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## Thermodynamics of reductions in multiscale dynamics

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**Abstract:** Thermodynamic formalism arises in multiscale dynamics as a mathematical expression of the compatibility of two dynamical theories describing the time evolution of the same macroscopic systems on two different levels of description.

**Keywords:** Thermodynamics, Contact geometry, Reductions in dynamical systems

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### 1. Introduction

Depending on our interests in the macroscopic systems under investigation and on the physics taking place in them, we choose an appropriate level of description to formulate models describing their behavior. For instance the behavior of water is found to be well described by the classical fluid mechanics if our interests are in the way it flows in rivers but the quantum mechanics is needed if we are interested in the structure of snow flakes. We also note that the more complex are the systems (as for example are the systems arising in biology and nanotechnology) the more it is difficult to satisfy our interests with only one level. A multilevel (also called a multiscale) descriptions are needed.

Our objective in this paper is to explore certain implications of the multiscale nature of modeling (in particular the thermodynamic formalism). In this investigation we continue the research reported previously in [1], [2].

Let

$$\dot{y} = G(y, \zeta) \quad (1)$$

be the dynamical system of our principal interest. We want to investigate solutions of (1). By  $y$  we denote the state variable,  $y \in N$ ,  $N$  denotes the state space,  $\dot{y}$  is the time derivative of  $y$ ,  $\zeta$  denotes a set of parameters.

Instead of specifying the vector field  $G$ , we introduce another dynamical system

$$\dot{x} = F(x, \xi) \quad (2)$$

and relate it to (1). The symbol  $x$  stands for a state variable,  $x \in M$ ,  $M$  denotes the state space, and  $\xi$  is a set of parameters. We assume that  $x \rightarrow y$  is a known mapping  $Y$

$$y = Y(x) \quad (3)$$

The dynamical systems (1) and (2) are related as follows. We assume that both (1) and (2) describe behavior of macroscopic systems observed in experiments. Moreover, we assume that they describe experimentally observed behavior of the same family of macroscopic systems but on two different levels of description. The model (2) includes more details than the model (1). In other words, the model (2) is more microscopic than the model (1). Hereafter, we shall call Level G the level of description on which the model (1) is formulated and Level F the level on which the model (2) is formulated. We shall also say that the two models (1) and (2) satisfying the above assumptions are mutually compatible.

The thermodynamic formalism presented below is a mathematical formulation of such compatibility. We shall see that one of its consequences is the emergence of a new potential on Level G. We shall denote it by the symbol  $S^{(G \leftarrow F)}(y)$ . In the context of the thermodynamic formalism this new potential has the physical interpretation of entropy on Level G that arises as a result of its compatibility with the model (2) formulated on Level F.

## 2. Thermodynamic formalism

The strategy that we follow in our search for the mathematical formulation of the compatibility of (1) and (2) is based on the following two observations.

### *Observation 1*

Let us assume that we have completely solved both (1) and (2). In other words, we assume that the phase portraits corresponding to both (1) and (2) are known. We recall that a phase portrait corresponding to (1) (we use the symbol  $(\mathcal{P}hp)_G$  to denote it) is a collection of all trajectories passing through all points  $y \in N$  for all values of the parameters  $\zeta$ . Similarly, the phase portrait corresponding to (2) (that is a collection of all trajectories passing through all points  $x \in M$  for all values of the parameters  $\xi$ ) is denoted by the symbol  $(\mathcal{P}hp)_F$ . Since both (1) and (2) describe the same behavior, the phase portrait  $(\mathcal{P}hp)_G$  has to be recognizable as a pattern in the phase portrait  $(\mathcal{P}hp)_F$ . The problem is thus to reformulate (2) in such a way that (1) becomes in it manifestly visible.

The strategy leading from more microscopic to less microscopic view is generally known as coarse graining. The coordinate dependence that this term immediately invokes does not serve well the investigation of reductions in dynamical systems. In fact, we all know from our innate ability to make passages from a detailed to an overall, and also reverse passages from an overall to a detailed, viewpoints (that we are making continuously in our visual perception) that these processes do not involve any coordinate dependent coarse graining. One of the main challenges in the investigation of reductions in dynamical systems is to introduce a really geometrical (i.e. in particular coordinate independent) definition of "coarse graining". We have called it above a "pattern recognition" but its precise mathematical definition remains an open problem.

### Observation 2

Where can we find a guide for such reformulation of (2)? We recall that the dynamical systems (1) and (2) describe behavior of real physical systems. They represent the experimentally observed physical phenomena, they are not just arbitrarily chosen dynamical systems. We can therefore ask the question of what is the most basic and the oldest physical theory describing the compatibility relation between two levels. In Section 2.1 below we argue that such theory is the classical thermodynamics. We shall base therefore our further investigation on this classical theory.

#### 2.1. Thermodynamics in $N$

The two levels that are compared in the classical equilibrium thermodynamics are the following: Level G is the macroscopic mechanics that includes heat and Level F is the microscopic mechanics of molecules and atoms.

The classical thermodynamics formulates the compatibility by ignoring Level F and only implicitly involving it in the formulation of Level G. The formulation on the Level G model proceeds as follows. The state variables in the macroscopic mechanics without heat and restricted only to statics are the energy per unit volume  $e$  and the number of moles per unit volume  $n$ . The heat is included by making two modifications. First, the energy  $e$  is let to include also the so called internal energy (speaking in terms of Level F, the internal energy is the energy of all atoms). The second modification is the emergence of a potential. This new potential is a real valued function of  $(e, n)$  satisfying certain properties that we shall list below. We shall see that one of the properties is that the potential has a tendency to reach always its maximal value allowed by imposed constraints. The potential is called entropy (we denote it by the symbol  $s$ ) and its tendency to reach maximum is often called the Maximum Entropy Principle or in an abbreviated form the MaxEnt principle [3], [4].

Level F enters explicitly the formulation only after we ask questions like: (i) what is the physical interpretation of the entropy  $s$ , where does this potential come from, (ii) given a macroscopic system, what is the functional relation  $s = s(e, n)$  representing it in the classical thermodynamics, (iii) why is the entropy always maximized. If we remain only on Level G then we are unable to find answers that could satisfy us. The viewpoint that includes Level F offers a deeper insight. Roughly speaking,  $s$  is the maximum value of a potential that originally arises in the reformulation of (2) in which the approach of Level F to Level G is manifestly displayed.

We now proceed to formulate the classical thermodynamics in the setting of contact geometry that appears to be the most convenient and natural to express the MaxEnt principle. It will become clear in Section 2.2 that such setting is also natural and convenient for formulating the time evolution expressing the compatibility of Level F and Level G.

In the particular case when Level G is the level of the classical equilibrium thermodynamic then  $y = (e, n)$ , where  $e$  is the energy per unit volume and  $n$  is the number of moles per unit volume. For later use, we shall formulate below the classical thermodynamics with a more general state variables  $y = (e, m); y \in N$ , where  $e$  is the total energy per unit volume and  $m$  stands for the remaining state variables. We introduce first thermodynamics into  $N$  formally and then, in Section 2.2, from the compatibility of Eq.(2) with Eq.(1).

Thermodynamics is formally introduced into  $N$  by introducing potential

$$s : N \rightarrow R; y \mapsto s(y) \in R \quad (4)$$

called an entropy per unit volume, and satisfying the following properties:

$$\begin{aligned} & s \text{ is a concave function} \\ & \frac{\partial s}{\partial e} > 0 \\ & s \text{ tends to its maximum allowed by constraints} \end{aligned} \quad (5)$$

The relation (4) is called a fundamental thermodynamic relation (see [5]).

The third property can also be alternatively formulated as a statement that the fundamental group of thermodynamics is the group of Legendre transformations. Indeed, the maximization allowed by constraints can also be cast into the following form. We introduce a new potential

$$\phi(y, y^*) = -s(y) + \langle y^*, y \rangle \quad (6)$$

called a thermodynamic potential in  $N$ ;  $y^* = (e^*, m^*)$ ,  $\langle, \rangle$  denotes pairing in  $N$ . The Legendre transformation  $s^*(y^*)$  of  $s(y)$  is made by passing through the following two steps: (*Step 1*) We note that finding a maximum of  $s(y)$  subjected to constraints fixing  $e$  and  $m$  is equivalent to finding a minimum of the thermodynamic potential  $\phi$ , where  $y^*$  play the role of Lagrange multipliers, i.e. to solving the equation  $\frac{\partial \phi}{\partial y} = 0$ ; let solutions to this equation be denoted by  $y_{eq}(y^*)$ . (*Step 2*)  $s^*(y^*) = \phi(y_{eq}(y^*), y^*)$ .

The natural mathematical setting for Legendre transformations is the space  $\mathbf{N} = T^*N \times R$  with element  $(y, y^*, \phi)$ ,  $y \in N$ ,  $y^* \in T_y^*N$ ,  $\phi \in R$ , where  $T_y^*N$  denotes the cotangent space over  $y \in N$ . The space  $\mathbf{N}$  is naturally equipped with the contact structure defined by 1-form  $\theta^N = d\phi - y^*dy$ . This 1-form is preserved in Legendre transformations. For the sake of simplicity we shall hereafter assume that  $N$  is a vector space equipped with the scalar product  $\langle, \rangle$ . By  $N^*$  we denote its dual. The space  $\mathbf{N}$  is now simply  $\mathbf{N} = N \times N^* \times R$ .

Having introduced the space  $\mathbf{N}$ , we can now see thermodynamics in  $N$  as a manifold  $\mathcal{N} \subset \mathbf{N}$  defined by

$$\mathcal{N} = \{(y, y^*, \phi) \in \mathbf{N} | y^* = \frac{\partial s}{\partial y}(y), \phi = s(y)\} \quad (7)$$

We call this manifold a **Gibbs-Legendre manifold in  $\mathbf{N}$**  because it naturally extends the Gibbs manifold  $\{(y, \phi) \in N \times R | \phi = s(y)\}$  [3] and because it is a Legendre manifold in the sense that  $[\theta^{(N)}]_{\mathcal{N}} = 0$ . If we replace the fundamental thermodynamic relation  $s = s(y)$  with its Legendre transform  $s^* = s^*(y^*)$  then the alternative representation of thermodynamics in  $N$  is the Gibbs-Legendre manifold as  $t \rightarrow \infty$

$$\mathcal{N}^* = \{(y, y^*, \phi) \in \mathbf{N} | y = \frac{\partial s^*}{\partial y^*}(y^*), \phi = s^*(y^*)\} \quad (8)$$

The contact-structure formulation of the classical thermodynamics has been introduced first in [6].

## 2.2. Thermodynamic time evolution

So far, the only knowledge that we have on Level G is the time evolution governed by (1). In addition, we know that the time evolution governed by (2), that takes place on a more microscopic level (Level F), is compatible with the time evolution governed by (1). We shall now use this additional information to increase our knowledge on Level G. From the compatibility of (2) and (1) we arrive at thermodynamics (in the sense of Section 2.1) on Level G.

Following the first observation that we made at the beginning of Section 2, we proceed by reformulating (2) into a fast time evolution approaching a submanifold  $\mathcal{M}_{th}$  followed by a slower time evolution on this submanifold. The slow time evolution governed by  $[Eq.(2)]_{\mathcal{M}_{th}}$  is then the time evolution on Level G governed by (1). The information that we have gained on Level G is the geometry of the manifold  $\mathcal{M}_{th}$  (playing now the role of the state space on Level G). The geometry is essentially, as we shall see below, the thermodynamics (in the sense of Section 2.1) on Level G.

Following the second observation that we made at the beginning of Section 2, we assume that the fact that (2) and (1) are compatible implies (irrespective of details of the time evolution equations (2) and (1)) that the fast time evolution has universal features of thermodynamics. We now proceed to formulate it.

### 2.2.1. Thermodynamics in $M$

We begin by formally introducing thermodynamics into  $M$  in the same way as we have formally introduced thermodynamics in Section 2.1 into  $N$ . We replace the space  $N$  by  $M$ , the state variables  $y$  by  $x$ , and the fundamental thermodynamic relation (4) by another fundamental thermodynamic relation

$$\begin{aligned}\eta : M &\rightarrow R; x \mapsto \eta(x) \in R \\ Y : M &\rightarrow N; x \mapsto Y(x) \in N\end{aligned}\tag{9}$$

Instead of the symbol  $s$  that we have used in Section 2.1 for the entropy in  $N$  (see (4)), we use in  $M$  the symbol  $\eta$ . The second line in (9) does not have an analogy in  $N$ . It is the mapping (3). Similarly as the space  $\mathbf{N}$  in Section 2.1, the space  $\mathbf{M} = T^*M \times R; (x, x^*, \varphi)$  is naturally equipped with the 1-form  $\theta^M = d\varphi - x^*dx$ .

Next, we start to build up a setting for the fast time evolution. We introduce a new space  $\mathbf{M}^N = T^*M \times N^* \times N \times R$  with elements  $(x, x^*, y^*, y, \varphi)$ ,  $x \in M, x^* \in T_x^*M, y^* \in N^*, y \in N, \varphi \in R$ . The space  $\mathbf{M}^N$  is naturally equipped with the 1-form  $\theta^{(M^N)} = d\varphi - x^*dx - y^*dy$ . Instead of the thermodynamic potential (6) we now introduce in  $\mathbf{M}^N$  the thermodynamic potential

$$\Phi(x, y^*) = -\eta(x) + \langle y^*, Y(x) \rangle\tag{10}$$

We shall assume that  $\eta$  and  $Y$  are such that  $\Phi$  defined in (10) is a convex function of  $x$ . The manifold representing thermodynamics in  $\mathbf{M}^N$  is now its submanifold

$$\begin{aligned}\mathcal{M} &= \{(x, x^*, y^*, y, \varphi) \in \mathbf{M}^N | x^* = \Phi_x(x, y^*), y = \Phi_{y^*}(x, y^*), \varphi = \Phi(x, y^*)\}; \\ &(x, y^*) \hookrightarrow (x, \Phi_x(x, y^*), y^*, \Phi_{y^*}(x, y^*), \Phi(x, y^*))\end{aligned}\tag{11}$$

called a **Gibbs-Legendre manifold in  $\mathbf{M}^N$** . We use hereafter the abbreviated notation  $\Phi_x = \frac{\partial \Phi}{\partial x}$ .

We note that in various projections of  $\mathcal{M}$  we see geometrically all the elements of the maximization of the entropy  $\eta(x)$  subjected to constraints  $Y(x)$ . Namely:

(i)

The manifold  $[\mathcal{M}]_{y^*=0}$  displays the fundamental thermodynamic relation (9). Indeed, the manifold  $[\mathcal{M}]_{y^*=0}$  is the image of the mapping  $x \mapsto (x, -\eta_x(x), 0, Y(x), -\eta(x))$ .

(ii)

The manifold  $[\mathcal{M}]_{x^*=0}$  displays the state  $x_{th}(y^*)$  in  $M$  at which  $\eta(x)$  subjected to constraints  $Y(x)$  reaches its maximum and also the fundamental thermodynamic relation (4) in  $N$  implied by the fundamental thermodynamic relation (9) in  $M$ . Indeed, the manifold  $[\mathcal{M}]_{x^*=0}$  is the image of the mapping  $(x, y^*) \mapsto (x_{th}(y^*), 0, y^*, Y(x_{th}(y^*)), \eta^*(y^*))$ , where  $\eta^*(y^*) = s^*(y^*)$  is the Legendre transformation of  $s = s(y)$ .

### 2.2.2. The time evolution in $\mathbf{M}^N$

Finally, we turn our attention to the time evolution describing approach of solutions to (2) to solutions to (1). We have seen that the space  $\mathbf{M}^N$  provides a suitable setting for MaxEnt passing from the fundamental thermodynamic relation (9) in  $M$  to the fundamental thermodynamic relation (4) in  $N$ . We shall use the same space and MaxEnt to formulate the time evolution providing the passage (2)  $\rightarrow$  (1).

In the static situation that we have discussed so far, the passage  $\eta(x) \rightarrow s(y)$  is made by Legendre transformation (i.e. by maximizing the entropy  $\eta(x)$  subjected to constraints  $Y(x)$ ). We recall that Legendre transformation in  $\mathbf{M}^N$  is a transformation preserving its contact structure (i.e. the 1-form  $\theta^{(M^N)} = d\varphi - x^*dx - y^*dy$ ). Let now construct a time evolution that makes the Legendre transformation leading from  $\eta(x)$  to  $s(y)$ . In other words, we look for a time evolution in  $\mathbf{M}^N$  that preserves its contact structure and brings  $\eta(x)$  to  $s(y)$  as  $t \rightarrow \infty$ . We shall call such time evolution a **thermodynamic time evolution**. To find it is our first problem. The second problem (discussed in Section 2.2.3) is then to relate the vector fields  $F$  and  $G$  appearing in (2), (1) to the quantities  $\eta(x)$ ,  $s(y)$  and others appearing in the thermodynamic time evolution.

The key result that allows us to tackle the first problem is the knowledge of the canonical form (see e.g. [7]) of the time evolution preserving the contact structure. In the particular case of  $\mathbf{M}^N$  equipped with the 1-form  $\theta^{(M^N)} = d\varphi - x^*dx - y^*dy$ , the time evolution preserving  $\theta^{(M^N)}$  is governed by

$$\begin{aligned}
 \dot{x} &= \Psi_{x^*} \\
 \dot{x}^* &= -\Psi_x + x^*\Psi_\varphi \\
 \dot{y}^* &= \Psi_y \\
 \dot{y} &= -\Psi_{y^*} + y\Psi_\varphi \\
 \dot{\varphi} &= -\Psi + \langle x^*, \Psi_{x^*} \rangle + \langle y, \Psi_y \rangle
 \end{aligned} \tag{12}$$

where

$$\Psi : \mathbf{M}^N \rightarrow R \tag{13}$$

is called a **contact Hamiltonian**.

The remaining problem is to identify the contact Hamiltonian  $\Psi$  satisfying the following three requirements:

$$\begin{aligned}
(1) & : [\Psi]_{\mathcal{M}} = 0 \\
(2) & : \mathcal{M} \text{ is an invariant manifold} \\
(3) & : \mathcal{M} \rightarrow \mathcal{N}^* \text{ as } t \rightarrow \infty
\end{aligned} \tag{14}$$

The first property is a general property of the contact Hamiltonian (see e.g. [7]), the second and the third properties are physical requirements. We want the thermodynamic time evolution to take place on the Gibbs-Legendre manifold representing the thermodynamics and we want the time evolution to bring the thermodynamics from the more microscopic Level F to the more macroscopic Level G.

The three properties (14) do not single out the contact Hamiltonian. Below, we present three examples of  $\Psi$ . In Section 2.2.3 we then discuss the physics involved in the process of choosing  $\Psi$ .

*Example 1*

$$\Psi(x, x^*, y^*, y, \varphi) = \frac{1}{2}(\langle \Phi_x, \Lambda \Phi_x \rangle - \langle x^*, \Lambda x^* \rangle) \tag{15}$$

where  $\Lambda : M^* \rightarrow M$  is an operator satisfying the following properties

$$\begin{aligned}
& \Lambda \text{ is independent of } (x, x^*, y^*, y, \varphi) \\
& \Lambda \text{ is symmetric and positive definite} \\
& \Lambda Y_x = 0
\end{aligned} \tag{16}$$

We now verify the properties (14). The first property is obviously satisfied. In order to investigate the second and the third properties, we evaluate (12) on  $\mathcal{M}$ . We obtain

$$\begin{aligned}
\dot{x} & = -\Lambda \Phi_x \\
\dot{x}^* & = -\Phi_{xx} \Lambda \Phi_x \\
\dot{y}^* & = 0 \\
\dot{y} & = 0 \\
\dot{\Phi} & = -\langle \Phi_x, \Lambda \Phi_x \rangle
\end{aligned} \tag{17}$$

We thus indeed see that the manifold  $\mathcal{M}$  is invariant and that the thermodynamic potential  $\Phi$  plays the role of the Lyapunov function for the approach  $x \rightarrow x_{th}(y^*)$  where  $x_{th}(y^*)$  is a solution of  $\Phi_x = 0$ . This proves that  $\mathcal{M} \rightarrow \mathcal{N}^*$  as  $t \rightarrow \infty$ .

We also note that from the mathematical point of view, the dynamics (17) is a gradient dynamics. The vector field is generated by gradient of a potential (the potential in our case is  $\Phi$ ) that is transformed into a vector by a metric tensor (in our case it is  $\Lambda$ ).

*Example 2*

The quadratic in  $x^*$  function  $\langle x^*, \Lambda x^* \rangle$  appearing in (15) can be replaced by a more general (convex in  $x^*$ ) function  $\Xi$  called a dissipation potential. We thus arrive at the second example of the contact Hamiltonian:

$$\Psi(x, x^*, y^*, y, \varphi) = [\Xi(x, x^*)]_{x^*=\Phi_x} - \Xi(x, x^*) \tag{18}$$



where the dissipation potential  $\Xi : T^*M \rightarrow R$  is required the following properties:

$$\begin{aligned}
& \Xi \text{ is independent of } (x, x^*, y^*, y, \varphi) \\
& \Xi, \text{ as a function of } x^* \text{ reaches its minimum at } (x, 0) \\
& \Xi \text{ is a convex function } x^* \text{ in a neighborhood of } (x, 0) \\
& \langle Y_x, [\Xi]_{x^*=\eta_x} \rangle = 0 \\
& [\Xi]_{x^*=Y_x} = 0
\end{aligned} \tag{19}$$

If (12) is restricted to  $\mathcal{M}$  we obtain

$$\begin{aligned}
\dot{x} &= -[\Xi_{x^*}]_{x^*=\Phi_x} \\
\dot{x}^* &= -\Phi_{xx}[\Xi_{x^*}]_{x^*=\Phi_x} \\
\dot{y}^* &= 0 \\
\dot{y} &= 0 \\
\dot{\Phi} &= -[\langle x^*, \Xi_{x^*} \rangle]_{x^*=\Phi_x}
\end{aligned} \tag{20}$$

The proof of the properties (14) follows closely the proof in the previous example.

From the mathematical point of view, the dynamical system (20) is a nonlinear generalization of the gradient dynamical system.

### Example 3

Having in mind the first property in (14), we note that we can add to (15) or (18) a term that, if evaluated on  $\mathcal{M}$ , becomes zero because of an antisymmetric multiplication rather than because of subtraction as it is in (15) or in (18). Such term is obviously  $\langle x^*, L\Phi_x \rangle$ , where  $L : M^* \rightarrow M$  is a skew-symmetric operator. If we take into account the physical context that we shall discuss in Section 2.2.3 then we propose

$$\Psi(x, x^*, y^*, y, \varphi) = -\mathcal{S}(x, x^*, y^*, y, \varphi) + \frac{1}{e^*} \mathcal{H}(x, x^*, y^*, y, \varphi) \tag{21}$$

where

$$\mathcal{S}(x, x^*, y^*, y, \varphi) = \Xi(x, x^*) - [\Xi(x, x^*)]_{x^*=\Phi_x} \tag{22}$$

and

$$\mathcal{H}(x, x^*, y^*, y, \varphi) = \langle x^*, L\Phi_x \rangle \tag{23}$$

where the dissipation potential  $\Xi$  is required to satisfy the properties (19) and the operator  $L$  the properties

$$\begin{aligned}
& L \text{ is skewsymmetric} \\
& L\eta_x = Lm_x = 0
\end{aligned} \tag{24}$$

We recall (see Section 2.1) that  $y = (e, m)$  and  $Y(x) = (e(x), m(x))$ , where  $e(x)$  is the energy per unit volume and  $m(x)$  are the remaining state variables in the space  $N$ .

If we evaluate now (12) with (21) playing the role of the contact Hamiltonian on  $\mathcal{M}$  we arrive at

$$\begin{aligned}
\dot{x} &= Le_x + [\Xi_{x^*}]_{x^*=\eta_x} \\
\dot{x}^* &= \Phi_{xx}(Le_x + [\Xi_{x^*}]_{x^*=\eta_x}) \\
\dot{y}^* &= 0 \\
\dot{y} &= 0 \\
\dot{\eta} &= [\langle x^*, \Xi_{x^*} \rangle]_{x^*=\eta_x}
\end{aligned} \tag{25}$$

From the mathematical point of view, the dynamics (25) is a combination of a Hamiltonian and gradient dynamics. We recall that in order that  $\dot{x} = Le_x$  be a Hamiltonian dynamics we need to assume that  $L$  satisfies an additional property, namely that  $\langle A_x, LB_x \rangle$ , where  $A$  and  $B$  are real valued sufficiently regular functions of  $x \in M$ , is a Poisson bracket (i.e. beside being antisymmetric it also satisfies the Jacobi identity). We note a very important mathematical difference between the contact-structure formulation (12), (21) and the explicit formulation (25). In the geometrical formulation (12), (21) the combination of the two types of dynamical systems is made by using one geometrical structure (namely the contact structure) to transform gradients of two potentials (namely  $\mathcal{S}$  and  $\mathcal{H}$ ). In the explicit formulation (25), the combination is made by using two geometrical structures (namely the symplectic structure  $L$  and the metric structure  $\Lambda$ ) to transform gradient of one potential (namely the thermodynamic potential  $\Phi$ ). The former formulation is clearly superior from the geometrical point of view.

Before leaving this section we make another comment indicating the advantage of the geometrical formulation (12), (21). We note that the first two equations in (12) can be obtained as Euler-Lagrange equations (variations are made with respect to  $x$  and  $x^*$ ) corresponding to the functional

$$\mathcal{I} = \int dt [\Psi(x, x^*, y^*) - \langle x^*, x \rangle] \tag{26}$$

We note that  $[\mathcal{I}]_{\mathcal{M}}$  has the physical interpretation of the total entropy generated during the approach from Level F to Level G. To the best of our knowledge there is no variational formulation of the explicit form (25) of the time evolution equations.

### 2.2.3. Relation of the thermodynamic time evolution to Eqs.(2) and (1)

In this section we make a few comments about the physical content of the above three examples of the contact Hamiltonian  $\Psi$ . The first one corresponds to a simple relaxation. The second one generates a more complex, nonlinear, relaxation needed for example in chemical kinetics (see [8]). The most important modification is made in the third example. If we take a completely microscopic viewpoint of macroscopic systems, their time evolution is Hamiltonian since the microscopic particles composing them evolve in time according to the classical or quantum mechanics that both are indeed Hamiltonian. It is therefore natural to expect that the mechanics (i.e. the Hamiltonian time evolution) will remain, at least partially, also in the macroscopic time evolution. In the absence of the first term on the right hand side of (21), the time evolution equations (12) represent indeed the Hamiltonian mechanics provided  $\langle A_x, LB_x \rangle$ , where  $A$  and  $B$  are real valued sufficiently regular functions of  $x \in M$ , is a Poisson

bracket. The formulation is different from but equivalent to the standard canonical formulation of the Hamiltonian dynamics. Its main advantage is that it naturally accepts (i.e. without a need of bringing into the formulation another geometry, just by adding another generating potential) gradient dynamics. This cannot be done in the setting (25). The two terms on the right hand side of (25) cannot be put into the setting involving only one geometrical structure.

Finally, we face the following problem. We know (2) and we want to reformulate it in the form (12) and (1). What is the relation between  $F$  appearing in (2) and the contact Hamiltonian  $\Psi$  appearing in (12)? To answer this question we need to enter into a detail analysis of solutions to (2). We have already commented about the difficulty of this type of analysis in the Observation 1 in Section 2 (see more in [9], [10]).

There is also an alternative point of view of (2) versus (12). We do not begin with the knowledge of (2). We assume that we just know (1) and the physics associated with it on Level G. Our goal is now to try to carry and appropriately adapt the same physics to the more microscopic Level F. Our starting assumption is that the model on Level F will have the form (12) and (1). It is thus the extension of the physics from Level G to Level F that will give us the contact Hamiltonian  $\Psi$ .

Neither the first nor the second routes are pursued in this paper. We make only a few observations regarding the first route in the illustration presented in the next section. As for the second route, we can illustrate it for example on the modeling of the flow behavior of soft and dense colloids in [11].

### 3. Illustration

The macroscopic system under investigation in this illustration is a solid heat conductor in which only heat conduction takes place and all the other possible changes associated with it are ignored.

The equation representing (1) is the Fourier equation

$$\frac{\partial e}{\partial t} = -\partial_i(\lambda^{(Four)}\partial_i h_e) \quad (27)$$

where  $e : R^3 \rightarrow R$ ;  $\mathbf{r} \mapsto e(\mathbf{r})$  is the internal energy. This is the state variable playing the role of  $y$  in (1). By the symbol  $\partial_i$  we denote  $\frac{\partial}{\partial r_i}$ ;  $i = 1, 2, 3$ . We use hereafter the summation convention. The symbol  $h$  stands for a potential  $h : R^3 \rightarrow R$  that is assumed to be sufficiently regular and concave;  $\lambda^{(Four)} > 0$  is a parameter called a Fourier heat conductivity coefficient.

A more microscopic viewpoint of heat conduction (needed for example if at least one dimension of the conductor is of the order of  $10^{-8}$  or  $10^{-9}$  meters) we take to be represented by the simplest version

$$\begin{aligned} \frac{\partial e}{\partial t} &= -\partial_i q_i \\ \frac{\partial q_i}{\partial t} &= \frac{1}{\tau}(-q_i + \lambda^{(Catt)}\partial_i h_e) \end{aligned} \quad (28)$$

of the Cattaneo theory [12]. We regard now (28) as (2). This means that  $x = (e, \mathbf{q})^T$ ;  $\mathbf{q} : R^3 \rightarrow R^3$  is called a heat flux. The mapping (3) is  $(e, \mathbf{q})^T \mapsto e$ . The potential  $h$  is the same as in (27), the parameters in (28) are  $\lambda^{(Catt)} > 0$  and  $\tau > 0$ .

An analysis of solutions to (28) is straightforward. If  $\tau \rightarrow 0$  then solutions to (28) tend to solutions to (27) with  $\lambda^{(Catt)} = \lambda^{(Four)}$ . It is also easy to identify the contact Hamiltonian in (12). We take

$$\Phi(x) = -h(e) - \int d\mathbf{r} \left( -\frac{\alpha}{2} \mathbf{q}^2 + \alpha \lambda^{(Four)} \partial_i(h_e) q_i \right) \quad (29)$$

and the contact Hamiltonian (15) with  $\Lambda = \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{2\tau} \end{pmatrix}$ . With these specifications, the fast time evolution is governed by

$$\frac{\partial q_i}{\partial t} = \frac{1}{\tau} (\Phi_{q_i}) \quad (30)$$

Solutions of  $\Phi_{\mathbf{q}} = 0$  is  $(q_i)_{th} = \lambda^{(Four)} \partial_i(h_e)$ . This means that the thermodynamic potential on the Fourier level arising from its compatibility with the Cattaneo level is

$$S^{(Four \leftarrow Catt)} = [\Phi]_{\mathbf{q}=\mathbf{q}_{th}} = -h(e) - \frac{\alpha(\lambda^{(Four)})^2}{2} \int d\mathbf{r} \partial_i(h_e) \partial_i(h_e) \quad (31)$$

Now we turn our attention to the analysis of solutions of Eq.(27). An important role in such investigation plays the potential  $h$ . Equation (27) implies  $\frac{dh}{dt} > 0$  provided the solid conductor under investigation is confined to  $\Omega \subset R^3$  and the boundary conditions on its boundary are periodic. Consequently,  $-h$  plays the role of the Lyapunov function for the approach, as  $t \rightarrow \infty$ , to solutions to  $h_e = constant$ . The potential  $S^{(Four \leftarrow Catt)}$  (see(31)), that we have obtained from the compatibility of the Fourier dynamical theory with the more microscopic Cattaneo dynamical theory, is a nonlocal extension of the potential  $h$ . In the context of equilibrium statistical mechanics this type of extensions are made phenomenologically and are known as Cahn-Hilliard nonlocal extensions [13]. Our arguments that led us to (31) are based on the other hand on dynamics, more specifically, on the comparison of two dynamical theories formulated on two different levels of description. The potential  $h$  does arise from an analysis of solutions of (27) but its extension (31) does not. The extended potential (31) arises from an analysis of solution to (28) that expresses a more detailed physics than the one expressed mathematically in (27). We can for example use (31) to construct a nonlocal extension of the Fourier equation (27). If we replace  $h$  in (27) by  $h + \frac{\alpha\lambda^{(Four)}}{4} \int d\mathbf{r} \partial_i(h_e) \partial_i(h_e)$  we arrive at

$$\frac{\partial e}{\partial t} = -\partial_i \left( \lambda^{(Four)} \partial_i \left( h_e - \alpha \lambda^{(Four)} \partial_i(h_e \partial_i h_e) \right) \right) \quad (32)$$

that can be seen as representing a nonlocal extension of the Fourier theory implied by its compatibility with the Cattaneo theory.

#### 4. Conclusion

Restriction to a single level of description means that details seen on other levels are ignored. To justify such assumption becomes particularly difficult in complex systems, as for instance biological systems. But even if the situation under investigation is such that the assumption is justified, the formulation on more levels brings a new information that can possibly be useful inside a single level analysis. In this paper we explore the concept of the compatibility of two dynamical theories formulated on two different levels of description. We argue that the mathematical formulation of such compatibility

is a general formulation of thermodynamics. We call it a thermodynamic formalism. Regarding its possible usefulness in the analysis of specific problems we mention two results: (i) The thermodynamic formalism provides a setting for a geometrical and also variational formulation of dynamics combining the symplectic and the gradient dynamics. (ii) The thermodynamic formalism provides a new potential on the more macroscopic level. The potential arises from the compatibility with a more microscopic level and is not directly related to the dynamics on the more macroscopic level. The latter result is illustrated on the analysis of the compatibility of the Cattaneo and the Fourier heat conduction theories.

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### Conflicts of Interest

The authors declare no conflict of interest.

### References

1. Grmela, M., Role of thermodynamics in multiscale physics. *Computers and Math. Appl.* **2008**, *65*, 1457-1470.
2. Grmela, M., Contact Geometry of mesoscopic Thermodynamics and Dynamics. *Entropy* **2014**, *16*, 1652-1686.
3. Gibbs, J. W., In *Collected Works*; Longmans: Green and Comp. New York, 1984.
4. Jaynes, E. T., In *Foundations of probability theory and statistical mechanics, in Delaware Seminar in the Foundation of Physics*; Editor, M. Bunge, ; Springer New York, 1967.
5. Callen, H. B., In *Thermodynamics*; Wiley: New York, 1960.
6. Hermann, R., In *Geometry, Physics and Systems*; Marcel Dekker: New York, 1973.
7. V.I. Arnold, In *Mathematical methods of classical mechanics*; Springer: New York, 1989.
8. Grmela, M., Fluctuations in extended mass-action-law dynamics. *Physica D* **2012**, *241*, 976-986.
9. Villani, C., Particle systems and nonlinear Landau damping. *Phys. Plasmas* **2014**, *21*, 030902.
10. Gorban, A.N.; Karlin, I.V., *Hilbert's 6th Problem: Exact and Approximate Hydrodynamic Manifolds for Kinetic Equations*; Bulletin (New Series) of the Am. Math. Soc. S, 2013; 0373-0979 Nov 20.
11. M. Grmela, A. Ammar, F. Chinesta, G. Maîtrejean, A mesoscopic rheological model of moderately concentrated colloids. *J. Non-Newtonian Fluid. Mech.* **2014**, *212*,1-12.
12. C. Cattaneo, Sulla conduzione del calore, Atti del Seminario Matematico e Fisico della Università di Modena, **3**, 83-101 (1948)
13. J.W. Cahn, J.E. Hilliard, Free Energy of a Nonuniform System. Interfacial Free Energy. *J. Chem. Phys.* **1958**, *28*,258.

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