})}$  is the energy of atoms generating their mesoscopic motion (heat flux);

$$E^{(\text{micint})} = \int d\mathbf{r} e^{(\text{micint})}(s, \varepsilon; \mathbf{r}),$$
  

$$E^{(\text{mesint})} = \int d\mathbf{r} e^{(\text{mesint})}(s, \varepsilon, \mathbf{w}; \mathbf{r}).$$
(32)

The mesoscopic local internal energy  $e^{(\text{mesint})}(s, \varepsilon, w; r)$  is a sum of the mesoscopic kinetic energy  $\frac{w^2}{2\mu(s,\varepsilon)}$  and the mesoscopic potential energy  $v(s, \varepsilon)\partial_i\varepsilon\partial_i\varepsilon$ . The quantity  $\mu > 0$  plays a role in the heat transfer that is analogous to the role that the mass plays in the mass transfer. As argued in [19–26],  $\mu$  is proportional to  $\varepsilon(r)$ . The mesoscopic potential energy, as also argued in [19–26], arises due to spacial inhomogeneities of the microscopic internal energy  $\varepsilon$ . Both  $\mu$  and v are real valued functions of the entropy field s(r) and the microscopic internal energy  $\varepsilon(r)$ . We assume that the energies in (32) are chosen in such a way that the equation  $S_w = 0$ is solved by w = 0. A more detailed specification of (32) requires a more detailed analysis of the atomic and molecular motion on the microscopic scale. In this paper we leave this problem open.

We note that if the entropy *S* in (29) depends on  $\varepsilon(\mathbf{r})$  nonlocally (i. e., the entropy at the point  $\mathbf{r}$  depends on  $\varepsilon(\mathbf{r})$  and also on  $\partial_i \varepsilon(\mathbf{r})$ ) then the local internal temperature defined in (30) becomes (the derivative with respect to  $\varepsilon(\mathbf{r})$  has to be changed into the variational derivative with respect to  $\varepsilon(\mathbf{r})$ )

$$\frac{1}{\vartheta(\mathbf{r})} = s_{\varepsilon(r)} - \partial_j(s_{\partial_j \varepsilon(r)}).$$
(33)

We recall that in this paper we do not consider imposed external forces (as for example an imposed internal temperature gradient) that prevent approach to equilibrium. An extension of the GENERIC type analysis to externally forced systems is presented for example in [44].

### 4.1 Hamiltonian time evolution

Our next task is to write down equations governing the time evolution of (28). As we did for the state variables (10) and (16), we require that the equations are compatible with mechanics and thermodynamics and consequently, we assume that they are a particular realization of the GENERIC equation (6). In order to write down the Hamiltonian part, we need to know the kinematics of (28), i. e., the Poisson bracket expressing it mathematically.

The kinematics of  $(s(\mathbf{r}), \mathbf{w}(\mathbf{r}))$  is expressed in (18). How does this Poisson bracket change when  $(s(\mathbf{r}), \mathbf{w}(\mathbf{r}))$  is replaced by  $(s(\mathbf{r}), \varepsilon(\mathbf{r}), \mathbf{w}(\mathbf{r}))$ ? As the scalar field  $s(\mathbf{r})$ , the scalar field  $\varepsilon(\mathbf{r})$  is assumed to be passively advected with the phonon momentum  $\mathbf{w}(\mathbf{r})$ . The same assumption is made about the mass field  $\rho(\mathbf{r})$  when we want to extend the Poisson bracket expressing kinematics of  $(s(\mathbf{r}), \mathbf{u}(\mathbf{r}))$ , where  $\mathbf{u}(\mathbf{r})$  is the mass momentum field, to the Poisson bracket expressing kinematics of the full set  $(s(\mathbf{r}), \rho(\mathbf{r}), \mathbf{u}(\mathbf{r}))$  of state variables of the classical hydrodynamics. Consequently, the Poisson bracket expressing kinematics of  $(s(\mathbf{r}), \varepsilon(\mathbf{r}), \mathbf{w}(\mathbf{r}))$  is (18) with an additional third line that is the same as the first line except that *s* is replaced by  $\varepsilon$ , so we have

$$\{A, B\}^{(2th)} = \int d\mathbf{r} \left[ s[\partial_j(A_s)B_{w_j} - \partial_j(B_s)A_{w_j}] + \varepsilon[\partial_j(A_\varepsilon)B_{w_j} - \partial_j(B_\varepsilon)A_{w_j}] + w_j[\partial_i(A_{w_j})B_{w_i} - \partial_i(B_{w_j})A_{w_i}] \right].$$
(34)

If  $\rho$  replaces  $\varepsilon$  and u replaces w, the Poisson bracket (34) is indeed the Poisson bracket expressing kinematics in the classical hydrodynamics (see [18] for original references and details).

Equation (2) corresponding to the Poisson bracket (34) is

$$\frac{\partial s}{\partial t} = -\partial_j (sE_{w_j}),$$

$$\frac{\partial \varepsilon}{\partial t} = -\partial_j (\varepsilon E_{w_j}),$$

$$\frac{\partial e}{\partial t} = -\partial_j (E_{w_j} (e + \pi)),$$

$$\frac{\partial w_i}{\partial t} = -\partial_j (w_i E_{w_j} + \pi \delta_{ij}),$$
(35)

$$\pi = -e + sE_s + \varepsilon E_{\varepsilon} + w_i E_{w_i}.$$
(36)

If the energy depends also on gradients of  $\varepsilon$  (as for instance the mesoscopic potential energy in (32)), then (see [45] where this type of analysis is made in the context of the mass transport) the heat pressure  $\pi$  changes into

$$\pi = -e + sE_s + \varepsilon E_{\varepsilon} + w_i E_{w_i} - \varepsilon \partial_i E_{\partial_i \varepsilon}$$
(37)

and the fourth equation in (35) turns into

$$\frac{\partial w_i}{\partial t} = -\partial_j (w_i E_{w_j} + \partial_i (\varepsilon) E_{\partial_j \varepsilon} + \pi \delta_{ij}).$$
(38)

We recall (see (30)) that  $E_s = \frac{1}{S_e} = T$  and  $E_{\varepsilon} = -\frac{S_{\varepsilon}}{S_e} = -\frac{T}{\vartheta}$ .

### 4.2 Gradient time evolution

As in the Cattaneo–Vernotte theory (see Section 3.2.2), we let the heat momentum *w* dissipate directly since *w* addresses more microscopic details than *e* and thus we expect *w* to relax more rapidly than *e*. Moreover, since

we expect that the energy dissipated in the time evolution of w will enter the microscopic internal energy  $\varepsilon$ , we also let  $\varepsilon$  dissipate correspondingly. Instead of the dissipation potential (22) we choose now

$$\Xi^{(2\text{temp})} = \frac{1}{2} \int d\mathbf{r} \frac{w_i^*}{\varepsilon^*} \Lambda^{(2\text{temp})} \frac{w_i^*}{\varepsilon^*},$$
(39)

where  $\Lambda^{(2\text{temp})}$  is a symmetric positive definite operator. The remaining state variable *e* will relax indirectly in the course of the time evolution through its coupling to w(r) in the vector field (35) (see Section 4.2.1).

The equations in (35) with the dissipation term become

$$\begin{aligned} \frac{\partial s}{\partial t} &= -\partial_j (sE_{w_j}) + \sigma, \\ \frac{\partial \varepsilon}{\partial t} &= -\partial_j (\varepsilon E_{w_j}) + \Xi_{\varepsilon^*} \\ &= -\partial_j (\varepsilon E_{w_j}) + \frac{\vartheta^3}{T^2} \Lambda^{(2\text{temp})} E_{w_i} E_{w_i}, \\ \frac{\partial e}{\partial t} &= -\partial_j (E_{w_j} (e + \pi)), \\ \frac{\partial w_i}{\partial t} &= -\partial_j (w_i E_{w_j} + \pi \delta_{ij}) + \Xi_{w_i^*} \\ &= -\partial_j (w_i E_{w_j} + \pi \delta_{ij}) - \frac{\vartheta^2}{T} \Lambda^{(2\text{temp})} E_{w_i}, \end{aligned}$$
(40)

with the entropy production

$$\sigma = w_i^* \Xi_{w_i^*} + \varepsilon^* \Xi_{\varepsilon^*} = 2\left(\frac{\vartheta}{T}\right)^2 \Lambda^{(2\text{temp})} E_{w_i} E_{w_i}.$$
(41)

An extra (viscosity type) dissipation of **w** can be added to the right hand side of the fourth equation in (40) by replacing the dissipation potential  $\Xi^{(2temp)}$  with  $\Xi^{(2temp)} + \Xi^{(GH)}$ , where  $\Xi^{(GH)}$  is the Guyer–Krumhansl dissipation potential given in (25).

#### 4.2.1 Compatibility with mechanics, thermodynamics, and the Fourier theory

Agreement of solutions to (35) with observations constituting the experimental basis for the compatibility with mechanics and thermodynamics is guaranteed since (35) is a particular realization of (6).

Now we turn to the compatibility with the Fourier theory. As in Section 3.2.3, we assume that w relaxes to equilibrium (i. e., to solutions to  $S_w = 0$ ) faster than e, s, and  $\varepsilon$ , and that we are already close to the equilibrium (i. e., w is small since the solution to  $S_w = 0$  is w = 0). If we neglect in the equation governing the time evolution of w the quadratic and higher order terms in w we arrive at

$$\frac{\partial \varepsilon}{\partial t} = -\partial_j (\varepsilon E_{w_j}) + \frac{\vartheta^3}{T^2} \Lambda^{(2\text{temp})} E_{w_i} E_{w_i},$$

$$\frac{\partial e}{\partial t} = -\partial_j ((e+\pi) E_{w_j}),$$

$$\frac{\partial w_i}{\partial t} = -\partial_i \pi - \frac{\vartheta^2}{T} \Lambda^{(2\text{temp})} E_{w_i},$$
(42)

where  $\pi = -e + Ts - \frac{T}{\vartheta}\varepsilon$ . Assuming that  $\frac{\partial w_i}{\partial t} = 0$  we arrive at

$$\frac{\partial \varepsilon}{\partial t} = \partial_i \left( \left( \frac{\varepsilon T}{\vartheta^2 \Lambda^{(2emp)}} \right) \partial_i \pi \right) + \frac{1}{\vartheta \Lambda^{(2temp)}} \partial_i (\pi) \partial_i (\pi),$$

$$\frac{\partial e}{\partial t} = \partial_i \left( \left( \frac{(e+\pi)T}{\vartheta^2 \Lambda^{(2temp)}} \right) \partial_i \pi \right),$$
(43)

where  $\partial_i \pi = s \partial_i T - \varepsilon \partial_i \left(\frac{T}{\vartheta}\right)$ . These two equations represent now the two temperature version of the Fourier theory. Instead of one equation governing the time evolution of the total energy density  $e(\mathbf{r})$ , the two temperature Fourier theory consists of two coupled equations governing the time evolution of the total energy density  $e(\mathbf{r})$  and the microscopic internal energy  $\varepsilon(\mathbf{r})$ . Asymptotically (as  $t \to \infty$ ) solutions to (43) tend to solutions to

$$\partial_i \pi = s \partial_i E_s + \varepsilon \partial_i E_\varepsilon = s \partial_i T - \varepsilon \partial_i \left(\frac{T}{\vartheta}\right) = 0.$$
(44)

The equilibrium states implied by the two temperature theory (40) are thus w = 0 and solutions to (44). The temperatures *T* and *9* become the same and independent of the position coordinate *r*.

More detailed properties of solutions to (40) can be discussed only after making a more detailed specification of the fundamental thermodynamic relation (29) and of the operators  $\Lambda^{(2tewmp)}$  entering the dissipation potential. Particularly interesting is the question of the measurability of the two temperatures T and  $\vartheta$ . A useful insight needed to answer this question can be gained by asking the analogous question in the context of the mass transfer: How do we measure the two chemical potentials in two component systems? What we need are membranes that are selectively permeable or impermeable for the two components. In the context of the two temperature viewpoint of the heat transfer the temperatures play the same role as chemical potentials and thus for measuring them separately we need thermodynamic walls (an analog to membranes) that selectively allow to pass or stop the microscale energy  $\varepsilon$  and the rest that drives the motion on the mesoscopic scale (i.e., the motion characterized by the heat flux). We suggest that with the readily available standard thermodynamic walls the standard thermometers measure the microscopic temperature  $\vartheta$ . The difference between T and  $\vartheta$  can be made visible, for instance, by observing the detailed time dependence of the equilibration taking place in the temperature measurement, or by observing fluctuations in the measurement results. The former method needs more detailed information about the nature of the thermodynamic walls and a detailed analysis of solutions to (40), the latter method needs an extension of the two temperature model to a more microscopic level. We intend to follow these indications in our future investigations.

# **5** Discussion

Investigations of the heat transfer on the micro and nanoscales are motivated by the importance that heat transfer plays in electronic devices. In this paper we are entering deeper into the microscopic nature of the heat transfer by distinguishing in the internal energy a part driving the motion on the microscopic (atomistic) scale and a part driving the motion on the mesoscopic scale (i. e., the scale on which we see the heat flux). Both energy fields play in our mathematical formulation the role of independent state variables. In the context of the mass transfer, this extension is analogous to recognizing that a one component system is in fact composed of two components. In the mathematical formulation of the time evolution the presence of two mass fields in the set of state variables brings about the presence of two chemical potentials (i. e., two conjugate mass fields). Analogically, the time evolution in the extended heat transfer with two energy fields involves two conjugate energy fields (i. e., two temperatures).

The time evolution equations are constructed as particular realizations of the GENERIC structure. The construction itself automatically implies agreement with all experimental observations addressing the compatibility with mechanics, thermodynamics, the Fourier theory, and the Cattaneo–Vernotte theory. Comparison with more detailed experimental observations requires more detailed specifications of the quantities entering the mathematical formulation (in particular the fundamental thermodynamic relation) and more detailed analysis of solutions of the governing equations. For example, we only suggest additions to the formulation and to the mathematical analysis of solutions of the governing equations of the governing equations that could make both temperatures directly measurable and comparable with theoretical predictions.

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