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Steepest Entropy Ascent Model for Far-Non-Equilibrium Thermodynamics. Unified Implementation of the Maximum Entropy Production Principle

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Abstract: We report on work published recently in Phys. Rev. E **90**, 042113 (2014), where by suitable reformulations, we cast the mathematical frameworks of several well-known different approaches to the description of non-equilibrium dynamics into a unified formulation valid in all these contexts, which extends to such frameworks the concept of Steepest Entropy Ascent (SEA) dynamics introduced by the present author in previous works on quantum thermodynamics. Actually, the present formulation constitutes a generalization also for the quantum thermodynamics framework. The analysis emphasizes that in the SEA modeling principle a key role is played by the geometrical metric with respect to which to measure the length of a trajectory in state space. In the near thermodynamic equilibrium limit, the metric tensor turns is directly related to the Onsager's generalized resistivity tensor. Therefore, through the identification of a suitable metric field which generalizes the Onsager generalized resistance to the arbitrarily far non-equilibrium domain, most of the existing theories of non-equilibrium thermodynamics can be cast in such a way that the state exhibits the spontaneous tendency to evolve in state space along the path of SEA compatible with the conservation constraints and the boundary conditions. The resulting unified family of SEA dynamical models are all intrinsically and strongly consistent with the second law of thermodynamics. The nonnegativity of the entropy production is a general and readily proved feature of SEA dynamics. In several of the different approaches to non-equilibrium description we consider here, the SEA concept has not been investigated before. We believe it defines the precise meaning and the domain of general validity of the so-called Maximum Entropy Production principle. Therefore, it is hoped that the present unifying approach may prove useful in providing a fresh basis for effective, thermodynamically consistent, numerical models and theoretical treatments of irreversible conservative relaxation towards equilibrium from far non-equilibrium states. The mathematical frameworks are: A) Statistical or Information Theoretic Models of Relaxation; B) Small-Scale and Rarefied Gases Dynamics (i.e., kinetic models for the Boltzmann equation); C) Rational Extended Thermodynamics, Macroscopic Non-Equilibrium Thermodynamics, and Chemical Kinetics; D) Mesoscopic Non-Equilibrium Thermodynamics, Continuum Mechanics with Fluctuations; E) Quantum Statistical Mechanics, Quantum Thermodynamics, Mesoscopic Non-Equilibrium Quantum Thermodynamics, and Intrinsic Quantum Thermodynamics.

Keywords: steepest entropy ascent; maximum entropy production; nonequilibrium thermodynamics

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1. Introduction

In Ref. [1], we reformulate with a somewhat unusual notation the essential mathematical elements of several different approaches to the description of non-equilibrium dynamics with the purpose of presenting a unified formulation which, in all these contexts, allows to implement the local Steepest Entropy Ascent (SEA) concept whereby the dissipative, irreversible component of the time evolution the local state is assumed to pull the state along the path in state space which, with respect to an underlying metric, is always tangent to the direction of maximal entropy increase compatible with the local conservation constraints.

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Such reformulations not only allow a precise meaning, general implementation, and unified treatment of the so-called Maximum Entropy Production (MEP) principle (for a recent review see [2]) in the various frameworks, but also extends to all frameworks an observation that we have been developing as part of an extreme view of the quantum thermodynamics context for the last three decades [3–8]. In doing so, Ref. [1] introduces an important generalization also for the quantum thermodynamics modeling framework.

The resulting SEA unified formulation allows us to extend at once to all the cited frameworks the SEA concept which has so far been considered only in the framework of quantum thermodynamics. However, a similar or at least closely related set of assumptions underlie the well-known GENERIC scheme [9–12] which developed independently.

An important observation that we emphasize in the SEA construction is that the entropy production cannot be meaningfully maximized subject just to a set of conservation constraints or boundary and symmetry conditions, but in order to identify a SEA path in state space we must equip the state space with a metric field with respect to which to compute the distance between states and hence the distance traveled during the time evolution. Thus, a key role is played by the geometrical metric with respect to which to measure the length of a trajectory in state space. Once this is done, the metric tensor turns out to be directly related to the Onsager's generalized resistivity tensor, which physically characterizes the system and, at least in the near-equilibrium regime, represents the strength of its reaction when pulled out of equilibrium.

In a forthcoming technical paper [13] we will prove that under broad conditions the description of dissipation assumed in GENERIC is equivalent (if not coincident) with the SEA principle. The formal relation between the SEA metric tensor $\hat{G}$ and the GENERIC dissipative tensor (usually denoted by M) can be established by means of a detailed technical analysis of the respective underlying mathematical landscapes. There, we discuss the analogies and differences of the SEA and GENERIC approaches and show under what conditions their descriptions of the dissipative part of the time evolution can be considered essentially equivalent.

In our previous work, we recognized the need for an explicit selection of a metric for the state space, but because in quantum thermodynamics the state representative, the density operator, is essentially a generalized probability distribution, we adopted the uniform metric for probability distributions, namely, the Fisher-Rao metric, which is appropriate [14–16] when no additional constraints due to symmetries and internal structure are introduced which effectively "distort" the uniformity of the state space. For example, the role of such symmetries has been discussed in the framework of Mesoscopic Non-Equilibrium Thermodynamics in Refs. [17,18] where it is shown that standard results such as the Fokker-Planck equation and Onsager theory emerge in the near-equilibrium limit. Our generalized SEA approach, could be used to extend such results into the far non-equilibrium domain, while maintaining full thermodynamic consistency.

In Ref. [1] we conclude that in most of the existing theories of non-equilibrium the time evolution of the local state representative can be seen to actually follow in state space the path of SEA with respect to a suitable metric connected with the generalized resistivity tensor of the fluid, material, or system. This is true in the near-equilibrium limit, where in all frameworks it is possible to show that the traditional assumption of linear relaxation coincides with the SEA result.

Far from equilibrium the SEA dynamical models may turn out to be a very fundamental as well as practical starting point to warrant an intrinsic consistency with the second law of thermodynamics which follows not only from the nonnegativity of the local entropy production density but also from other interesting features. For example, as required by the second law [19,20], we prove the instability of the equilibrium states that do not have the maximum local entropy density for the given local values of the densities of the conserved properties. Such conclusions are general and emerge from the SEA construction in a relatively straightforward way, and hold regardless of the details of the underlying metric tensor.

In a variety of fields of application, the present unifying approach may prove useful in providing a new basis for effective numerical and theoretical models of irreversible, conservative relaxation towards equilibrium from far non-equilibrium states as well as of far-from-equilibrium steady states such as in shocks. For example, see Refs. [21,22]

Future work is needed to address also the relationships and establish differences and similarities between the SEA description of far from equilibrium dissipation and other closely related approaches, such as the recent Contact Geometry of Mesoscopic Thermodynamics and Dynamics [23–25], the general ideas of the Rate-Controlled Constrained-Equilibrium Approach to Far-From-Local-Equilibrium Thermodynamics [26,27] of the Quasi-Equilibrium approximation of Invariant Manifolds [28], of the MEP formulations of chemical kinetics by Ziegler [29,30] and others [31–34] as well as the works of Edelen [35].

We conclude with a more philosophical note, again from Ref. [1], about the question of what is the scope and physical significance of the SEA principle.

The question of what is "the physical basis" for the SEA scheme (or for that is the same, for the GENERIC scheme) is tricky and in philosophically ill posed. It is as if one would ask what is the physical basis for believing that a classical system should obey Hamilton's equations or the equivalent minimum action principle. The meaning of "physical reality" is well explained in the classic book on this subject by Henry Margenau [36]. There is a level of perceptions, the empirical world, that we try to describe by defining concepts, their relations with the plane of perceptions (operational measurement procedures), and relations among concepts that we call laws or principles (often using the language of mathematics to express them efficiently). The farther the construction goes from the plane of perceptions the more "abstract" it becomes, but the advantage is that more abstraction may allow to encompass and regularize a broader set of less abstract theories, in short, to unify them. At any level of abstraction, what makes a theory "physical" are its links to the plane of perception, namely the fact that the theory allows to model some empirical evidence with some reasonable level of approximation.

Paraphrasing words of Feynman, what makes a particular law or principle "great", such as the great conservation principles or the second law of thermodynamics, is the fact that they hold for whatever level of description of whatever empirical reality, provided the model has some basic structure and obeys some reasonable conditions, such as those that grant and give meaning to the concept of separability between the object of study and its surroundings. The spirit of the SEA construction is precisely this. We consider a number of frameworks that have successfully modeled non-equilibrium systems at some level of description, we focus on how these successful models of physical reality describe entropy production by irreversibility, and we cast them in a way that allows us to see that they can all be encompassed and regularized by the unifying geometrical SEA construction. The GENERIC construction is even more ambitious in that it attempts to unify at once also the reversible and transport contributions by recognizing their common Hamiltonian structure and their relations with the irreversible aspects of the dynamics.

Being more abstract (i.e., farther from Margenau's plane of perceptions) than the various physical theories they unify, the SEA and GENERIC constructions emerge as general dynamical principles which operate within the same domain of validity and hence a similar level of "greatness" of the second law of thermodynamics, by complementing it with the additional essential elements about non-equilibrium behavior.

An important fraction of the greatness of the second law of thermodynamics stems from the fact that it supports the operational definition of entropy [37,38] as a property of any well-defined system and in any of its equilibrium and non-equilibrium states. Other good fractions that have direct impact also on the near-equilibrium description of dynamics derive from the stability and maximal entropy features of the equilibrium states.

An important fraction of the greatness of the SEA principle stems from the fact that for any well-defined system it supports the operational definition of the metric field $\hat{G}$ over its entire state space, which characterizes even in the far non-equilibrium domain all that can be said about the spontaneous, irreversible, entropy generating tendency towards stable equilibrium. Another good fraction derives from the fact that within the SEA construction the maximum entropy production (MEP) principle acquires a precise and general validity whereby, in any well-defined model, the entropy producing component of the dynamics effectively pulls the state of the system in the direction of steepest entropy ascent compatible with the metric field $\hat{G}$ and the imposed conservation laws.

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