

Research Article

Miroslav Grmela*, Michal Pavelka, Václav Klika, Bing-Yang Cao, and Nie Bendian

Entropy and Entropy Production in Multiscale Dynamics

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Abstract: Heat conduction is investigated on three levels: equilibrium, Fourier, and Cattaneo. The Fourier level is either the point of departure for investigating the approach to equilibrium or the final stage in the investigation of the approach from the Cattaneo level. Both investigations bring to the Fourier level an entropy and a thermodynamics. In the absence of external and internal influences preventing the approach to equilibrium the entropy that arises in the latter investigation is the production of the classical entropy that arises in the former investigation. If the approach to equilibrium is prevented, then the entropy that arises in the investigation of the approach from the Cattaneo level to the Fourier level still brings to the Fourier level the entropy and the thermodynamics even if the classical entropy and the classical thermodynamics are absent. We also note that vanishing total entropy production as a characterization of equilibrium state is insufficient.

Keywords: non-equilibrium thermodynamics, heat transfer, constitutive relations, entropy production, dissipation potential

1 Introduction

Macroscopic systems that are free from external forces and from external and internal constraints reach states, called equilibrium states, at which their behavior is found to be well described by the classical equilibrium thermodynamics (ET). This is the experimental observation on which ET stands. For one component macroscopic systems, the variables parametrizing the equilibrium states are the volume V , the number of moles N , and the energy E . A more detailed investigation of the time evolution bringing the macroscopic systems to the equilibrium states (i. e., a more detailed investigation of the process of preparation of macroscopic systems for ET) reveals that the time evolution describing it is driven by a potential. This potential, if evaluated at the asymptotically reached equilibrium states, becomes the equilibrium entropy $S^{(ET)}$. The preparation process thus plays two roles: (i) it brings the macroscopic systems to equilibrium states where ET is applicable, and (ii) it also determines the fundamental thermodynamic relation $S^{(ET)} = S^{(ET)}(V, N, E)$ in which the individual nature of macroscopic systems is expressed in ET . Formally, we represent the process of preparing macroscopic systems to ET by the diagram

$$\begin{array}{c} M \\ \downarrow \\ ET \end{array} \quad (1)$$

*Corresponding author: Miroslav Grmela, École Polytechnique de Montréal, C.P. 6079 suc. Centre-ville, Montréal, H3C 3A7, Québec, Canada, e-mail: miroslav.grmela@polymtl.ca

Michal Pavelka, Mathematical Institute, Faculty of Mathematics and Physics, Charles University, Sokolovská 83, 186 75 Prague, Czech Republic, e-mail: pavelka@karlin.mff.cuni.cz

Václav Klika, Department of Mathematics – FNSPE, Czech Technical University in Prague, Trojanova 13, 120 00 Prague, Czech Republic, e-mail: vaclav.klika@fjfi.cvut.cz

Bing-Yang Cao, Nie Bendian, Department of Engineering Mechanics, Tsinghua University, Beijing, 100084 China, e-mails: caoby@tsinghua.edu.cn, niebendian@sina.com

where M represents the mesoscopic theory on which the preparation process is observed. The dynamics involved in (1) will be called *reducing dynamics*.

Historically, the first mathematical formulation of (1) was made by Boltzmann with M being the kinetic theory (with one particle distribution function playing the role of state variables) and with the Boltzmann kinetic equation governing the time evolution equation. The mathematical structure extracted from the Boltzmann equation and from many other well-investigated examples of the passage (1) was identified in [1], in [2] (that was presented at the AMS-IMS-SIAM Joint Summer Research Conference in the Mathematical Sciences on Fluids and Plasmas: Geometry and Dynamics, held at the University of Colorado, Boulder, CO, USA, 17–23 July 1983), and in [3–9]. In [7, 8] it has been called GENERIC. The potential generating (1) is called $M \rightarrow ET$ entropy. If this entropy is evaluated at the state reached in the preparation process, it becomes the equilibrium entropy $S^{(ET)}$.

Let us now consider two mesoscopic theories: M and m . Both are assumed to be well established and the mesoscopic theory m is more macroscopic than M . We say that m is more macroscopic (or equivalently less microscopic) than M if some details seen in M are not seen in m . We say that a mesoscopic theory is well established if its consequences agree with experimental observations from which the theory sprang out. For example, we can think of M as being the kinetic theory and m as fluid mechanics. Note that the experimental observations on which M is based are different from those on which m is based. Since both M and m are well established, it must be possible to prepare the macroscopic systems for the mesoscopic theory m . The preparation process (the reducing dynamics)

$$\begin{array}{c} M \\ \downarrow \\ m \end{array} \quad (2)$$

has to be seen in M .

It has been suggested in [10] that the mathematical structure collected in GENERIC (i. e., the mathematical structure extracted from investigations of many examples of the passage (1)) also applies, with an appropriate adjustment, to the passage (2). The structure has been called in [10] CR-GENERIC. The reducing dynamics describing mathematically (2) is also driven by a potential that is interpreted as an $(M \rightarrow m)$ -entropy. If this potential is evaluated at the asymptotically reached state (i. e., the states arrived by completing the preparation process) it becomes an entropy on the level “ m ,” denoted $S^{(Mm)}$. The main objective of this paper is to investigate this type of entropy.

In order to be able to put the entropy $S^{(Mm)}$ into the context of the $M \rightarrow ET$ entropy and $S^{(ET)}$ entropy that we encountered in the investigation of the passage (1), we consider three well-established theories M , m , and ET and investigate relations depicted in the diagram

$$\begin{array}{c} M \\ \downarrow \\ m \\ \downarrow \\ ET \end{array} \quad (3)$$

We note that the passage (3) can be made only for systems that are allowed to reach the equilibrium level “ ET ” while the passage (2) can also be made for open (externally forced) systems that are prevented by external influences to reach the level “ ET .” As an example we recall the Rayleigh–Bénard system (a horizontal layer of a fluid heated from below). It is well established that the observed behavior of this system can be well described on the level of fluid mechanics (by Boussinesq equations). If we thus take the level “ m ” to be the level of fluid mechanics and the level “ M ” to be a more microscopic level (e. g., the level of kinetic theory), then the passage (2) does exist. However, the passage (3) cannot be made since the external forces, namely, the temperature gradient and the force of gravitation, prevent the approach to thermodynamic equilibrium

states. We shall see in Section 6 that in the context of (3), the entropy $S^{(Mm)}$ is the production of the $m \rightarrow ET$ entropy.

In this paper we illustrate the passages (1), (2), and (3) on the particular example in which the system under investigation is a rigid heat conductor, the level “ M ” is the Cattaneo theory, and the level “ m ” is the Fourier theory. Because of the recent realization [11] that a still more microscopic description on what we call an extended Cattaneo level (“ \mathfrak{M} ”) is very pertinent, we include it in our analysis in Section 7.

Before entering into details of the illustration, we make a comment about general versus specific formulations of the passages (1), (2), and (3). As we already noted in the context of the passage (1), the first was the Boltzmann equation representing a particular example of (1). The general (GENERIC) formulation has appeared later when trying to formulate in abstract mathematical (in particular geometrical) terms a common structure extracted from the Boltzmann equation and many equations addressing (1) (e. g., the Navier–Stokes–Fourier equations). Having now GENERIC, all the particular examples of (1) can be regarded as its particular realizations. However, every new realization is very important for the following three reasons. First, it connects GENERIC with a particular physical context and thus brings a new insight into the physical content of the abstract concepts introduced in GENERIC. Second, it provides a new motivation and a new guide for a further development of the general formulation. Third, it contributes to the particular theory discussed in the illustration by bringing a unification that allows to benefit from results and physical insights obtained in other fields. For instance, we shall see later that the Hamiltonian structure is one element of the element of GENERIC. This then means that all the results obtained for abstract Hamiltonian systems are immediately available.

In this paper we put into focus the CR-GENERIC structure of the passage (2). There are much fewer well-studied examples of (2) than of (1). Illustrations are thus particularly important. All the passages appearing in (1), (2), (3) are formulated and investigated in the setting of the rigid-body heat conduction. The general formulation of GENERIC and CR-GENERIC (which can be found in [12]) makes its bottom-up appearance implicitly as a common structure of all the passages. We discuss below all the passages in a way that their common structure is manifestly visible. The unified analysis of equilibrium, Fourier, Cattaneo, and extended Cattaneo levels, as well as of their relations, represents also a new contribution to the physics of heat conduction. To the best of our knowledge, a systematic and unified investigation of four levels and passages among them is made in this paper for the first time.

2 Equilibrium theory: ET

We limit ourselves to processes in which the volume V and the number of moles N remain unchanged. Hereafter, we therefore omit V and N and consider only the energy E as the state variable in ET . The physical system under consideration is thus a rigid heat conductor. The fundamental thermodynamic relation in ET is

$$S^{(ET)} = S^{(ET)}(E). \quad (4)$$

We call hereafter the quantity $S^{(ET)}$ an ET -entropy and the function $S^{(ET)}(E)$ an “ ET ” fundamental thermodynamic relation.

The Legendre transformation $S^{*(ET)}(E^*)$ of $S^{(ET)}(E)$ is obtained as follows. First, we introduce the “ ET ” thermodynamic potential

$$\Phi^{(ET)}(E, E^*) = -S^{(ET)}(E) + E^* E. \quad (5)$$

Next, we find E at which $\Phi^{(ET)}$ reaches its minimum (i. e., we solve $\Phi_E^{(ET)} = \frac{\partial \Phi^{(ET)}}{\partial E} = 0$), and we denote it $E^{(ET)}(E^*)$. Finally, $S^{*(ET)}(E^*) = [\Phi^{(ET)}(E, E^*)]_{E=E^{(ET)}}$.

We now ask the question of what could be the time evolution of E for which $E \rightarrow E^{(ET)}$ as $t \rightarrow \infty$. With such time evolution, the Legendre transformation described above is made simply by following the evolution

to its conclusion. But on the equilibrium level there is no time evolution. In isolated systems the energy E , that is, the only state variable on the level “ ET ,” does not change in time. On the more microscopic levels that we shall discuss in next sections the time evolution does take place even when E remains constant. The Legendre transformations that will arise in the next sections will indeed be made by following appropriate time evolutions. From the physical point of view, the time evolutions will describe the process of preparing the systems for using the equilibrium level or more generally a level that involves fewer details. When we are already on the equilibrium level, as is the case in this section, we have no details to lose. The energy E , that is, the only state variable, remains constant. No time evolution takes place. In order to see the Legendre transformation $S^{(ET)}(E) \rightarrow S^{*(ET)}(E^*)$ as a result of a time evolution, we have to open our system and we have to let it interact with a thermal bath of the temperature $T = \frac{1}{E}$. From the physical point of view, the time evolution that we are looking for will describe the equilibration process bringing our system to equilibrium with the thermal bath. The simplest equation governing such time evolution (and thus also making the Legendre transformation $S^{(ET)}(E) \rightarrow S^{*(ET)}(E^*)$) is

$$\dot{E} = -\Lambda^{(ET)} \Phi_E^{(ET)}, \quad (6)$$

where the dot denotes the time derivative, $\Phi_E^{(ET)} = \frac{\partial \Phi^{(ET)}}{\partial E}$, and $\Lambda^{(ET)} > 0$ is a parameter. The Lyapunov theorem ($\Phi^{(ET)}$ serves as the Lyapunov function) implies that $E \rightarrow E^{(ET)}$ as $t \rightarrow \infty$, where $E^{(ET)}(E^*)$ is the energy E at which $\Phi^{(ET)}$ reaches its minimum, i. e., $E^{(ET)}(E^*)$ is a solution of $\Phi_E^{(ET)} = 0$.

3 Fourier theory: $m \rightarrow ET$

Now we turn to the Fourier theory “ m .” There is only one state variable in the Fourier theory. It is the field of the internal energy $e(\mathbf{r})$; $\mathbf{r} \in \mathbb{R}^3$ is the position vector. The state space in m will be denoted by $U^{(m)}$ (i. e., $e(\mathbf{r}) \in U^{(m)}$).

The time evolution of $e(\mathbf{r})$ (i. e., the time evolution in the reducing dynamics (1) in which the level M is replaced by the level m) is governed by

$$\frac{\partial e}{\partial t} = -\nabla \cdot (\Lambda^{(m)} \nabla e^*). \quad (7)$$

We explain the meaning of the symbols introduced in (7).

By $e^*(\mathbf{r})$ we denote a state variable that is conjugate to $e(\mathbf{r})$. We define it as follows. We introduce first

$$s^{(m)} : U^{(m)} \rightarrow \mathbb{R}, \quad (8)$$

called an m -entropy. We assume that $s^{(m)}$ is a sufficiently regular and concave function. We shall call $s^{(m)}(\mathbf{r}) = s^{(m)}(e; \mathbf{r})$ introduced in (8) an “ m ” thermodynamic relation similarly as we call (4) $S^{(ET)} = S^{(ET)}(E)$ an “ ET ” fundamental thermodynamic relation. The conjugate state variable $e^*(\mathbf{r})$ is introduced as $e^*(\mathbf{r}) = s_{e(\mathbf{r})}^{(m)}$, where we use the notation $e^*(\mathbf{r}) = s_{e(\mathbf{r})}^{(m)} = \frac{\delta s^{(m)}}{\delta e(\mathbf{r})}$, with $\delta \dots / \delta \dots$ an appropriate functional derivative. The symbol ∇ stands for $\partial / \partial \mathbf{r}$. By $\Lambda^{(m)}(e(\mathbf{r}))$ we denote a positive definite operator. Hereafter, we shall use the summation convention: $\nabla \cdot (\Lambda^{(m)} \nabla e^*) = \partial_i (\Lambda_{ik}^{(m)} \partial_k e^*) = \sum_{i=1}^3 \sum_{k=1}^3 \partial_i (\Lambda_{ik}^{(m)} \partial_k e^*)$, where $\partial_i = \partial / \partial r_i$, $i = 1, 2, 3$.

3.1 Properties of solutions to eq. (7)

We make a few observations about solutions to (7). First, we note that

$$\dot{E} = 0 \quad (9)$$

(where the dot means the time derivative and $E = \int d\mathbf{r} e(\mathbf{r})$) provided the boundary conditions are chosen (in accordance with the assumption of the absence of external influences) in such a way that the integrals

over the boundary equal zero. Therefore the ET level corresponding to the reduction of the Fourier m level that is compliant with the Fourier evolution equation (7) is the fixed equilibrium $E^{(ET)}$ with the fundamental thermodynamic relation $S^{(ET)} = S^{(ET)}(E^{(ET)})$.

The second observation is about the time evolution of the m -level entropy $s^{(m)}$. We note that

$$\dot{S}^{(m)} > 0n, \quad (10)$$

where $S^{(m)} = \int drs^{(m)}(e; \mathbf{r})$. Indeed,

$$\dot{S}^{(m)} = \langle e^*, \partial_t e \rangle = - \int dr e^* \nabla \cdot (\Lambda^{(m)} \nabla e^*) = \int dr (\nabla e^*) \cdot \Lambda^{(m)} (\nabla e^*) \geq 0,$$

due to the assumption that $\Lambda^{(m)}$ is a positive definite operator. The entropy production is thus equal to $\dot{S}^{(m)}$ as there is no entropy flux at the boundary assumed, and on the m -level it is thus $\int dr (\nabla e^*) \cdot \Lambda^{(m)} \cdot \nabla e^* > 0$.

With an introduction of an “ m ”-thermodynamic potential

$$\Phi^{(m)}(E^*) = \int dr \phi^{(m)}(\mathbf{r}; E^*), \quad (11)$$

where

$$\phi^{(m)}(\mathbf{r}; E^*) = -s^{(m)}(e; \mathbf{r}) + E^* e(\mathbf{r}), \quad (12)$$

the above two observations (9) and (10) then imply

$$\dot{\Phi}^{(m)} < 0. \quad (13)$$

(i) *The approach to equilibrium*

The asymptotic, $t \rightarrow \infty$, solutions to (7), denoted $e^{(ET)}(\mathbf{r}; E^*)$, are minima of $\Phi^{(m)}$ (i. e., solutions to $\Phi_{e(\mathbf{r})}^{(m)} = 0$). Indeed, the m -level thermodynamic potential $\Phi^{(m)}$ plays the role of the Lyapunov function for the $t \rightarrow \infty$ approach to the equilibrium states $e^{(ET)}(\mathbf{r}; E^*)$.¹

(ii) *The “ ET ” fundamental thermodynamic relation (4) implied by the “ m ” fundamental thermodynamic relation (8)*

The approach to equilibrium $E^{(ET)}$ from level m should be compliant with the ET description, i. e., $\Phi^{(m)}(E^*) = \Phi^{(ET)}(E^*)$, where $\Phi^{(ET)}(E^*)$ is the Legendre transformation of $S^{(ET)}(E)$ and similarly $\Phi^{(m)}(E^*)$ is the Legendre transformation of $s^{(m)}(e)$. Then

$$-S^{(ET)}(E) + E^* E|_{E=E^{(ET)}(E^*)} = \Phi^{(ET)}(E^*) = \Phi^{(m)}(E^*) = - \int dr s^{(m)}(e^{(ET)}(E^*, \mathbf{r}); \mathbf{r}) + E^* E, \quad (14)$$

and we see that E^* introduced in (12) is the conjugate variable to E on the level ET (i. e., $E^* = S_E$), equilibrium variables from the two levels satisfy the following correspondence $E^{(ET)} = E = \int dr e(\mathbf{r})|_{e=e^{(ET)}} = \int dr e^{(ET)}(\mathbf{r}; E^*)$, and entropies are related as $S^{(ET)}(E^*) = S^{(m)}(e^{(ET)}(\mathbf{r}; E^*); \mathbf{r}) = \int dr s^{(m)}(e^{(ET)}(E^*, \mathbf{r}); \mathbf{r})$.

We also note that if we choose the m -entropy $s^{(m)}(e(\mathbf{r}))$ to be pointwise (in energy e) the same function as $S^{(ET)}(E)$ (the so-called local equilibrium assumption), then $S^{(ET)} = S^{(ET)}(E)$ is the “ ET ” fundamental thermodynamic relation implied by the “ m ” fundamental thermodynamic relation.

Note also that it is possible to construct a “Lyapunov potential” $\Phi(e) - \langle \Phi_e|_{e_0}, (e - e_0) \rangle$ which leads to a non-equilibrium steady state (energy density field e_0); see [15].

Finally, we note that the Fourier equation (7) can also be written in the form

$$\frac{\partial e}{\partial t} = \nabla \cdot (\Lambda^{(m)} \nabla \Phi_e^{(m)}), \quad (15)$$

with the “ m ” thermodynamic potential $\Phi^{(m)}$ given in (12).

¹ Lyapunov theory per se is not available in this generality. Although the problem of stability in (nonlinear) partial differential equations is more complex and requires tailored analysis to a given problem, we propose to consider the existence of Lyapunov type functional as a strong indication of stability of equilibrium point. This is supported by extensions of Lyapunov theory to certain classes of partial differential equations [13, 14].

3.2 Generalized Fourier theory: $m \rightarrow ET$

Still another way to write the Fourier time evolution equation (7) is

$$\frac{\partial e}{\partial t} = \Psi_{e^*(\mathbf{r})}^{(m)}, \quad (16)$$

where $\Psi^{(m)} = \frac{1}{2} \int d\mathbf{r} (\nabla e^*) \cdot \Lambda^{(m)} \cdot (\nabla e^*)$. We call $\Psi^{(m)}$ an “ m ” dissipation potential.

We note that both (9) and (10) and thus also (13) remain to hold also for more general dissipation potentials Ψ . The properties that guarantee (9), (10), (13) are the following: (i) $\Psi^{(m)}$ is a sufficiently regular function $\Psi^{(m)} : U^{(m)} \times U^{(X)} \rightarrow \mathbb{R}$, $(e(\mathbf{r}), X^{(m)}(\mathbf{r})) \mapsto \Psi^{(m)}(e, X)$, with $X^{(m)} = \nabla e^*$; (ii) $\Psi^{(m)}(e(\mathbf{r}), 0) = 0$; (iii) $\Psi^{(m)}$ as a function of $X^{(m)}(\mathbf{r}) \in U^{(X)}$ reaches its minimum at 0; and (iv) $\Psi^{(m)}$ as a function of $X^{(m)}(\mathbf{r}) \in U^{(X)}$ is a convex function in a neighborhood of 0.

We indeed easily verify that (9) and (10) hold and that $\Psi^{(m)} = \frac{1}{2} \int d\mathbf{r} (\nabla e^*) \cdot \Lambda^{(m)} \cdot (\nabla e^*)$ is a particular case of the dissipation potential satisfying the four properties of $\Psi^{(m)}$ listed above. The quantity $X^{(m)}$ is called an “ m ” dissipative thermodynamic force or just simply an “ m ” thermodynamic force. We note that $X^{(m)} = \nabla e^*$ can also be written as $X^{(m)} = -\nabla \Phi_e^{(m)}$ and that entropy production can be calculated in this generalized version as

$$\dot{S}^{(m)} = \langle e^*, \partial_t e \rangle = \langle e^*, \Psi_{e^*}^{(m)} \rangle. \quad (17)$$

The generalization from (15) to (16) can be motivated by results in statistics. It was shown in [16, 17] that a generalized gradient dynamics (dissipative dynamics generated by a dissipation potential) is implied by the large deviation principle with the rate function (Lagrangian) dependent on the state variables and fluxes of the state variables. Therefore, it would make sense to investigate also reduction methods working directly with the Lagrangian instead of the implied dissipation potential. In the present work, however, we focus directly on the dissipation potentials.

4 Cattaneo theory: $M \rightarrow ET$

In order to extend the range of applicability of the Fourier theory (e. g., to investigations of the heat conduction in electronic devices) we follow Cattaneo [18] and extend the state space of the Fourier theory $U^{(m)}$ to a larger state space $U^{(M)}$. The elements of $U^{(M)}$ are the fields $e(\mathbf{r})$, which serve as the state variables in the Fourier theory, and an additional vector field $\mathbf{J}(\mathbf{r})$, i. e.,

$$(e(\mathbf{r}), \mathbf{J}(\mathbf{r})) \in U^{(M)}. \quad (18)$$

The physical interpretation of $\mathbf{J}(\mathbf{r})$ will be revealed later in this section in the investigation of the time evolution of (18).

Similarly as in ET or in the Fourier theory, we introduce the M -entropy

$$s^{(M)} : U^{(M)} \rightarrow \mathbb{R} \quad (19)$$

and call $s^{(M)}(\mathbf{r}) = s^{(M)}(e, \mathbf{J}; \mathbf{r})$ an “ M ” fundamental thermodynamic relation. Again, keeping the notation introduced in ET and in the Fourier theory, we introduced the conjugate state variables $e^* = s_{e(\mathbf{r})}^{(M)}$, $\mathbf{J}^* = s_{\mathbf{J}(\mathbf{r})}^{(M)}$ and the “ M ” thermodynamic potential $\Phi^{(M)} = -S^{(M)} + E^* E$, where $S^{(M)} = \int d\mathbf{r} s^{(M)}(e, \mathbf{J}; \mathbf{r})$ and $E = \int d\mathbf{r} e(\mathbf{r})$.

In the time evolution of the Cattaneo state variables (18), we want first of all to preserve (9) and (10) but with $S^{(M)}$ replacing $S^{(m)}$. It is easy to verify that in the time evolution governed by

$$\frac{\partial}{\partial t} \begin{pmatrix} e \\ J_i \end{pmatrix} = \begin{pmatrix} \partial_i \left(\frac{1}{(e^*)^2} J_i^* \right) \\ \frac{1}{(e^*)^2} \partial_i (e^*) \end{pmatrix} + \begin{pmatrix} 0 \\ \Psi_{J_i^*}^{(M)} \end{pmatrix} \quad (20)$$

both (9) and (10) with $S^{(M)}$ replacing $S^{(m)}$ remain valid. By $\Psi^{(M)}$ we denote that “ M ” dissipation potential satisfying the properties listed in Section 3.2 with the “ M ” thermodynamic force $X^{(M)} = \mathbf{J}^*$. We shall discuss the properties of solutions to (20) in Section 4.1 and derive (20) in Section A.

4.1 Properties of solutions to eq. (20)

The energy conservation (9) of the energy $E = \int d\mathbf{r}e(\mathbf{r})$ is manifestly visible in (20). The “ M ” energy flux (i. e., the heat flux on the M -level denoted by the symbol $\Omega^{(M)}$) is related to the vector field \mathbf{J} (which serves as the extra state variable) by

$$\Omega^{(M)} = -\frac{1}{(e^*)^2}\mathbf{J}^*. \quad (21)$$

Now we turn to the entropy inequality (10) with $s^{(m)}$ replaced by $s^{(M)}$. We see immediately that $\frac{\partial s^{(M)}}{\partial t} = \partial_i \left(\frac{1}{e^*} J_i^* \right) + J_i^* \Psi_{J_i^*}^{(M)}$. The “ M ” entropy flux, denoted by the symbol $\mathfrak{S}^{(M)}$, is thus given by

$$\mathfrak{S}^{(M)} = -\frac{1}{e^*}\mathbf{J}^*. \quad (22)$$

From (21) and (22) we then see that $\mathfrak{S}^{(M)} = e^* \Omega^{(M)}$, which is indeed the classical relation between the heat flux and the entropy flux.

The “ M ” entropy production implied by (20) is given by

$$J_i^* \Psi_{J_i^*}^{(M)} > 0, \quad (23)$$

as change of “ M ” entropy is

$$\dot{s}^{(M)} = e^* \partial_i e + J_i^* \partial_i J_i = e^* \partial_i \left(\frac{1}{(e^*)^2} J_i^* \right) + J_i^* \frac{1}{(e^*)^2} \partial_i (e^*) + J_i^* \Psi_{J_i^*}^{(M)} = \partial_i \left(\frac{1}{e^*} J_i^* \right) + J_i^* \Psi_{J_i^*}^{(M)}.$$

The inequality sign in (23) is a direct consequence of the four properties of dissipation potentials listed in Section 3.2. Since both $\dot{E} = 0$ and $\dot{S}^{(M)} > 0$ hold, also the inequality $\dot{\Phi}^{(M)} < 0$ holds. This inequality then implies (see more in Section 4.1.1) the approach to equilibrium and the “ ET ” fundamental thermodynamic relation implied by the “ M ” fundamental thermodynamic relation (19). We note that the “ ET ” fundamental thermodynamic relations obtained in Section 3.1 and in this section are identical if $\mathbf{J}^{(ET)} = 0$ and $[s^{(M)}]_{J=0} = s^{(m)}$.

In order for the Cattaneo equation (20) to be regarded as an extension of the Fourier equation (7) or (16), we have to show that solutions to (7) approximate well asymptotic solutions to (20). If this is the case then the macroscopic system under investigation can be prepared (by letting the time evolution to take its course for a sufficiently long time) for the m -level description. We shall investigate this question in Section 6.

Now we return to the question of what is the physical interpretation of the vector field $\mathbf{J}(\mathbf{r})$ that serves on the level “ M ” as the extra state variable. We see from (21) and (22) that $\mathbf{J}(\mathbf{r})$ is related to but is not the same as either heat flux or the entropy flux. The relation involves the fundamental thermodynamic relation (19). More information about the physical interpretation of $\mathbf{J}(\mathbf{r})$ will arise in Section A, where we discuss the derivation of (20).

4.1.1 Rigorous derivation of the approach to ET : Open problem

In the context of the Fourier equations (7) and (16) (considered together with the boundary conditions expressing the absence of external forces), the entropy production disappears (i. e., $\dot{\Phi}^{(m)} = -\dot{S}^{(m)} = 0$ due to energy conservation $\dot{E}^{(m)} = 0$ and as entropy production corresponds to the whole time derivative of entropy $S^{(m)}$ due to zero entropy flux) only at the equilibrium states (i. e., the states at which the thermodynamic potential $\Phi^{(m)}$ reaches its minimum). This then makes a strong indication of the approach to equilibrium via Lyapunov theory as discussed above. The situation is different in the context of the Cattaneo equation (20). The entropy production disappears (i. e., $\dot{\Phi}^{(M)} = -\dot{S}^{(M)} = 0$ again due to conservation of total energy and because the system is assumed closed resulting in zero total entropy flux; finally note that a total entropy

production rather than local is considered) on the manifold $\{(e, \mathbf{J}) \in U^{(M)} | \mathbf{J}^* = 0\}$ while the equilibrium states form a smaller submanifold $\{(e, \mathbf{J}) \in U^{(M)} | \mathbf{J}^* = 0, e^* = E^*\}$. It is the mutual interaction of the dissipative (governed by the second term on the right-hand side of (20)) and the nondissipative (governed by the first term on the right-hand side of (20)) time evolutions that is expected to drive solutions to the Cattaneo equation to the equilibrium states, i. e., vanishing entropy production is not providing a characterization of equilibrium. A similar situation arises in the context of the Boltzmann kinetic equation where the entropy production disappears at the local Maxwell distribution functions and the equilibrium states are the total Maxwell distribution functions that are a small submanifold of the manifold formed by the local Maxwell distribution functions. An interesting open problem is to adapt the rigorous proof [19] of the approach to equilibrium for the Boltzmann equation to the Cattaneo equation (20).

5 $M \rightarrow m$

The Fourier theory represented by (7), (15), and (16) addresses systems that are allowed to approach equilibrium. We can however also include into the Fourier theory systems that, due to the presence of external and internal constraints, are prevented from approaching equilibrium and thus from preparing them for ET level of description. We shall denote the external and internal influences preventing the approach to ET by the symbol \mathcal{P} . If we still limit ourselves only to the processes that preserve the energy, the equation replacing (7) and (15) will take the form

$$\frac{\partial e}{\partial t} = -\partial_i \mathcal{J}_i, \quad (24)$$

where the energy flux \mathcal{J} remains unspecified. Its specification $\mathcal{J} = \mathcal{J}^{CR}(e(\mathbf{r}), \mathcal{P})$, where \mathcal{P} are internal constraints, will be called (in accordance with the established terminology) *constitutive relation* (CR).

We now assume that a comparison of results of experimental observations with solutions to eq. (24) (that is equipped with an appropriate CR $\mathcal{J} = \mathcal{J}^{CR}(e, \mathcal{P})$) shows an agreement. This then means that any other well-established description that is more microscopic (more detailed) than the one provided by (24) has to show an approach to (24).

The next question is which more microscopic theory (more microscopic level M) we choose. In the illustration discussed in this paper we choose a theory in which a flux $\Upsilon(\mathbf{r})$ plays the role of the state variable. The simplest time evolution equation for Υ describing the approach to \mathcal{J}^{CR} as $t \rightarrow \infty$ is a direct adaptation of the Fourier equation (15) to the state variable Υ , i. e.,

$$\frac{\partial \Upsilon_i}{\partial t} = -\Lambda_{ik}^{(Mm)} \Phi_{\Upsilon_i}^{(Mm)}, \quad (25)$$

where

$$\Phi^{(Mm)}(\Upsilon; J^{CR}) = -S^{(Mm)}(\Upsilon) + J_j^{CR} \mathfrak{J}_j(\Upsilon) \quad (26)$$

is an “ Mm ” thermodynamic potential, $\Lambda^{(Mm)}$ is a positive definite operator. The specification of both the entropy $S^{(Mm)}$ that is associated with the $M \rightarrow m$ time evolution (we call it, in accordance with the terminology used in the previous sections, an “ Mm ” entropy) and $\mathfrak{J}(\Upsilon) = \mathcal{J}$ must come from physical considerations in which new experimental observations of heat transfer (observations that are more detailed than those on which the Fourier theory is based) and associated with them new physical insight are expressed in terms of the state variable Υ . The vector $J^{(CR)}$ is related to the constitutive relations \mathcal{J}^{CR} by (27) below.

We shall see in the next section that for externally unforced systems that are allowed to reach the equilibrium level “ ET ,” such more microscopic viewpoint can be the viewpoint offered by the Cattaneo theory. If we make this choice, then we can see the physical meaning of Υ and identify the functions $S^{(Mm)}$ and $\mathcal{J}(J^{CR})$. At this point we leave both $S^{(Mm)}(\Upsilon)$ and $\mathcal{J}(\Upsilon)$ unspecified.

Now, we investigate solutions to (25). Since we assume that $\Phi^{(Mm)}$ is a convex function of Y and $\dot{\Phi}^{(Mm)} = -\int d\mathbf{r} \Phi_{Y_i}^{(Mm)} \Lambda_{ik}^{(Mm)} \Phi_{Y_k}^{(Mm)} < 0$, the Lyapunov theory implies that $Y \rightarrow Y^{(m)}(J^{CR})$ as $t \rightarrow \infty$, where $Y^{(m)}(J^{CR})$ is a solution to $\Phi_Y^{(Mm)} = 0$.

The passage $Y \rightarrow Y^{(m)}$, made by following the time evolution governed by (25), can also be seen as a result of the reducing Legendre transformation $S^{(Mm)}(Y) \rightarrow S^{+(m)}(J^{CR})$, where $S^{+(m)}(J^{CR}) = [\Phi^{(Mm)}(Y; J^{CR})]_{Y=Y^{(m)}(J^{CR})}$. Indeed, making the Legendre transformation of $S^{(Mm)}(Y)$ means to find the minimum of the thermodynamic potential (26). Note that $\Phi^{(Mm)}$ reaches its minimum at $Y^{(m)}$.

Consequently, we arrive at

$$\mathcal{J}^{CR} = \mathfrak{J}(Y^{(m)}) = S_{J^{CR}}^{+(m)}, \quad (27)$$

relating $J^{(CR)}$ introduced in (26) to constitutive relations in (24). After the time evolution making the passage $M \rightarrow m$ (i. e., the time evolution governed by (25)) has been completed, the time evolution on the level “ m ” is governed by

$$\frac{\partial e}{\partial t} = -\partial_i \left(S_{J_i^{CR}}^{+(m)} \right). \quad (28)$$

The relation (27) between the constitutive relations J^{CR} and the quantities $S^{(Mm)}(Y)$, $\mathfrak{J}(Y)$ appearing in (25) become more explicit if we choose $J_i^{CR} = \partial_i e^*$. With this choice, eq. (28) takes the form

$$\frac{\partial e}{\partial t} = S_{e^*}^{+(m)} \quad (29)$$

and thus, if we compare it with (16), we arrive at $S^{+(m)}(e^*) = \Psi^{(m)}(e^*)$.

The most important result of this section is the “ m ” level entropy $S^{+(m)}(J^{CR}(e^*))$. We recall that we have obtained this potential on the level “ m ” from the assumption that the “ m ” level is well established (i. e., results of “ m ” level experimental observations agree with predictions made on the “ m ” level). This assumption then implies that in the context of another well-established level “ M ,” that is more microscopic than the level “ m ,” we have to be able to see an approach to the level “ m .” If we assume that this approach is governed by (25), then we arrive at the potential $S^{+(m)}(J^{CR}(e^*))$ on the level “ m .”

If the system under investigation is closed (i. e., the system eventually reaches the level “ ET ”), then we have on the level “ m ” two entropies: $S^{(m)}(e)$ and $S^{+(m)}(J^{CR}(e^*))$. The former is generating entropy driving the passage $m \rightarrow ET$ and the latter is the entropy that arises from the passage $M \rightarrow m$. In the next section, we shall investigate their relation in the context of the Cattaneo theory addressing the passage $M \rightarrow ET$.

If the system under investigation is open (i. e., external influences prevent the approach to the thermodynamic equilibrium), then the generating entropy $S^{(m)}(e)$ does not exist, but the target entropy $S^{+(m)}(J^{CR}(e^*))$ still exists. The appearance of two entropies on the level “ m ,” one from the passage $M \rightarrow m$ (the target entropy) and the other from the passage $m \rightarrow ET$ (the generating entropy), is the main result of this paper.

6 $M \rightarrow m \rightarrow ET$

In this section we consider closed systems and compare the passage $M \rightarrow ET$ to the passage $M \rightarrow m \rightarrow ET$. The time evolution ensuring the former passage is governed by (20) and the time evolution ensuring the latter passage is a sequence of two time evolutions, of which the first, fast, is governed by (25) and the second, slow, which follows after the fast one, is governed by (24) (or (16)). The objective is to relate the quantities entering the Cattaneo equations (20) to the quantities entering the fast (25) and the slow (24) (or (16)) Fourier equations. We have already seen in the previous section relations between the quantities entering the fast (25) and the slow (24) (or (16)) Fourier equations. We shall include now in our investigation also the Cattaneo equations.

The problem that we face is to investigate solutions to (20). Our objective is to show that solutions to (20) can be well approximated by solutions to (25) followed by solutions to (24) with appropriate relations among

the quantities entering these equations. In order to analyze asymptotic solutions to (20) we note its formal similarity to the Hamilton equations in particle mechanics. The first equation corresponds to $\dot{r} = p^*$, and the second corresponds to $\dot{p} = -r^* - \lambda p^*$, where r is the position vector, p is the momentum, (r^*, p^*) are the conjugate variables, and λp^* , $\lambda > 0$, represents the friction. In this context, we know that if the mass m of the particle (that is involved in the relation between p and p^*) is sufficiently small and λ (that is involved in the friction) is sufficiently large, then p evolves faster than r . After some time, p settles at (or in the vicinity of) the quasi-equilibrium manifold determined by $r^* - \lambda p^* = 0$. The time evolution then continues on the quasi-equilibrium manifold and is governed by the inertialess dynamics $\dot{r} = -\frac{1}{\lambda}r^*$.

Analogically in the context of (20), with an appropriate choice of $s^{(M)}$ (determining the relation between the variables and their conjugates) and $\Psi^{(M)}$ (determining the dissipation), \mathbf{J} evolves in time faster than e and consequently, at the later stage of the time evolution \mathbf{J} relaxes to a constant, $\partial\mathbf{J}/\partial t$ is small, and the second equation in (20) reduces to

$$\frac{1}{(e^*)^2} \partial_i(e^*) + \Psi_{J_i^*}^{(M)} = 0. \quad (30)$$

We note that with the same choice of $s^{(M)}$ and $\Psi^{(M)}$ and at the same stage of the time evolution, the second term on the right-hand side of the Poisson bracket (46) will be smaller than the first term. Indeed, the governing equations implied by the Poisson bracket (46) are

$$\frac{\partial}{\partial t} \begin{pmatrix} e \\ J_i \end{pmatrix} = \begin{pmatrix} \partial_i \left(\frac{1}{(e^*)^2} J_i^* \right) \\ \frac{1}{(e^*)^2} \partial_i(e^*) \end{pmatrix} - \boxed{\frac{1}{s^{(M)}} (\partial_{J_j} - \partial_{J_i}) \left(\frac{J_i^*}{J_i^*} \right)^2} + \begin{pmatrix} 0 \\ \Psi_{J_i^*}^{(M)} \end{pmatrix},$$

where the boxed terms are contributions from the second term of the Poisson bracket. One can see that near the “ m ” level (Fourier manifold), where J_i is a constant (MaxEnt value of \mathbf{J} in the transition $M \rightarrow m$ while again assuming no outer or inner effects are considered), we may assume derivatives of \mathbf{J} to be subleading to the other contributions, justifying their omission above. In the one-dimensional setting, moreover, the terms are exactly equal to zero. Similarly, time evolution of the flux \mathbf{J} near the Fourier manifold is well approximated by the algebraic constraint (30).

Summing up, the above considerations imply that (with an appropriate choice of $s^{(M)}$ and $\Psi^{(M)}$ and limiting ourselves to only the later stage of the time evolution) the time evolution governed by (20) proceeds in two stages.

In the first (fast) stage the state variables approach the vicinity of the quasi-equilibrium manifold determined by (30). The time evolution in this stage (describing the approach $M \rightarrow m$) is governed by (25) with $\mathbf{Y} = \mathbf{J}^*$, the CR $\mathcal{J}_i^{CR} = -\frac{1}{(e^*)^2} \partial_i e^*$, and

$$S^{(Mm)} = \Psi^{(M)}. \quad (31)$$

These relations follow from $M \rightarrow ET$ and their choices can be verified from the fast (reducing) evolution equation, which then reads

$$\dot{J}_i^* = \frac{\partial \delta S^{(M)} / \delta J_i}{\partial t} = \frac{\delta^2 S}{\delta J_i \delta J_j} \dot{J}_j = s_{J_i J_j}^{(M)} \frac{\delta}{\delta J_j} \left(\Psi^{(M)} + \int \mathbf{dr} \left(\frac{1}{(e^*)^2} \partial_i e^* \right) J_i^* \right), \quad (32)$$

while $\dot{J}_i^* = \dot{Y}_i = -\Lambda_{ij}^{(Mm)} \Phi_{J_i^*}^{(Mm)}$ and $\Lambda_{ij}^{(Mm)} = -s_{J_i J_j}^{(M)}$ is a symmetric positive definite operator (due to concavity of entropy). Therefore

$$\Phi^{(Mm)} = -\Psi^{(M)} + \int \mathbf{dr} \left(-\frac{1}{(e^*)^2} \partial_i e^* \right) J_i^* \quad (33)$$

plays the role of thermodynamic potential and the M force satisfies $X_i^{(M)} = -\frac{1}{(e^*)^2} \partial_i e^* = \partial_i \frac{1}{e^*}$ in contrast to the m force $X_i^{(m)} = \partial_i e^*$; see Section 3.2.

In the second stage the time evolution is governed by (16) with $\Psi^{(m)}$ that we aim to identify by a relation to $\Psi^{*(M)}$, if possible. Let us explore the simplest and most natural case,

$$\Psi^{(M)} = \int \mathbf{dr} \frac{1}{2} \lambda \mathbf{J}^* \cdot \mathbf{J}^*,$$

and thus $\Psi^{*(M)} = \int \mathbf{dr} \frac{1}{2} \lambda \mathbf{X}^{(M)} \cdot \mathbf{X}^{(M)}$, where $\Psi^{*(M)}$ is the dissipation potential conjugate to $\Psi^{(M)}$ via Legendre transformation

$$0 = \frac{\delta}{\delta \mathbf{J}^*} \left(-\Psi^{(M)} + \mathbf{X}^{(M)} \cdot \mathbf{J}^* \right) \Big|_{\mathbf{J}^* = \mathbf{J}^*(\mathbf{X}^{(M)})} \quad \text{and} \quad \Psi^{*(M)} = -\Psi^{(M)}(\mathbf{J}^*) + \mathbf{X}^{(M)} \cdot \mathbf{J}^* \Big|_{\mathbf{J}^* = \mathbf{J}^*(\mathbf{X}^{(M)})}. \quad (34a)$$

The inverse transformation reads

$$0 = \frac{\delta}{\delta \mathbf{X}^{(M)}} \left(-\Psi^{*(M)} + \mathbf{X}^{(M)} \cdot \mathbf{J}^* \right) \Big|_{\mathbf{X}^{(M)} = \mathbf{X}^{(M)}(\mathbf{J}^*)} \quad \text{and} \quad \Psi^{(M)} = -\Psi^{*(M)}(\mathbf{X}^{(M)}) + \mathbf{X}^{(M)} \cdot \mathbf{J}^* \Big|_{\mathbf{X}^{(M)} = \mathbf{X}^{(M)}(\mathbf{J}^*)}. \quad (34b)$$

Note that the conjugate dissipation potential $\Psi^{*(M)}$ is exactly the thermodynamic potential $\Phi^{(Mm)}$.

Further, solutions to (30) are

$$J_i^* = \left[\Psi_{X_i^{(M)}}^{*(M)} \right]_{X_i^{(M)} = -\frac{1}{(e^*)^2} \partial_i e^*}, \quad (35)$$

and hence the evolution equation for energy density in eq. (20) becomes

$$\partial_t e = \partial_i \left(\frac{1}{(e^*)^2} \Psi_{X_i^{(M)}}^{*(M)} \Big|_{\mathbf{X}^{(M)} = \nabla \frac{1}{e^*}} \right), \quad (36)$$

guaranteeing energy conservation.

Let us now find a relation between the two entropies $S^{(Mm)}$ and $S^{(m)}$ on the Fourier m level, i. e., in the situation at which the second equation in (20) reduces to its equilibrium form (30) we also replace the $s_e^{(M)}$ with $s_e^{(m)}$ (i. e., e^* on the “ M ” level is the same as e^* on the “ m ” level) in accordance with MaxEnt reduction [20]. On the one hand entropy connecting the Cattaneo and Fourier levels satisfies

$$S^{(Mm)} \Big|_{\mathbf{X}^{(M)} = \nabla \frac{1}{e^*}} = \Psi^{(M)} \Big|_{\mathbf{X}^{(M)} = \nabla \frac{1}{e^*}} = \int \mathbf{dr} \frac{1}{2} \lambda \mathbf{J}^* \cdot \mathbf{J}^* = \int \mathbf{dr} \frac{1}{2} \mathbf{X}^{(M)} \cdot \mathbf{J}^* = \int \mathbf{dr} \left[\frac{1}{2} X_i^{(M)} \Psi_{X_i^{(M)}}^{*(M)} \right]_{\mathbf{X}^{(M)} = \nabla \frac{1}{e^*}} > 0,$$

as $\mathbf{X}^{(M)}(\mathbf{J}^*) = \lambda \mathbf{J}^*$, which follows from the Legendre transformation mentioned above, and using eq. (35). On the other hand, entropy production linked with the evolution from Fourier level to equilibrium satisfies

$$\begin{aligned} \dot{S}^{(m)} &= \langle e^*, \partial_t e \rangle = \int \mathbf{dr} e^* \partial_i \left(\frac{1}{(e^*)^2} \Psi_{X_i^{(M)}}^{*(M)} \Big|_{\mathbf{X}^{(M)} = \nabla \frac{1}{e^*}} \right) = \int \mathbf{dr} - (\partial_i e^*) \frac{1}{(e^*)^2} \Psi_{X_i^{(M)}}^{*(M)} \Big|_{\mathbf{X}^{(M)} = \nabla \frac{1}{e^*}} \\ &= \int \mathbf{dr} \left[X_i^{(M)} \Psi_{X_i^{(M)}}^{*(M)} \right]_{\mathbf{X}^{(M)} = \nabla \frac{1}{e^*}} = 2S^{(Mm)} > 0. \end{aligned} \quad (37)$$

Note that entropy inequality is thus satisfied but, more importantly, we have shown that in systems that are not prevented from reaching equilibrium, the entropy that arises in the investigation of the passage $M \rightarrow m$ is a quantity directly related to the production of the entropy that arises in the investigation of the passage $m \rightarrow ET$.

Further, the Mm -entropy $S^{(Mm)}$ that arises in the analysis of the passage $M \rightarrow m$ becomes directly related to the “ m ” dissipation potential $\Psi^{(m)}$ that arises in the analysis of the passage $m \rightarrow ET$. The relation is given by (31) and (37). However, note that such a relation is quite complicated and finally note that one cannot use projections via MaxEnt to obtain the dissipation potential $\Psi^{(m)}$ on the lower level from the upper level $\Psi^{(M)}$ or $\Psi^{*(M)}$. Indeed if one would use such a relation via projection, i. e.,

$$\Psi^{(m)} = \left[\Psi^{*(M)}(X^{(M)}) \right]_{X_i^{(M)} = -\frac{1}{(e^*)^2} \partial_i e^*},$$

one would not obtain the evolution of energy on the Fourier m level, as a direct calculation reveals.

7 Extended Cattaneo level \mathfrak{M}

It was shown for instance in [11] that good agreement with experiments is obtained when working with not only the \mathbf{J} field (Cattaneo M level), but also with an additional tensor field \mathbf{Q} coupled to the \mathbf{J} field. The level with $(e, \mathbf{J}, \mathbf{Q})$ (or alternatively $(s, \mathbf{J}, \mathbf{Q})$) involves thus more details than the levels “ M ” and “ m .” We shall denote it by the symbol \mathfrak{M} and call it an extended Cattaneo level. Below, we shall investigate the passages $\mathfrak{M} \rightarrow ET$ and $\mathfrak{M} \rightarrow M$.

Let us now show how to derive the equations using CR-thermodynamics [10]. A natural CR-extension of the Cattaneo M -level is the extended Cattaneo level \mathfrak{M} with state variables $(s, \mathbf{J}, \mathbf{Q})$, \mathbf{Q} being a symmetric tensor field. The Poisson bracket is an extension of bracket (46) (disregarding the higher-order terms in that bracket as above),

$$\begin{aligned} \{A, B\} = & \int \mathbf{dr} (\partial_k A_{s^{(M)}} B_{J_k} - \partial_k B_{s^{(M)}} A_{J_k}) \\ & + \int \mathbf{dr} ((\partial_j A_{J_i} + \partial_i A_{J_j}) B_{Q_{ij}} - (\partial_j B_{J_i} + \partial_i B_{J_j}) A_{Q_{ij}}). \end{aligned} \quad (38)$$

Note that one can also proceed in the spirit of the original Guyer–Krumhansl works [21] from the level of kinetic theory of phonons. For instance, two particle kinetic theory or Grad hierarchy for phonons leads to additional state variables coupled to the heat flux; see [12]. The reversible evolution equations implied by the Poisson bracket (38) are

$$\partial_t s = -\partial_i E_{J_i}, \quad (39a)$$

$$\partial_t J_i = -\partial_i E_s - \partial_j E_{Q_{ij}} - \partial_j E_{Q_{ji}}, \quad (39b)$$

$$\partial_t Q_{ij} = -\partial_j E_{J_i} - \partial_i E_{J_j}. \quad (39c)$$

Transformation from this energetic representation to the entropic representation turns the evolution equations to

$$\frac{\partial e}{\partial t} = \partial_i \left(\frac{1}{(e^*)^2} J_i^* \right) - \partial_i \left(\frac{J_j^* Q_{ij}^*}{(e^*)^2} \right) - \partial_j \left(\frac{J_i^* Q_{ji}^*}{(e^*)^2} \right), \quad (40a)$$

$$\frac{\partial J_i}{\partial t} = \frac{1}{(e^*)^2} \partial_i (e^*) + \partial_j \frac{Q_{ij}^*}{e^*} + \partial_j \frac{Q_{ji}^*}{e^*}, \quad (40b)$$

$$\frac{\partial Q_{ij}}{\partial t} = \partial_j \frac{J_i^*}{e^*} + \partial_i \frac{J_j^*}{e^*}, \quad (40c)$$

where the conjugate variables e^* , \mathbf{J}^* , and \mathbf{Q}^* can be interpreted as derivatives of an $S^{(EC)}$ entropy living on the EC level. Note that the relation between heat flux (flux of energy) and entropy flux becomes more complex in the presence of the extra variable \mathbf{Q} .

Dissipation is included through a dissipation potential on the EC level $\Psi^{(EC)}(\mathbf{J}^*, \mathbf{Q}^*)$, and the evolution equations become

$$\frac{\partial e}{\partial t} = \partial_i \left(\frac{1}{(e^*)^2} J_i^* \right) - \partial_i \left(\frac{J_j^* Q_{ij}^*}{(e^*)^2} \right) - \partial_j \left(\frac{J_i^* Q_{ji}^*}{(e^*)^2} \right), \quad (41a)$$

$$\frac{\partial J_i}{\partial t} = \frac{1}{(e^*)^2} \partial_i (e^*) + \partial_j \frac{Q_{ij}^*}{e^*} + \partial_j \frac{Q_{ji}^*}{e^*} + \Psi_{J_i^*}^{(EC)}, \quad (41b)$$

$$\frac{\partial Q_{ij}}{\partial t} = \partial_j \frac{J_i^*}{e^*} + \partial_i \frac{J_j^*}{e^*} + \Psi_{Q_{ij}^*}^{(EC)}. \quad (41c)$$

The choice

$$\Psi^{(EC)}(\mathbf{J}^*, \mathbf{Q}^*) = \int \mathbf{dr} \frac{1}{2} \lambda (\mathbf{J}^*)^2 + \int \mathbf{dr} \frac{1}{2} \alpha Q_{ij}^* Q_{ij}^* \quad (42)$$

makes the evolution equations explicit (up to the specification of entropy), i. e.,

$$\frac{\partial e}{\partial t} = \partial_i \left(\frac{1}{(e^*)^2} J_i^* \right) - \partial_i \left(\frac{J_j^* Q_{ij}^*}{(e^*)^2} \right) - \partial_j \left(\frac{J_i^* Q_{ji}^*}{(e^*)^2} \right), \quad (43a)$$

$$\frac{\partial J_i}{\partial t} = \frac{1}{(e^*)^2} \partial_i(e^*) + \partial_j \frac{Q_{ij}^*}{e^*} + \partial_j \frac{Q_{ji}^*}{e^*} + \lambda J_i^*, \quad (43b)$$

$$\frac{\partial Q_{ij}}{\partial t} = \partial_j \frac{J_i^*}{e^*} + \partial_i \frac{J_j^*}{e^*} + \alpha Q_{ij}^*. \quad (43c)$$

These equations are comparable with equations (16) of the paper [11].

Now we proceed to the passage $\mathfrak{M} \rightarrow M$. The evolution equation for the \mathbf{Q} field in eqs. (43) can be seen as the reducing evolution when assuming fast relaxation of \mathbf{Q} and leading (after the relaxation) to the equation

$$0 = \partial_j \frac{J_i^*}{e^*} + \partial_i \frac{J_j^*}{e^*} + \alpha Q_{ij}^*, \quad (44)$$

which is a constitutive relation for \mathbf{Q}^* in the evolution equation for \mathbf{J} . After plugging this constitutive relation into the evolution equation for \mathbf{J} we obtain

$$\frac{\partial e}{\partial t} = \partial_i \left(\frac{1}{(e^*)^2} J_i^* \right) + \partial_i \left(\frac{J_j^*}{(e^*)^2} \frac{2}{\alpha} \left(\partial_i \frac{J_j^*}{e^*} + \partial_j \frac{J_i^*}{e^*} \right) \right), \quad (45a)$$

$$\frac{\partial J_i}{\partial t} = \frac{1}{(e^*)^2} \partial_i(e^*) - \partial_j \left(\frac{2}{\alpha e^*} \left(\partial_j \frac{J_i^*}{e^*} + \partial_i \frac{J_j^*}{e^*} \right) \right) + \lambda J_i^*, \quad (45b)$$

which can be interpreted as the Guyer–Krumhansl equation; see, e. g., [21–23], when dropping nonlinear terms (see also Section B).

One can again compare entropy production on the Cattaneo level with the potential driving the reducing evolution from the extended Cattaneo level to Cattaneo. The latter at the Cattaneo level (using constitutive relation (44)) is

$$\Psi^{(EC)} = \int d\mathbf{r} \frac{1}{2} \lambda (J^*)^2 + \frac{1}{\alpha} \left[\partial_j \frac{J_i^*}{e^*} + \partial_i \frac{J_j^*}{e^*} \right] \left[\partial_j \frac{J_i^*}{e^*} + \partial_i \frac{J_j^*}{e^*} \right],$$

while the former reads

$$\dot{S}^{(C)} = \langle e^*, \partial_t e \rangle + \langle J^*, \partial_t J^* \rangle = \operatorname{div}(J_i^*/e^*) + \Psi^{(EC)},$$

as direct calculation reveals.

In summary, another extension of the Cattaneo level by adding an extra tensor field \mathbf{Q} leads to a nonlinear generalization of equations that have been shown to be in good agreement with flash experimental data. By reduction of the fast evolution we obtain a generalization of the Guyer–Krumhansl equations. Again as above in the transition from the Cattaneo to the Fourier level, the reducing evolution is governed by an entropy-production-like quantity from the reduced level.

8 Conclusion

Emergence of various entropies in the analysis of the time evolution of both externally unforced and driven systems has already been discussed in [10], [24]. In this paper we have worked out a simple illustration. A systematic investigation of relations among the heat conduction theories formulated on four levels, namely, the equilibrium “*ET*”, the Fourier “*m*”, the Cattaneo “*M*”, and the extended Cattaneo \mathfrak{M} levels, led us to nine entropies, three on “*ET*”, two on “*m*”, two on “*M*”, and two on \mathfrak{M} . Let us now discuss entropies pertinent for the *ET*, *m*, and *M* levels (as the \mathfrak{M} level would be analogical).

8.1 *ET*-entropies

The first *ET*-entropy, introduced in (4), arises as a result of experimental observations (listed in Thermodynamic Tables). The second and the third *ET*-entropies arise in Sections 3 and 4 in the analysis of solutions to the Fourier and the Cattaneo heat conduction equations. Their origin is thus dynamical. It is the process that is needed to prepare the systems to the *ET*-level that is giving rise to the *ET*-entropies.

8.2 *m*-entropies; the main result

The first *m*-entropy arises in Section 3 as a potential generating the preparation process for using the equilibrium level of description. This entropy therefore does not exist if the system under consideration is prevented from reaching the thermodynamic equilibrium. The second *m*-entropy, which arises in Section 5 in the analysis of the passage from the Cattaneo to the Fourier description of the heat conduction, however, exists also in the presence of external forces and external and internal constraints preventing the approach to the thermodynamic equilibrium. *The second m-entropy thus provides thermodynamics also to systems for which the classical ET does not exist. If the approach to equilibrium is permitted, then both m-entropies exist and the latter (i.e., the one associated with the passage $M \rightarrow m$) turns out to be production of the former (i.e., the one associated with the passage $m \rightarrow ET$).* The *m*-entropy that arises in the passage $M \rightarrow m$ can therefore be called an entropy production but such terminology is confusing since such entropy production does not have to be production of any entropy (as is indeed the case when the approach to equilibrium does not exist and thus the classical entropy does not exist). We therefore suggest to call the entropy that arises in the analysis of $M \rightarrow m$ a CR-entropy, i.e., the entropy determining the CRs. The realization that the classical entropies and the CR-entropies have very different origins brings also a clarification to discussions about the maximum-entropy and the maximum-entropy production principles (for example in their use in determining the constitutive relations in fluid mechanics of complex fluids [25, 26]).

Note that we showed that vanishing of entropy production does not characterize the equilibrium fully (in Section 4.1.1).

8.3 *M*-entropies

There are two *M*-entropies, one arising in the analysis of $M \rightarrow ET$ and the other in the analysis of $M \rightarrow m$. We note that the transformation of the *M*-entropy corresponding to the passage $M \rightarrow ET$ to the resulting *ET*-entropy, which is made by following the time evolution on the level “*M*” to its conclusion, is also a reducing Legendre transformation. This is true also for the transformation from the *m*-entropy to the corresponding *ET*-entropy in the analysis of $m \rightarrow ET$ and the transformation from the *Mm*-entropy to the *m*-entropy in the passage $M \rightarrow m$.

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Appendix A. Derivation of the Cattaneo equation (20)

Both the Fourier (7) and the Cattaneo (20) time evolution equations have been derived in the previous sections by investigating their consequences. We have first proposed the equations and then we have shown that they

both generate the time evolution describing the approach to equilibrium at which the classical ET applies. In addition, in Section 6, we have also shown that solutions to (20) agree with solutions to (7) provided the parameters entering (20) and the initial condition are chosen appropriately. Now, we turn to the derivation of (20) that begins with some fundamental principles and eq. (20) arises from an investigation of their consequences. The fundamental principles can be found either in the very microscopic (atomistic) viewpoint of heat or in some general considerations about the mathematical structure of mesoscopic theories. We shall now derive (20) from the principles that have arisen on the latter route.

As argued in [9, 12, 27, 28], the mesoscopic time evolution equations describing the approach to equilibrium all have a general structure called GENERIC. The vector field generating the mesoscopic time evolution (i. e., the right-hand side of the time evolution equation) is a sum of two parts, one (being a remnant of the Hamiltonian dynamics of the fundamental particles composing the macroscopic system under investigation) is Hamiltonian, and the other (driving the system to the thermodynamic equilibrium) is gradient. We now proceed to recognize the GENERIC structure in (20).

The second term on the right-hand side of (20) represents a general gradient dynamics. The requirement of the GENERIC structure thus does not bring anything new to the second term on the right-hand side of (20). The different situation is however with the first term on the right-hand side of (20). According to GENERIC, this term has to be Hamiltonian with the energy $E = \int d\mathbf{r}e(\mathbf{r})$ serving as the generating potential and the entropy $S^{(M)} = \int d\mathbf{r}s^{(M)}(\mathbf{r})$ playing the role of the Casimir potential (i. e., a potential that is different from the energy but, as the energy, remains unchanged during the Hamiltonian time evolution). We recall that the Hamiltonian vector field is a covector field (that is, the gradient of the energy E) transformed into a vector field by a Poisson bivector \mathcal{L} . The Poisson bivector is then expressed mathematically in the Poisson bracket $\{A, B\} = \int d\mathbf{r}(A_e, A_J)^T \mathcal{L}(B_e, B_J)$, where A and B are real-valued and sufficiently regular functions of $(e(\mathbf{r}), \mathbf{J}(\mathbf{r}))$, and the vector $(A_e, A_J)^T$ is the transpose of the vector (A_e, A_J) . A bivector \mathcal{L} is a Poisson bivector if the bracket $\{A, B\}$ is the Poisson bracket (i. e., $\{A, B\} = -\{B, A\}$ and the Jacobi identity $\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0$ holds). With the Poisson bracket $\{A, B\}$ we can write the Hamiltonian time evolution as $\dot{A} = \{A, E\}$, $\forall A$ and the Casimir potential C as the potential for which $\{A, C\} = 0$, $\forall A$.

We now proceed to show that the first term on the right-hand side of (20) is Hamiltonian. To construct a Hamiltonian vector field we need a potential (that has the physical interpretation of the energy E) and a Poisson bivector \mathcal{L} (that has the physical interpretation of kinematics). Having chosen the state variables $(e(\mathbf{r}), \mathbf{J}(\mathbf{r}))$, the energy is given by $E = \int d\mathbf{r}e(\mathbf{r})$ (i. e., the gradient of the energy is $(E_{e(\mathbf{r})}, E_{\mathbf{J}(\mathbf{r})}) = (1, 0)$). It remains thus to identify the Poisson bivector \mathcal{L} expressing kinematics of the state variables $(e(\mathbf{r}), \mathbf{J}(\mathbf{r}))$. To find it, we turn to the physical origin of heat.

We begin with seeing the heat as a gas of phonons. Since we require that the entropy $S^{(M)}$ is the Casimir, it is useful to start the search for kinematics of the state variables $(s^{(M)}(\mathbf{r}), \mathbf{J}(\mathbf{r}))$ rather than the state variables $(e(\mathbf{r}), \mathbf{J}(\mathbf{r}))$. The relation between $(e(\mathbf{r}), \mathbf{J}(\mathbf{r}))$ and $(s^{(M)}(\mathbf{r}), \mathbf{J}(\mathbf{r}))$ is given by $\mathbf{J}(\mathbf{r}) = \mathbf{J}(\mathbf{r})$ and the “ M ” fundamental thermodynamic relation (19). We shall assume that the relation between $(e(\mathbf{r}), \mathbf{J}(\mathbf{r}))$ and $(s^{(M)}(\mathbf{r}), \mathbf{J}(\mathbf{r}))$ is one-to-one. This assumption restricts the choice of the “ M ” fundamental thermodynamic relations. The restriction is in fact a weak version of the local equilibrium assumption. Indeed, if we interpret $e^*(\mathbf{r})$ as an inverse of the local absolute temperature, then $e^*(\mathbf{r}) > 0$ and the transformation $(e(\mathbf{r}), \mathbf{J}(\mathbf{r})) \rightleftharpoons (s^{(M)}(\mathbf{r}), \mathbf{J}(\mathbf{r}))$ is one-to-one.

The Poisson bracket expressing kinematics of $(s^{(M)}(\mathbf{r}), \mathbf{J}(\mathbf{r}))$, where the field $\mathbf{J}(\mathbf{r})$ has the physical interpretation of the phonon momentum divided by $s^{(M)}$, is given by

$$\{A, B\} = \int d\mathbf{r}(\partial_k A_{s^{(M)}} B_{J_k} - \partial_k B_{s^{(M)}} A_{J_k}) + \int d\mathbf{r} \frac{1}{s^{(M)}} (\partial_i J_j - \partial_j J_i) A_{J_i} B_{J_j}. \quad (46)$$

This has been shown in Section 3.9 of [12]. We then directly verify that the bracket obtained by transforming the first term on the right-hand side of (46) from the state variables $(s^{(M)}(\mathbf{r}), \mathbf{J}(\mathbf{r}))$ to the state variables $(e(\mathbf{r}), \mathbf{J}(\mathbf{r}))$ (we recall that we are assuming that the transformation is one-to-one) implies (by using $\dot{A} = \{A, E\}$, $\forall A$) the time evolution governed by (20) (without the second term on its right-hand side). As for the second term on the right-hand side of (46), we have shown in Section 6 that if we limit ourselves to states that are not too far from states at which the time evolution is governed by the Fourier equation (7), then the

second term is negligible, which is also the setting of the Symmetric Hyperbolic Thermodynamically Compatible (SHTC) or Godunov–Peshkov–Romenski (GPR) equations [29, 30], developed by the Godunov school of thermodynamics.

Summing up, we have shown that (20) possesses a GENERIC structure, with the vector field $\mathbf{J}(\mathbf{r})$ having the physical interpretation of the phonon momentum divided by entropy, provided we limit our investigation to the stage in the time evolution in which solutions to the Fourier equation (7) provide a good approximation to solutions to the Cattaneo equation (20).

An alternative investigation of the kinematics of $(e(\mathbf{r}), \mathbf{J}(\mathbf{r}))$ can be based on the analogy between the time evolution of the mass density and the mass flux and the time evolution of the energy density and the energy flux. This analogy has already been noted and exploited in three different and apparently independent investigations. In [31], it was an attempt to develop a Lagrangian formulation of the Cattaneo hydrodynamics, in [32], it was the formulation of the thermo-mass viewpoint of heat, and in [33], it was an investigation of the Grad hierarchy (the distinction made between the material F-fields and the caloric G-fields). In this paper we mention only some results. Instead of starting with the Poisson bracket (46), we start with the standard mass-momentum Poisson bracket [12, 34]

$$\{A, B\} = \int d\mathbf{r} \left[\hat{\mathbf{J}}_i \left(\partial_j (A_{j_i}) B_{j_i} - \partial_j (B_{j_i}) A_{j_i} \right) + s^{(M)} \left(\partial_i (A_{s^{(M)}}) B_{j_i} - \partial_i (B_{s^{(M)}}) A_{j_i} \right) \right], \quad (47)$$

where the field $s^{(M)}$ replaces the mass density and $\hat{\mathbf{J}}$ the momentum density related to the above vector field \mathbf{J} through $\hat{\mathbf{J}} = s^{(M)} \mathbf{J}$. Brackets (47) and (46) are equivalent (being transformations of each other).

Appendix B. Dynamic MaxEnt reduction of extended Cattaneo

Equations (39), which express reversible evolution on the extended Cattaneo level of description, can be equipped with dissipative terms also in the energetic representation, i. e.,

$$\partial_t s = -\partial_j J_i^\dagger + \frac{1}{\tau_J} \frac{(\mathbf{J}^\dagger)^2}{s^\dagger} + \frac{1}{\tau_Q} \frac{(\mathbf{Q}^\dagger)^2}{s^\dagger}, \quad (48a)$$

$$\partial_t J_i = -\partial_i s^\dagger - \partial_j Q_{ij}^\dagger - \partial_j Q_{ji}^\dagger - \frac{1}{\tau_J} J_i^\dagger, \quad (48b)$$

$$\partial_t Q_{ij} = -\partial_j J_i^\dagger - \partial_i J_j^\dagger - \frac{1}{\tau_Q} Q_{ij}^\dagger, \quad (48c)$$

where x^\dagger stands for derivative of energy with respect to x and where τ_J and τ_Q represent relaxation times. The equations for \mathbf{J} and for \mathbf{Q} contain dissipative terms and the equation for entropy contains entropy production. This dissipation can be seen as gradient dynamics in entropic representation, as shown in [30].

We will, however, proceed in the energetic representation in this section. When the energy is quadratic in \mathbf{Q} , the MaxEnt value of the \mathbf{Q} field is zero. The equation for \mathbf{Q} at this MaxEnt manifold becomes an equation for \mathbf{Q}^\dagger ,

$$0 = -\partial_j J_i^\dagger - \partial_i J_j^\dagger - \frac{1}{\tau_Q} Q_{ij}^\dagger. \quad (49)$$

Plugging the solution to this equation (constitutive relation) into the remaining equations leads to

$$\partial_t s = -\partial_j J_i^\dagger + \frac{1}{\tau_J} \frac{(\mathbf{J}^\dagger)^2}{s^\dagger} + \tau_Q \frac{(\nabla \mathbf{J}^\dagger + (\nabla \mathbf{J}^\dagger)^T)^2}{s^\dagger}, \quad (50a)$$

$$\partial_t J_i = -\partial_i s^\dagger + 2\tau_Q \partial_j (\partial_i J_j^\dagger + \partial_j J_i^\dagger) - \frac{1}{\tau_J} J_i^\dagger. \quad (50b)$$

The former equation is the entropy balance while the latter is the Guyer–Krumhansl equation (assuming τ_Q constant and proportionality between \mathbf{J} and \mathbf{J}^\dagger) [21]. The procedure just carried out is called Dynamic MaxEnt Reduction [12], and can be seen as equivalent to the CR-thermodynamic reduction presented above.

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