

THERMODYNAMICS OF HEAT FLUX IMPLIED BY REDUCING THE PHONON AND THE CATTANEO HEAT CONDUCTION THEORIES TO THE FOURIER THEORY

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ABSTRACT

We investigate heat conduction in the multiscale setting involving the Fourier, the Cattaneo, and the Peierls theories. Thermodynamics emerges in the passages among the scales. The time evolution appearing in the more microscopic theory (i.e. the theory involving more microscopic details) is split into the fast (reducing) and the slow (reduced) time evolution. During the reducing time evolution the extra state variables chosen to characterize the details become completely subjugated to the state variables used in the reduced time evolution. The reducing time evolution is generated by a potential that, if evaluated at the state reached asymptotically in the reducing time evolution, becomes a novel thermodynamic potential on the reduced level.

1 Introduction

Our objective is to illustrate the provenance of thermodynamics (both externally unforced and externally driven macroscopic systems) in the multiscale theory of heat conduction. The theories that are included in our investigation are the classical equilibrium thermodynamics (with only energy as the state variable), the classical Fourier theory (in which the energy field serves as the state variable and the Fourier equation governs its time evolution), the Cattaneo theory (in which a vector field related to the heat flux joins the set of state variables and the Cattaneo equations govern the time evolution), and the Peierls theory (in which the heat is seen as a phonon gas and the Boltzmann-like equation governs the time evolution). It is the reducing time evolution (i.e. the time evolution in which the system under consideration becomes prepared to be investigated on a single level of description, called a reduced level of description) that provides the thermodynamic potential on the chosen reduced level. The thermodynamic potential is the entropy if the reduced level is the level of the classical equilibrium thermodynamics, and the entropy production (or a potential closely related to it) if the reduced level is a level on which the time evolution takes place and on which also external driving forces can be considered. The relation between dynamics and thermodynamics, that we use in this paper, has been introduced in a general context in Refs.[1],[2]. The extended heat conduction theories that are presented in this paper have been discussed in more detail in [3].

The paper is organized as follows. First, in Section 2, we introduce the four levels in our multiscale setting as theories describing the preparation process for the application of the classical equilibrium thermodynamics. Subsequently, in Section 3, we discuss the reducing time evolutions to the Fourier heat conduction theory and the implied by it thermodynamics of heat flux.

The multiscale setting in which this paper is written requires a very careful choice of **the terminology and the notation**. We now explain their main features. Remaining details are explained in the text when new symbols are introduced. We use four levels of description: $\mathcal{L}^{(E)}$, $\mathcal{L}^{(F)}$, $\mathcal{L}^{(C)}$, $\mathcal{L}^{(P)}$ denoting the level of the equilibrium thermodynamics, the Fourier level, the Cattaneo level, and the Peierls level respectively. The level $\mathcal{L}^{(E)}$ includes the least number of details, it is the most macroscopic level among the four levels. The amount of details increases as we proceed in the order the levels are written and the most microscopic level is the Peierls level $\mathcal{L}^{(P)}$. We shall investigate passages from a level $\mathcal{L}^{(B)}$ to a less microscopic levels $\mathcal{L}^{(A)}$. The quantities that arise in the investigation of the passage $\mathcal{L}^{(B)} \rightarrow \mathcal{L}^{(A)}$ are denoted by the upper index (BA) . If these quantities are evaluated at the states on the level $\mathcal{L}^{(A)}$ that are reached in the passage $\mathcal{L}^{(B)} \rightarrow \mathcal{L}^{(A)}$ then they are denoted by the upper index (AB) . The entropy is denoted by the symbol S , the thermodynamic potential arising in Legendre transformations by the symbol Φ . We use a shorthand notation $f_x(x)$ to denote the derivative of the function $f(x)$ with respect to x . By $r = (r_1, r_2, r_3)$ we denote the position vector; we use the Einstein summation convention over the repeated indices. We also use the shorthand notation $\partial_j = \frac{\partial}{\partial r_j}$; $j = 1, 2, 3$. In order to simplify the presentation, we consider the systems under investigation in this paper to be confined to a region in \mathbb{R}^3 with the volume equals to one and the boundary conditions that make all the integrals over the boundary that arise in by parts integrations equal to zero (e.g. the periodic boundary conditions).

2 Static and Dynamic Reduction to the Equilibrium Thermodynamics of Heat

We limit ourselves to a pure heat conduction. Only the internal energy of macroscopic systems under consideration can change. In all other aspects, the systems remain unchanged in all

transformations and the time evolutions considered in this paper. We allow however the internal energy to be described in four different ways. The difference is in the amount of details used to characterize it. The theories involving more details, called more microscopic theories of heat, are needed in the investigation of heat transfer at micro and nano scales and, as we shall see below, in the introduction of the thermodynamics of heat flow.

We begin to investigate systematically the passages $\mathcal{L}^{(E)} \rightarrow \mathcal{L}^{(E)}$, $\mathcal{L}^{(F)} \rightarrow \mathcal{L}^{(E)}$, $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(E)}$, $\mathcal{L}^{(P)} \rightarrow \mathcal{L}^{(E)}$, describing the preparation processes for the application of the level $\mathcal{L}^{(E)}$. We are making the passages both by the Maximum Entropy Principle (MaxEnt Principle) and by following the time evolution involved in the preparation process.

Passage $\mathcal{L}^{(E)} \rightarrow \mathcal{L}^{(E)}$

The transformation considered in the passage $\mathcal{L}^{(E)} \rightarrow \mathcal{L}^{(E)}$ is the transformation obtained by putting a system into the contact with another system that serves as a thermal bath of the temperature T . The contact is such that the internal energy can freely pass from the system to the thermal bath and also in the opposite direction.

Static Legendre Reduction

On the level of the classical equilibrium thermodynamics, $\mathcal{L}^{(E)}$, the only state variable is the internal energy per unit volume,

$$\begin{aligned} & \text{the state variable on } \mathcal{L}^{(E)} \text{ associated with } \mathcal{L}^{(E)} \rightarrow \mathcal{L}^{(E)} : \\ & E \in \mathbb{R} \end{aligned} \quad (1)$$

The remaining state variables used in the classical equilibrium thermodynamics, namely the volume and the number of moles, will be constant and will be hereafter omitted on all levels. The state space on $\mathcal{L}^{(E)}$ that is associated with $\mathcal{L}^{(E)} \rightarrow \mathcal{L}^{(E)}$ is denoted $M^{(EE)}$ (i.e. $E \in M^{(EE)}$).

Thermodynamics is introduced by introducing the fundamental thermodynamic relation (we use the terminology of [4])

$$\begin{aligned} & \text{the fundamental thermodynamic relation associated with} \\ & \mathcal{L}^{(E)} \rightarrow \mathcal{L}^{(E)} : \\ & S^{(EE)} : M^{(EE)} \rightarrow \mathbb{R} \end{aligned} \quad (2)$$

The function $S^{(EE)}$ is called an entropy associated with the passage $\mathcal{L}^{(E)} \rightarrow \mathcal{L}^{(E)}$. We shall assume in this paper that $-S^{(EE)}$ is a convex function. It is in the fundamental thermodynamic relation (2) where the individual nature of the systems investigated on the level $\mathcal{L}^{(E)}$ is expressed.

In order to make the passage from an isolated system to the system coupled to a thermal bath, we shall use first the MaxEnt Principle (maximization of the entropy subjected to constraints). To formulate the MaxEnt principle we introduce the thermody-

namic potential

$$\Phi^{(EE)}(E; T) = -S^{(EE)}(E) + \frac{1}{T}E \quad (3)$$

find its minimum (as a function of E) and evaluate $\Phi^{(EE)}$ at the minimum. This then becomes the fundamental thermodynamic relation, denoted $S^{*(EE)}(T)$, of the system coupled to the thermal bath with the temperature T . Expressing this procedure (called a Legendre transformation $S^{(EE)}(E) \rightarrow S^{*(EE)}(T)$) in mathematical terms, we first solve the equation $\Phi_E^{(EE)} = 0$. We denote its solution by the symbol $E_{red}(T)$. The Legendre transformation $S^{*(EE)}(T)$ of $S^{(EE)}(E)$ is then $S^{*(EE)}(T) = \Phi^{(EE)}(E_{red}(T); T)$. The quantity $\Phi_E^{(EE)}$ will be called a conjugate of E and will be denoted by the symbol E^* . We note that the Legendre transformation of $S^{*(EE)}(T)$ gives back the original entropy $S^{(EE)}(E)$ (i.e. $S^{(EE)}(E) = [-S^{*(EE)}(T) + E \frac{1}{T}]_{T=T_{red}(E)}$, where $T_{red}(E)$ is a solution of $[-S^{*(EE)}(T) + E \frac{1}{T}]_E = 0$).

Dynamic Legendre Reduction

The time evolution during which the system under consideration and the thermal bath become a single system that can be investigated on the level $\mathcal{L}^{(E)}$ is the time evolution bringing E to $E_{red}(T)$. We ask thus the question of what is the time evolution of E that brings the system to the minimum of the free energy $\Phi^{(EE)}(E)$ and thus makes the Legendre transformation described above. There are clearly many time evolutions that answer the question. The simplest among them is

$$\frac{dE}{dt} = -\Lambda^{(EE)} E^* \quad (4)$$

where $\Lambda^{(EE)} > 0$ is a parameter. We see immediately that (4) implies $\frac{d\Phi^{(EE)}}{dt} = -\Lambda^{(EE)} (E^*)^2 < 0$ which then means that the free energy $\Phi^{(EE)}$ plays the role of the Lyapunov function for the approach $E \rightarrow E_{red}(T)$ as $t \rightarrow \infty$. This means that we have replaced the MaxEnt Principle as the argument for minimizing the free energy $\Phi^{(EE)}$ by the time evolution governed by (4).

Passage $\mathcal{L}^{(F)} \rightarrow \mathcal{L}^{(E)}$

From the physical point of view, this passage represents the preparation process for using the level $\mathcal{L}^{(E)}$ to describe the behavior of the system under consideration. The states reached in this preparation process are called thermodynamic equilibrium states. The quantities playing the role of state variables on the Fourier level $\mathcal{L}^{(F)}$ (see more details in [3]) is the field $e(r)$:

$$\begin{aligned} & \text{the state variable on } \mathcal{L}^{(F)} \text{ associated with } \mathcal{L}^{(F)} \rightarrow \mathcal{L}^{(E)} : \\ & e : \mathbb{R}^3 \rightarrow \mathbb{R}; r \mapsto e(r) \end{aligned} \quad (5)$$

The state space on the level $\mathcal{L}^{(F)}$ that is associated with the passage $\mathcal{L}^{(F)} \rightarrow \mathcal{L}^{(E)}$ is denoted by the symbol $M^{(FE)}$ (i.e. $e(r) \in$

$M^{(FE)}$). The fundamental thermodynamic relation on $\mathcal{L}^{(F)}$ is given by

$$\begin{aligned} & \text{the fundamental thermodynamic relation associated with} \\ & \mathcal{L}^{(F)} \rightarrow \mathcal{L}^{(E)} : \\ & S^{(FE)} : M^{(FE)} \rightarrow \mathbb{R} \\ & E : M^{(FE)} \rightarrow \mathbb{R} \end{aligned} \quad (6)$$

The quantity $S^{(FE)}(e)$ is the entropy on $\mathcal{L}^{(F)}$ associated with the passage $\mathcal{L}^{(F)} \rightarrow \mathcal{L}^{(E)}$, $E(e)$ is the energy playing the role of the state variable on the level $\mathcal{L}^{(E)}$. We shall assume that $-S^{(FE)}(e)$ is a convex function. The physical meaning of the field $e(r)$ in (5) can vary but the physical meaning of the quantities appearing in the fundamental thermodynamic relation (6) is fixed.

The passage $\mathcal{L}^{(F)} \rightarrow \mathcal{L}^{(E)}$ is made again by the reducing Legendre transformation. We introduce

$$\Phi^{(FE)}(e; T) = -S^{(FE)}(e) + \frac{1}{T}E(e) \quad (7)$$

and solve $\Phi_{e(r)}^{(FE)} = 0$. Solutions of this equation are denoted e_{red} . The reduced Legendre transformation of $S^{(FE)}(e)$ is $S^{*(FE)}(T) = [\Phi^{(FE)}(e; T)]_{e=e_{red}}$. The quantity $\Phi_{e(r)}^{(FE)}$ will be called conjugate of $e(r)$ and denoted by the symbol $e^\dagger(r)$.

Dynamic Legendre Reduction

The time evolution during which the system under investigation becomes prepared for using the level $\mathcal{L}^{(E)}$ to describe its behavior is the time evolution bringing e to $e_{red}(T)$. We thus look for the time evolution taking place on the level $\mathcal{L}^{(F)}$ that brings about the minimization of the free energy $\Phi^{(FE)}(e; T)$ and consequently replaces the MaxEnt Principle as the answer to the question of why the free energy is minimized. Again, there are many time evolutions on the level $\mathcal{L}^{(FE)}$ that will drive the field e to $e_{red}(T)$. The simplest among them is the Fourier time evolution governed by

$$\frac{\partial e}{\partial t} = \partial_j (\Lambda^{(FE)} \partial_j e^\dagger) \quad (8)$$

where $\Lambda^{(FE)} > 0$ is a parameter. We note that (8) implies $\frac{d\Phi^{(FE)}}{dt} = -\int dr \partial_j (e^\dagger) \Lambda^{(FE)} \partial_j (e^\dagger) < 0$ and consequently $\Phi^{(FE)}$ plays the role of the Lyapunov function for the approach $e \rightarrow e_{red}(T)$ as $t \rightarrow \infty$. Moreover, we note that $\int e(r) dr$ is conserved during the time evolution and thus in the fundamental thermodynamic relation (6) $E(e) = \int dr e(r)$ then the energy is conserved during the time evolution governed by (8).

Passage $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(E)}$

This is the same preparation process as the one discussed above except that the initial state is described in more details on

the level Cattaneo $\mathcal{L}^{(C)}$. The quantities playing the role of state variables on the level $\mathcal{L}^{(C)}$ (see more details in [3]) are two fields

$$\begin{aligned} & \text{the state variable on } \mathcal{L}^{(C)} \text{ associated with } \mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(E)} : \\ & e : \mathbb{R}^3 \rightarrow \mathbb{R}; r \mapsto e(r) \\ & q : \mathbb{R}^3 \rightarrow \mathbb{R}^3; r \mapsto q(r) \end{aligned} \quad (9)$$

The state space on the level $\mathcal{L}^{(C)}$ that is associated with the passage $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(E)}$ is denoted by the symbol $M^{(CE)}$ (i.e. $(e(r), q(r)) \in M^{(CE)}$). The fundamental thermodynamic relation on $\mathcal{L}^{(C)}$ is given by

$$\begin{aligned} & \text{the fundamental thermodynamic relation associated with} \\ & \mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(E)} : \\ & S^{(CE)} : M^{(CE)} \rightarrow \mathbb{R} \\ & E : M^{(CE)} \rightarrow \mathbb{R} \end{aligned} \quad (10)$$

The quantity $S^{(CE)}(e, q)$ is the entropy on $\mathcal{L}^{(C)}$ associated with the passage $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(E)}$, $E(e, q)$ is the energy playing the role of the state variable on the level $\mathcal{L}^{(E)}$. We shall assume that $-S^{(CE)}(e, q)$ is a convex function. The physical meaning of the state variables (9) can vary but the physical meaning of the quantities appearing in the fundamental thermodynamic relation (10) is fixed.

The passage $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(E)}$ is made again by the reducing Legendre transformation. We introduce

$$\Phi^{(CE)}(e, q; T) = -S^{(CE)}(e, q) + \frac{1}{T}E(e, q) \quad (11)$$

and solve $\Phi_{e(r)}^{(CE)} = 0, \Phi_{q(r)}^{(CE)} = 0$. Solutions of these equations are denoted $(e(r), q(r))_{red}$. The reduced Legendre transformation of $S^{(CE)}(e, q)$ is $S^{*(CE)}(T) = [\Phi^{(CE)}(e, q; T)]_{(e, q)=(e, q)_{red}}$. The quantities $(\Phi_{e(r)}^{(CE)}, \Phi_{q(r)}^{(CE)})$ will be called conjugates of $(e(r), q(r))$ and denoted $(e^\ddagger(r), q^\ddagger(r))$.

Dynamics Legendre Reduction

The simplest among the time evolutions that make the passage $(e, q) \rightarrow (e, q)_{red}$ is the time evolution governed by

$$\begin{aligned} \frac{\partial e}{\partial t} &= -\partial_j q_j^\ddagger \\ \frac{\partial q_i}{\partial t} &= -\partial_i e^\ddagger - \Lambda^{(CE)} q_i^\ddagger \end{aligned} \quad (12)$$

where $\Lambda^{(CE)} > 0$ is a parameter. We see indeed that $\frac{d\Phi^{(CE)}}{dt} = -\int dr q_j^\ddagger \Lambda^{(CE)} q_j^\ddagger < 0$ and consequently the thermodynamic potential $\Phi^{(CE)}$ plays the role of the Lyapunov function for the approach $(e, q) \rightarrow (e, q)_{red}$ as $t \rightarrow \infty$. We see

moreover that if the energy E in the fundamental thermodynamic relation (10) is $E = \int dre(r)$ then also the E is conserved during the time evolution governed by (12). A more general family of the Cattaneo equations governing the time evolution of $(e(r), q(r))$ is introduced in [3].

Passage $\mathcal{L}^{(P)} \rightarrow \mathcal{L}^{(E)}$

We still consider the preparation process for using the level $\mathcal{L}^{(E)}$, but we are describing it in more details. In the Peierls theory the heat is seen as a phonon gas. The new state variable that is adopted to characterize the internal energy is the phonon energy distribution function $f(r, v)$, v denotes the momentum of the phonon. The quantities playing the role of state variables on the Peierls level $\mathcal{L}^{(P)}$ (see more details in [3]) are thus

the state variable on $\mathcal{L}^{(P)}$ associated with $\mathcal{L}^{(P)} \rightarrow \mathcal{L}^{(E)}$:

$$\begin{aligned} e &: \mathbb{R}^3 \rightarrow \mathbb{R}; r \mapsto e(r) \\ f &: \mathbb{R}^3 \times \mathbb{R}^3 \rightarrow \mathbb{R}^3; (r, v) \mapsto f(r, v) \end{aligned} \quad (13)$$

The state space on the level $\mathcal{L}^{(P)}$ that is associated with the passage $\mathcal{L}^{(P)} \rightarrow \mathcal{L}^{(E)}$ is denoted by the symbol $M^{(PE)}$ (i.e. $(e(r), f(r, v)) \in M^{(PE)}$). The fundamental thermodynamic relation on $\mathcal{L}^{(P)}$ is given by

$$\begin{aligned} &\text{the fundamental thermodynamic relation associated with} \\ &\mathcal{L}^{(P)} \rightarrow \mathcal{L}^{(E)}: \\ &S^{(PE)}: M^{(PE)} \rightarrow \mathbb{R} \\ &E: M^{(PE)} \rightarrow \mathbb{R} \end{aligned} \quad (14)$$

The quantity $S^{(PE)}(e, f)$ is the entropy on $\mathcal{L}^{(P)}$ associated with the passage $\mathcal{L}^{(P)} \rightarrow \mathcal{L}^{(E)}$, $E(e, f)$ is the energy playing the role of the state variable E on the level $\mathcal{L}^{(E)}$. We assume that $-S^{(PE)}(e, f)$ is a convex function. The physical meaning of the state variables (13) can vary but the physical meaning of the quantities appearing in the fundamental thermodynamic relation (14) is fixed.

The passage $\mathcal{L}^{(P)} \rightarrow \mathcal{L}^{(E)}$ is made again by the reducing Legendre transformation. We introduce

$$\Phi^{(PE)}(e, f; T) = -S^{(PE)}(e, f) + \frac{1}{T}E(e, f) \quad (15)$$

and solve $\Phi_{e(r)}^{(PE)} = 0, \Phi_{f(r, v)}^{(PE)} = 0$. Solutions of these equations are denoted $(e, f)_{red}$. The reduced Legendre transformation of $S^{(PE)}(e, f)$ is $S^{*(PE)}(T) = [\Phi^{(PE)}(e, f; T)]_{(e, f) = (e, f)_{red}}$. The quantities $(\Phi_{e(r)}^{(PE)}, \Phi_{f(r, v)}^{(CE)})$ will be called conjugates of $(e(r), f(r, v))$ and denoted $(e^\ddagger(r), f^\ddagger(r, v))$.

Dynamic Legendre Reduction

The simplest time evolution making the passage $(e, f) \rightarrow (e, f)_{red}$ is governed by the following version of the Peierls kinetic equation (see more details in [3])

$$\begin{aligned} \frac{\partial e}{\partial t} &= -\partial_j \left(\int dv f \frac{\partial f^\ddagger}{\partial v_j} \right) \\ \frac{\partial f}{\partial t} &= \frac{\partial}{\partial v_j} \left(f \partial_j e^\ddagger \right) + \frac{\partial}{\partial v_j} \left(\Lambda^{(PE)} \frac{\partial f^\ddagger}{\partial v_j} \right) \end{aligned} \quad (16)$$

Indeed, (16) implies $\frac{d\Phi^{(PE)}}{dt} = -\int dr \int dv \frac{\partial f^\ddagger}{\partial v_j} f \Lambda^{(PE)} \frac{\partial f^\ddagger}{\partial v_j} < 0$ which means that the thermodynamic potential $\Phi^{(PE)}$ plays the role of the Lyapunov function for the approach $(e, f) \rightarrow (e, f)_{red}$ as $t \rightarrow \infty$. If the energy E in the fundamental thermodynamic relation (14) is given by $E = \int dre(r)$ then (16) implies also the energy conservation (i.e. $\frac{dE}{dt} = 0$).

3 Static and Dynamic Reduction to the Thermodynamics of Heat Flux

The systems discussed in the previous section were not prevented (either by external forces or by internal constraints) to reach thermodynamic equilibrium states at which their behavior is well described on the level $\mathcal{L}^{(E)}$. Now, we consider a situation when the systems are prevented from reaching the equilibrium states and consequently the level $\mathcal{L}^{(E)}$ is not available to them. We assume however that the Fourier level $\mathcal{L}^{(F)}$ is found to provide the setting describing well the experimentally observed behavior. We shall thus investigate two reductions: $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(F)}$ and $\mathcal{L}^{(P)} \rightarrow \mathcal{L}^{(F)}$. The main difference between these two reductions and the reductions discussed in the previous section is in the final destination of the reduction. In the reductions in Section 2 it was a subspace (composed of the equilibrium states) of the space serving as the state space on the level at which the reduction begins. In the reductions $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(F)}$ and $\mathcal{L}^{(P)} \rightarrow \mathcal{L}^{(F)}$ it is the vector field generating the time evolution on the reduced level. Since such vector field is determined (if we use the established terminology of fluid mechanics) by constitutive relations, the final destination of the reductions $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(F)}$ and $\mathcal{L}^{(P)} \rightarrow \mathcal{L}^{(F)}$ are not invariant or quasi-invariant subspaces of the state spaces $M^{(CE)}$ and $M^{(PE)}$ but constitutive relations on the Fourier level $\mathcal{L}^{(F)}$. Below, we shall describe briefly only the reduction $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(F)}$. The reduction $\mathcal{L}^{(P)} \rightarrow \mathcal{L}^{(F)}$ will be worked out in a separate paper.

Passage $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(F)}$

We shall follow closely the formulation of the reduction that we established in Section 2.

First, we turn to the specification of the state variables.

the state variable on $\mathcal{L}^{(C)}$ associated with $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(F)}$:

$$Q: \mathbb{R}^3 \rightarrow \mathbb{R}^3; r \mapsto Q(r) \quad (17)$$

The state space on the level $\mathcal{L}^{(C)}$ that is associated with the passage $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(F)}$ is denoted by the symbol $M^{(CF)}$ (i.e. $Q \in$

$M^{(CF)}$). The quantity $Q(r)$ is the heat flux appearing in the equation $\frac{\partial e}{\partial t} = -\partial_j Q_j$ governing the time evolution on the Fourier level $\mathcal{L}^{(F)}$.

The fundamental thermodynamic relation on $\mathcal{L}^{(C)}$ is given now by

$$\begin{aligned} & \text{the fundamental thermodynamic relation associated with} \\ & \mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(F)} : \\ & S^{(CF)} : M^{(CF)} \rightarrow \mathbb{R} \end{aligned} \quad (18)$$

The quantity $S^{(CF)}(Q)$ is the entropy on $\mathcal{L}^{(C)}$ associated with the passage $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(F)}$.

The passage $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(F)}$ is made by the reducing Legendre transformation. We introduce

$$\Phi^{(CF)}(Q; \Omega) = -S^{(CF)}(Q) + \Omega_j Q_j \quad (19)$$

and solve $\Phi_{Q(r)}^{(CF)} = 0$. Solution of this equation is denoted $Q_{red}(r)$. The reduced Legendre transformation of $S^{(CF)}(Q)$ is $S^{*(FC)}(\Omega) = [\Phi^{(CF)}(Q; \Omega)]_{Q=Q_{red}}$. The quantity $\Phi_Q^{(CF)} = Q^b$ is called a conjugate of Q .

Dynamics Legendre Reduction

The simplest among the time evolutions that make the passage $Q \rightarrow Q_{red}$ is the time evolution governed by

$$\frac{\partial Q}{\partial t} = -\Lambda^{(CF)} Q^b \quad (20)$$

where $\Lambda^{(CF)} > 0$ is a parameter. Since $\frac{d\Phi^{(CF)}}{dt} = -\int dr Q_j^b \Lambda^{(CF)} Q_j^b < 0$, the thermodynamic potential $\Phi^{(CF)}$ plays the role of the Lyapunov function for the approach $Q \rightarrow Q_{red}$ as $t \rightarrow \infty$.

Eq.(20) governs the fast time evolution in the time evolution governed by Eq.(12)

The choice of the the entropies S and the parameters Λ appearing in the reductions discussed in Section 2 are based solely on the evidence collected in experimental observations. When discussing the reduction $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(F)}$, we have an additional argument that helps us to make the choice. We require that the time evolution governed by (12) splits into the fast time evolution governed by (20) followed by the slow time evolution governed by (8). From this requirement we then expect to express the quantities appearing in (20) in terms of the quantities appearing in (12). In order to achieve it, we have to make a detailed analysis of solutions to (12) in which we recognize the fast and the slow parts of the time evolution. Below, we shall suggest a very simple solution that can however serve as the first approximation in a more detailed analysis.

We relate the quantities appearing in (20) to the quantities appearing in (12) as follows:

$$\begin{aligned} Q &= q^\ddagger; \quad S^{(CF)}(Q) = -\frac{1}{2} \int dr Q_j \Lambda^{(CE)} Q_j; \quad \Lambda^{(CF)} = (\Lambda^{(CE)})^{-1}; \\ \Omega_i &= -\partial_i e^\ddagger \end{aligned} \quad (21)$$

With these identifications, we see clearly that the first equation in (12) is $\frac{\partial e}{\partial t} = -\partial_j Q_j$. The second equation in (12) becomes $\frac{\partial q}{\partial t} = -\Phi_{Q(r)}^{(CF)}$. If we regard this equation as the equation governing the fast time evolution, then the states to which it approaches are solutions to $\Phi_{Q(r)}^{(CF)} = 0$. Such states are constitutive relations. This is because the last equality in (21) is the constitutive relation. Indeed, if we approximate e^\ddagger by e^\dagger then, as we see in (8), $-\partial_i e^\dagger$ is the thermodynamic force driving the time evolution of the internal energy in the Fourier theory. The second line in (21) is thus the Fourier constitutive relation. In the case of the externally imposed temperature gradient, the right hand side of the second line in (21) becomes the imposed temperature gradient.

The resulting entropy on the level $\mathcal{L}^{(F)}$ implied by the passage $\mathcal{L}^{(C)} \rightarrow \mathcal{L}^{(F)}$ is thus (we are making the approximation $e^\ddagger \sim e^\dagger$)

$$S^{*(FC)}(\nabla e^\dagger) = -\frac{1}{2} \int dr \partial_i (e^\dagger) (\Lambda^{(CE)})^{-1} \partial_i (e^\dagger). \quad (22)$$

We note that the entropy $S^{*(FC)}$ on the level $\mathcal{L}^{(F)}$, serving as the entropy in the thermodynamics of heat flow, equals the entropy production $\frac{dS^{(FE)}}{dt}$ multiplied by minus one.

4 Concluding Remarks

The well known motivation for going beyond the Fourier theory in the modeling of the heat conduction is the need to deal with the heat transfer in small electronic devices. We have shown that the formulation of more microscopic theories is also essential for the formulation of the thermodynamics of heat flux. A class of such type of extended thermodynamic theories has been introduced, probably for the first time, by Prigogine but it is the multiscale hierarchy of dynamical theories with established transitions among the levels where such theories find their foundation. The potential that generates the reducing dynamics (i.e. the potential generating the passage from a more microscopic to a less microscopic level) is the potential that, after completing the reducing time evolution, becomes the entropy on the reduced level.

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