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A hierarchy of Poisson brackets in non-equilibrium thermodynamics

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HIGHLIGHTS

- A natural hierarchy of Poisson brackets is explained in the context of non-equilibrium thermodynamics.
- A novel grand-canonical hierarchy of Poisson brackets is proposed.
- New Poisson brackets for non-local phenomena are derived from the hierarchy.
- Some of the projections of Poisson brackets are formulated as Lie–Poisson reductions.

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ABSTRACT

Reversible evolution of macroscopic and mesoscopic systems can be conveniently constructed from two ingredients: an energy functional and a Poisson bracket. The goal of this paper is to elucidate how the Poisson brackets can be constructed and what additional features we also gain by the construction. In particular, the Poisson brackets governing reversible evolution in one-particle kinetic theory, kinetic theory of binary mixtures, binary fluid mixtures, classical irreversible thermodynamics and classical hydrodynamics are derived from Liouville equation. Although the construction is quite natural, a few examples where it does not work are included (e.g. the BBGKY hierarchy). Finally, a new infinite grand-canonical hierarchy of Poisson brackets is proposed, which leads to Poisson brackets expressing non-local phenomena such as turbulent motion or evolution of polymeric fluids. Eventually, Lie–Poisson structures standing behind some of the brackets are identified.

1. Introduction

The principal goal of statistical mechanics is to extract pertinent features from the complete microscopic information contained in trajectories of microscopic particles composing macroscopic systems under consideration. The pertinent features are those seen in mesoscopic and macroscopic experimental observations. We look for a reduced (mesoscopic) time evolution which concentrates only on the pertinent features and ignores the irrelevant details. The reduction process from the micro to the meso dynamics (consisting of three steps, (i) finding microscopic trajectories, (ii) extracting from them the pertinent pattern, and (iii) constructing mesoscopic dynamics whose trajectories reproduce the pattern) is, in general, very complex. It is therefore very useful to realize that the microscopic, the mesoscopic, and the macroscopic time evolutions share a common structure, namely that the reversible evolution is expressed by means of a Poisson bracket and energy, see [1–7].

The two latter references introduce the General Equation for Non-Equilibrium Reversible–Irreversible Coupling (GENERIC). The GENERIC framework contains a large amount of mesoscopic models, e.g. classical hydrodynamics, Boltzmann equation, classical irreversible thermodynamics (CIT), extended irreversible thermodynamics (EIT), see [8], models for polymer flows, visco-elasto-plastic solids [9], etc. The main features of GENERIC are that the reversible part of the evolution equations is constructed from a Poisson bracket while the irreversible from a dissipation potential (or dissipative bracket when thermodynamic forces are small), and

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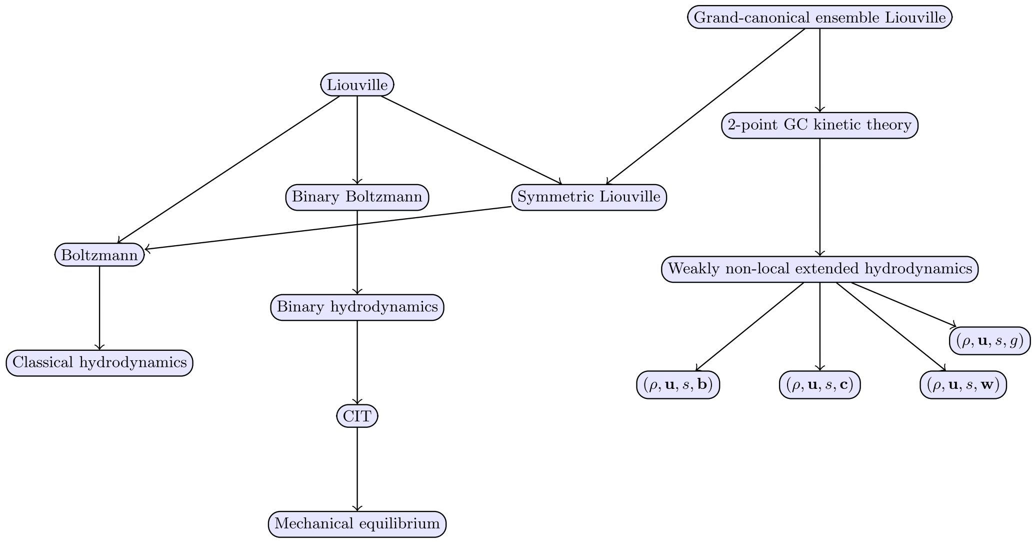

Fig. 1. Map of demonstrated projections. Note that if there is a projection from A to B and from B to C, then there is a projection from A to C. Starting from Liouville equation (or Liouville–Poisson bracket), Poisson brackets of Boltzmann equation and classical hydrodynamics are given by a straightforward projection. Similarly, Poisson bracket governing reversible evolution in kinetic theory of binary mixtures (binary Boltzmann equation) follows from the Liouville–Poisson bracket and it yields Poisson brackets for binary hydrodynamics (with two densities, momentum densities and entropy densities or temperatures) and for classical irreversible thermodynamics. Grand-canonical ensemble of Liouville equations, where number of particles can vary, can be simplified to the standard N-particle Liouville equation or it can be projected to a two-point kinetic theory, to weakly non-local extended hydrodynamics possibly useful in turbulence modeling or to the Poisson bracket coupling a spatial correlation function with hydrodynamic fields.

that the equations are also automatically compatible with equilibrium thermodynamics as they gradually approach equilibrium. The Hamiltonian structure of reversible evolution is common to a large class of models in continuum physics on many levels of description, see also [10], and we shall thus require that passages from levels with more details to levels with less details preserve the structure.

In this paper we focus on relations between Hamiltonian structures governing reversible evolution on different levels of description. This means that on the level of the microscopic dynamics of all particles composing macroscopic systems we consider the complete dynamics but on mesoscopic levels we consider only a part of the dynamics—the reversible part. For example, on the level of fluid mechanics, we consider only the Euler part and on the level of kinetic theory only the free flow without collisions. Moreover, we investigate only the Poisson brackets of the Hamiltonian structures, not the energy functionals. Our goal is to construct Poisson brackets as reductions of a known Poisson bracket expressing kinematics on a more detailed (more microscopic) level.

For example, we can start on the Liouville level, i.e. on the level on which N-particle distribution functions serve as state variables. The time evolution on the Liouville level, governed by the Liouville equation (see e.g. [11]), is Hamiltonian and reversible[1] time evolution. The right hand side of the Liouville equation (Liouville vector field) is gradient of energy transformed into a vector by the Liouville–Poisson structure (expressed mathematically in the Liouville–Poisson bracket—see Section 2.1.1). Projections from the N-particle distributions to lower (less detailed) levels of description then induce projections of the Liouville–Poisson bracket to Poisson brackets on the lower levels. The method of projection that we employ is quite natural and was already used for example in [13,5,14] and in [15]. In this paper we present it in its full generality within the context of non-equilibrium thermodynamics and investigate its geometric interpretation in appendices and Electronic supplementary (ES). We also employ it to develop new levels suitable for applications in the theory of turbulence. Various reductions demonstrated in this paper are presented in Fig. 1.

It sometimes happens that reversible evolution is not given by projection of the Liouville–Poisson bracket, as for example in an EIT theory of mixtures and BBGKY hierarchy (see Section 3). What is then the common structure shared by the reversible evolution on different levels of description? In general this question still remains an open problem in non-equilibrium thermodynamics as it is not for example clear whether validity of Jacobi identity is necessary when the reversible evolution is accompanied by an irreversible counterpart. In particular examples, for example the BBGKY hierarchy, the common structure is again the Poisson bracket as the terms containing higher-order distribution functions can be replaced by a constitutive relation (closure) while the rest remains Hamiltonian. That is how the Boltzmann collision term comes into play while the reversible part of Boltzmann equation is Hamiltonian. The BBGKY hierarchy however is not part of the present hierarchy of Poisson brackets. It is thus still unclear whether the Hamiltonian structure should be a necessary feature of all consistent reversible dynamics describing real physical systems compatible with non-equilibrium thermodynamics or not, but even if it is, the Poisson bracket can be out of the present hierarchy of Poisson brackets.

When starting from the N-particle Liouville–Poisson bracket, the number of particles is inherently incorporated into the Poisson brackets. To remove this dependence, we develop a grand-canonical hierarchy of Poisson brackets in Section 4.1. This hierarchy can be then reduced to a two-point kinetic theory or to a Poisson bracket coupling hydrodynamic fields with a conformation tensor, Reynolds stress and non-local vorticity. Such an extended hydrodynamics should be useful in modeling of fluids where non-local effects play an important role.

Contribution of this paper can be seen in the following points. Firstly, the natural hierarchy of Poisson brackets generated by projections from N-particle distribution functions to less detailed levels of description is investigated in the context of non-equilibrium thermodynamics. Various thermodynamically

[1] The reversibility can be checked the same way as for the reversible part of Boltzmann equation in [12] or it can be seen from compatibility of Liouville equation and Hamilton canonical equations.