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CR THERMODYNAMICS OF EXTERNALLY DRIVEN MACROSCOPIC SYSTEMS

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ABSTRACT

Let the time evolution of an externally driven macroscopic system be found to be well described by two different dynamical systems (*MESO-dynamics* and *meso-dynamics*) formulated on two different levels of description. One of the levels (*MESO-level*) takes into account more details (or in other words, is more microscopic) than the other (*meso-level*). If this is the case then the *meso-leve*l becomes equipped, in addition to the *meso-dynamics*, also with a *meso-thermodynamics*. The abstract mathematical setting for the *MESO* $\to$ *meso* passage leading to thermodynamics on the *meso-level* is illustrated on two examples: *MESO* $\to$ *equilibrium* reduction, and the *MESO* $\to$ *meso* reduction of externally driven systems. Details can be found in [1].

Static Legendre reduction

Let x denote the state variables on the *MESO-level*; $x \in M$, M denotes the state space on the *MESO-level*. We introduce three functions (V,W,Y): $V : M \to \mathbb{R};\ \ W : M \to \mathbb{R};\ \ Y : M \to N$, where N is a space associated with the target level (i.e. the *meso-level*) of the reduction. Next, we introduce

$$\Phi(x;v^*,w^*,Y^*) - -V(x) + < Y^*, Y(x) > \tag{1}$$

where $Y^* \in N^*$, $<,>$ is the pairing in N, and N^* is the dual of N. We shall call Φ a thermodynamic potential on the *MESO-level*. We assume that $-V$ is a convex function and Y is such that $\Phi_x = 0$ has only one solution denoted $x_0(Y^*)$. By Φ_x we denote $\frac{\partial \Phi}{\partial x}$. If M is an infinite dimensional space then $\frac{\partial}{\partial x}$ denotes an appropriate functional derivative. The function

$$\varphi(Y^*) = [\Phi(x;Y^*)]_{x=x_0(Y^*)} \tag{2}$$

is a Legendre reduction of the potential Φ. We shall call φ a thermodynamic potential on the *meso-level*. The Legendre reduction thus transfers thermodynamics on the *MESO-level*, expresse in the thermodynamic potential Φ, to thermodynamics on the *meso-level* expressed in the thermodynamic potential φ.

Dynamic Legendre reduction

The passage $x \to x_0(Y^*)$ made in the static Legendre reduction by minimizing the potential Φ is made in the dynamic Legendre reduction by following the time evolution of x. From the physical point of view, the time evolution represents the process of preparing the macroscopic system under investigation for the *meso-level* description of its behavior. The time evolution that makes the $x \to x_0(Y^*)$ passage is governed by

$$\dot{x} = -\mathcal{L}\Phi_x \tag{3}$$

where $\mathcal{L}$ is a bivector transforming the covector Φ_x into a vector. In addition, we require that $\mathcal{L}$ is such that $\dot{\Phi} = - < \Phi_x, \mathcal{L}\Phi_x > \leq 0$ and that the thermodynamics potential Φ_x plays the role of the Lyapunov function for the $t \to \infty$-approach to $x_0(Y^*)$.

Summing up, in order to formulate the preparation process leading from *MESO-level* to *meso-level* we need to equipp the state space M with the following structure: (i) the thermodynamic potential Φ and (ii) the geometrical structure, mathematically expressed in the operator $\mathcal{L}$, providing the passage from covectors to vectors. In the next two paragraphs we work out two specific illustrations.

MESO* $\to$ *equilibrium

The reduced *meso-level* is in this illustration the level of the classical equilibrium thermodynamics. We shall call it *equilibrium-level*. All quantities arising in this illustration are equipped with the superscript (Me). The macroscopic systems under consideration in this illustration are externally unforced. No time evolution takes place on the *equilibrium-level*. The time evolution governed by (3) represents the preparation process for applicability of the equilibrium thermodynamics (implicitly included in *Postulate 0* of the equilibrium thermodynamics) consisting of leaving the system without external influences for sufficiently long time.

The potential V is in this illustration the entropy $S^{(Me)}$, N is a two dimensional space of the equilibrium state variables (E,N) denoting the energy and the number of moles per unit volume, $Y(x) = (E(x),N(x))$, $Y^* - (\frac{1}{T}, -\frac{\mu}{T})$, where T is the equilibrium temperature and μ the chemical potential. The thermodynamic potential (1) takes the form

$$\Phi^{(Me)}(x;T,\mu) = -S^{(Me)}(x) + \frac{1}{T}E(x) - \frac{\mu}{T}N(x) \tag{4}$$

The time evolution equation (3) becomes

$$\dot{x} = TL\Phi_x^{(Me)} - [\Xi_{x^*}(x,x^*)]_{x^*=\Phi_x^{(Me)}} \tag{5}$$

that is known as GENERIC equation [2], [3]. The first term on the right hand side of (5) represents the Hamiltonian time evolution (the operator L is a Poisson bivector), the second term represents a generalized gradient dynamics (Ξ is called a dissipation potential). One particular example of

(5) is the Boltzmann kinetic equation. In this particular illustration, x is one particle distribution function, $S^{(Me)}$ is the Boltzmann entropy, E is the kinetic energy, and N is the normalization of the distribution function. The reduced thermodynamics expressed in the thermodynamic potential (2) is in this example the equilibrium thermodynamics of the ideal gas. The expressions for L and Ξ can be found in [1].

MESO* $\rightarrow$ *meso

Macroscopic systems subjected to external forces do not reach equilibrium sates and their behavior cannot be thus described on the *equilibrium-level* (i.e. by the classical equilibrium thermodynamics). Very often however a mesoscopic level (*meso-level*) providing a good description of the experimentally observed behavior is found. For instance, the observed behaviour of the Rayleight-Bénard system (a horizontal layer of fluid heated from below) is found to be well described on the level fluid mechanics, that thus plays in this example the role of the *meso-level*. If we then choose for the description a more detailed *MESO-level*, we should be able to prepare the system (by following the time evolution governed by (3)) to states $x_0(Y^*)$ at which the *meso-level* becomes applicable.

How shall we choose the space N? There are in fact two possibilities: (i) we choose it to be the state space of the *meso-level*, or (ii) we choose it to be the vector field of the *meso-dynamics* (or in other the fluxes arising on the right hand side of the equations governing the time evolution on the *meso-level*). In the former case, $Y(x)$ are the *meso-level* state variables expressed in terms of the the *MESO-level* state variables, Y^* are the conjugate *meso-level* state variables, and φ given in (2) is the thermodynamic potential on the *meso-level* that is implied by the thermodynamic potential Φ on the *MESO-level*. In the latter case, $Y(x)$ are the *meso-level* fluxes expressed in terms of the the *MESO-level* state variables, Y^* are forces (both externally imposed forces and the forces introduced in constitutive relations), φ given in (2) has the physical interpretation of the entropy production rather then of the entropy and it represents a novel thermodynamics of driven systems whose behavior can be well described on both *MESO-level* and *meso-level*. With this choice of the space N, the time evolution equation (3) has been called in [1] CR-GENERIC (CR stands for Constitutive Relations).

References

[1] M. Grmela, Externally driven macroscopic systems: Dynamics versus Thermodynamics, J.Stat.Phys. **166**, 282-316 (2017).

[2] M. Grmela, H.C. Öttinger, Dynamics and thermodynamics of complex fluids: I general formulation, Phys. Rev. E 56 (1997) 66206633.

[3] H.C. Öttinger, M. Grmela, Dynamics and thermodynamics of complex fluids. II. Illustrations of a general formalism. Phys. Rev. E 1997, 56, 66336655