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Reductions and extensions in mesoscopic dynamics

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Reduction of a mesoscopic level to a level with fewer details is made by the time evolution during which the entropy increases. An extension of a mesoscopic level is a construction of a level with more details. In particular, we discuss extensions in which extra state variables are found in the vector fields appearing on the level that we want to extend. Reductions, extensions, and compatibility relations among them are formulated first in an abstract setting and then illustrated in specific mesoscopic theories.

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I. INTRODUCTION

Macroscopic systems have always been investigated, both experimentally and theoretically, on several levels that differ in the amount of details. Hydrodynamics, equilibrium thermodynamics, and the Boltzmann kinetic theory of gases are examples of such levels. Each level has evolved from a particular physical insight and from an experience acquired in a collection of experimental observations. The type of observations differs for different levels. The levels are autonomous and each of them has its own domain of applicability. Among all the levels there is one on which all details (provided we remain inside the domain of classical physics) are taken into account. The state variables on this level are position coordinates and momenta of all (i.e., $\sim 10^{23}$) particles composing the macroscopic systems, the time evolution equations are Newton's equations, and the complete dynamical information consists of trajectories (experimentally observed or obtained by solving the Newton equations) of all the particles. All other levels ignore some details in order to provide a setting in which the overall features seen in macroscopic and mesoscopic experimental observations become recognizable. In the family of levels, the one with more details will be called more microscopic (or, equivalently, less macroscopic).

The most important discovery made in the investigation of macroscopic systems is the maximum entropy principle (MEP). According to this principle (that is, at least implicitly, present already in the Gibbs formulation of thermodynamics [1] but appearing first in a more general context in Ref. [2]) the ignored details influence the time evolution of the features that are explicitly kept and observed (both experimentally and theoretically) on a given level in such a way that the time evolution is a reduction during which entropy reaches its maximum allowed by constraints.

By *reduction* we mean a time evolution in which the macroscopic systems under investigation are approaching states at which more macroscopic descriptions become applicable. For instance, in the absence of external influences, the time evolution brings eventually most macroscopic systems to states at which the classical equilibrium thermodynamics is found to describe well the observed behavior. External forces may stop the reduction time evolution on an intermediate (called a mesoscopic) level. For example, the force of gravitation and temperature gradient, both imposed on a horizontal layer of a fluid (such a system is called the Rayleigh-Bénard system), stop the reduction on the level of fluid mechanics (recall that the Rayleigh-Bénard system is indeed found to be well described by the Boussinesq hydrodynamic equations and not by the classical thermodynamics). We begin to investigate the reduction in Sec. II by concentrating only on the entropy maximization and ignoring the time evolution that creates it. We call such a reduction a *static reduction*. In order to avoid a possible misunderstanding, we recall that the word "reduction" is often used in nonequilibrium statistical mechanics in a more general context for any passage from a microscopic or mesoscopic description to descriptions that ignore some details (by making some kind of pattern-recognition process—see Refs. [3,4] for examples of recent contributions to this type of investigation). In this paper we see a reduction in a more narrow sense as a process that is actually observed in the time evolution of macroscopic systems.

Entropy is a new potential, of nonmechanical origin, that has emerged in mesoscopic dynamics in order to deal with ignored details. All entropies share a core of common properties but otherwise they depend on the starting and the target levels and also on the macroscopic system under consideration. Both of these dependencies will be illustrated below. We can see the entropy in two ways. Either we consider it as given at the outset of the investigation and we look for the time evolution that maximizes it or, inversely, we regard the time evolution as given at the outset and look for the entropy that

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is maximized in it. In this paper we take mainly the former viewpoint.

Now we explain the meaning of *extension* of a mesoscopic theory. For a given mesoscopic level, we can attempt to identify more microscopic levels that reduce to it. Such theoretical construction leading from a mesoscopic level to more microscopic levels that reduce to it is called an extension. The extended models are needed if experimental observations show that some of the details ignored on a chosen mesoscopic level become important and cannot be therefore ignored. As an example, we recall the extension from the classical fluid mechanics to fluid mechanics of complex fluids (known as rheology) that was motivated by the impossibility to predict flows of melted plastic occurring in processing operations in the plastics industry. The ignored details that have to be taken into account in this case are some characterizations of the internal (polymeric) structure of plastic melts. We shall discuss several other examples of extension below.

An abstract equation expressing the mathematical structure that has been found to be common to a large class of mesoscopic dynamical equations is called the general equation for nonequilibrium reversible-irreversible coupling (GENERIC) (see Sec. III D). By investigating its solutions, we are uncovering new physics that it expresses. First, we note that solutions to GENERIC represent always a reduction from an (initial) mesoscopic level to another (target) mesoscopic level involving fewer details. Second, we relate GENERIC to two large subjects of classical nonequilibrium thermodynamics, namely the dissipation thermodynamics [5–8] and extended thermodynamics [9–12]. Third, we investigate modifications of entropies corresponding to modifications of target levels in the investigations of *initial level* → *target level* reductions. The abstract formulations and investigations are illustrated on a finite-dimensional toy example and in the context of several well-established mesoscopic theories. In particular, we discuss the reduction from Maxwell-Cattaneo heat transfer to Fourier heat conduction.

In this paper we present a unified formulation of thermodynamics that encompasses static reduction, dynamic reduction, and extensions. It has been realized for a long time that in mesoscopic dynamics there are in fact three potentials that play a significant role. They are the energy, the entropy, and the entropy production. The first generates the mechanical time evolution and the remaining two enter the time evolution caused by the incompleteness of the setting of mechanics. Details that are ignored in mesoscopic descriptions still influence the time evolution of the features that are chosen to be explicitly followed. The influence is expressed in the behavior of the entropy and the entropy production. Our main objective is to throw a new light on the roles that these three potentials play in reductions and extensions of mesoscopic dynamical theories. The abstract formulation is illustrated on a finite-dimensional toy example and in the context of several well-established mesoscopic theories. In particular, we discuss the reduction from Maxwell-Cattaneo heat transfer to Fourier heat conduction.

Since we investigate macroscopic systems on several different levels of description, we need a systematic notation. Each level will be denoted by an Arabic numeral. The numeral, in the subscript or the superscript in parenthesis, will then signify the level denoted by the numeral. In the examples we use, as much as possible, the traditional notation. Altogether, we discuss three levels: Level 1 is a chosen mesoscopic level, Level 0 is a level that is more macroscopic than Level 1, and Level 2 is the level obtained from Level 1 by an extension. In the examples, Level 0 is often, but not always, chosen to be the level of the classical equilibrium thermodynamics.

II. STATIC REDUCTION: LEVEL 1 → LEVEL 0

In this section we extract from the equilibrium statistical mechanics and the classical equilibrium thermodynamics a mathematical structure that we shall call a static reduction. Both of the equilibrium theories are its particular realizations. Other realizations include passages between two general levels, for instance, the passage between the level of kinetic theory and the level of fluid mechanics. We begin with the abstract mathematical formulation, and then its physical content is gradually revealed in examples provided in Sec. II A.

The state variables on Level 1 will be denoted by the symbol $x_1 \in M_1$, and by M_1 we denote the Level 1 state space. Similarly, on Level 0 we have $x_0 \in M_0$. Now we define the static reduction from Level 1 to Level 0.

We begin with a function $S^{(1\to 0)} : M_1 \to \mathbb{R}$ on Level 1 and with a mapping $\Pi^{(1\to 0)} : M_1 \to M_0$ relating state variables on Level 1 to state variables on Level 0. This mapping is onto but typically not one-to-one. We look for a function $S^{(0\leftarrow 1)} : M_0 \to \mathbb{R}$ that is an image of $S^{(1\to 0)}$ under the mapping $\Pi^{(1\to 0)}$. We call $S^{(1\to 0)}$ an entropy on Level 1 addressing its relation to Level 0 and $S^{(0\leftarrow 1)}$ an entropy on Level 0 that is reduced from $S^{(1\to 0)}$ by the mapping $\Pi^{(1\to 0)}$. Both entropies depend on both levels. In our notation we express this dependence by upper indices $(1 \to 0)$ and $(0 \leftarrow 1)$. The first numeral denotes always the level on which the entropy is defined [i.e., $S^{(1\to 0)}$ is a function of x_1 and $S^{(0\leftarrow 1)}$ is a function of x_0].

We shall find $S^{(0\leftarrow 1)}$ by use of the MEP. According to this principle, $S^{(0\leftarrow 1)}$ is a maximum of $S^{(1\to 0)}$ subject to the constraint $\Pi^{(1\to 0)}$. Hereafter, we assume that $S^{(1\to 0)}$ is a sufficiently regular and concave function of x_1. We make the passage $M_1 \to M_0$ in two steps as follows.

Step 1. We introduce a function

$$\Phi^{(1\to 0)}(x_1,x_0^*) = -S^{(1\to 0)}(x_1) + \langle x_0^*, \Pi^{(1\to 0)}(x_1)\rangle, \tag{2.1}$$

where $\langle,\rangle$ denotes the inner product in M_0 and x_0^* are Lagrange multipliers. We call $\Phi^{(1\to 0)}$ a *thermodynamic potential relating Level 1 to Level 0*. Next we find a minimum of $\Phi^{(1\to 0)}$, i.e., we solve equation

$$\frac{\partial \Phi^{(1\to 0)}}{\partial x_1} = 0. \tag{2.2}$$

We have already assumed that $S^{(1\to 0)}$ is a concave function of x_1. We shall, moreover, assume that the mapping $\Pi^{(1\to 0)}$ is such that the thermodynamic potential $\Phi^{(1\to 0)}(x_1,x_0^*)$ is a convex function of x_1.

Let the solution to (2.2) be $(x_1)_{\mathrm{eq}}(x_0^*)$. If we evaluate $\Phi^{(1\to 0)}$ at this state, we obtain

$$S^{(0)*}(x_0^*) = \Phi^{(1\to 0)}[(x_1)_{\mathrm{eq}}(x_0^*),x_0^*]. \tag{2.3}$$

Step 2. We introduce a function

$$\Phi^{(0)*}(x_0^*,x_0) = -S^{(0)*}(x_0^*) + \langle x_0^*,x_0\rangle. \tag{2.4}$$

Let the solution of

$$\frac{\partial \Phi^{(0)*}}{\partial x_0^*} = 0 \tag{2.5}$$

be $(x_0^*)_{\mathrm{eq}}(x_0)$. The function $S^{(0\leftarrow 1)}(x_0)$ defined by

$$S^{(0\leftarrow 1)}(x_0) = \Phi^{(0)*}[(x_0^*)_{\mathrm{eq}}(x_0),x_0] \tag{2.6}$$

is then the maximum entropy (MaxEnt) image of $S^{(1\to 0)}(x_1)$ under the mapping $\Pi^{(1\to 0)}$. The procedure indeed ends with the same result as the maximization of entropy $S^{(1\to 0)}$ with constraints given by requiring the projection $\Pi^{(1\to 0)}$ to have a constant image, see Appendix.

The state variables with star in the position of the upper index are called conjugate variables. We note that $x_0^* = \frac{\partial S^{(0\leftarrow 1)}}{\partial x_0}$. Similarly, we introduce $x_1^* = \frac{\partial S^{(1\to 0)}}{\partial x_1}$. A direct consequence of this definition is the *Maxwell relation*,

$$\frac{\partial (x^*)_i}{\partial (x)_k} = \frac{\partial (x^*)_k}{\partial (x)_i}, \tag{2.7}$$

where $x = [(x)_1,\dots,(x)_K]$ and $x^* = [(x^*)_1,\dots,(x^*)_K]$ are considered to be K-dimensional vectors. We do not distinguish in (2.7) between x_0 and x_1 since the relation holds for both x_0 and x_1. Other versions of the Maxwell relations (2.7) can be obtained from all possible Legendre transformations of the entropy.

A further insight into the mathematics involved in the passage $S^{(1\to 0)}(x_1) \to S^{(0\leftarrow 1)}(x_0)$ described in the two steps above is obtained by placing the formulation into the setting of contact geometry (see Ref. [13]). This is because in such a setting the Legendre transformations that, as we have shown above as the transformations involved in the MEP, are the natural transformations (they preserve the contact structure). An insight into the physics involved in $S^{(1\to 0)}(x_1) \to S^{(0\leftarrow 1)}(x_0)$ described in Eqs. (2.1)–(2.5) is best revealed in examples addressing familiar settings. We now proceed to develop some of them.

A. Examples

We present three particular realizations of the static reduction in which Level 0 is always the level of the classical equilibrium thermodynamics. Several other realizations (some of them with a different Level 0) will be shown in Sec. IV.

1. Classical equilibrium thermodynamics

In the examples discussed in this section we take Level 0 to be the level of the classical equilibrium thermodynamics. We now describe it. The only thing that is seen on this level is the size (characterized by the volume V) of the macroscopic system under investigation, its quantity (characterized by the number of particles N), and its energy, denoted by E. The energy includes the macroscopic mechanical energy of the macroscopic systems under consideration (as, for instance, the overall kinetic energy and potential energy) and also the energy (called internal energy) that manifests itself in macroscopic observations as heat. We thus have $x_0 = (V,N,E)$. This level is, in fact, the most macroscopic level so mapping Π [which we denote in this setting as $\Pi^{(0)}$] is an identity mapping $M_0 \to M_0$. The entropy [denoted in this case $S^{(0)}$] is a real valued and sufficiently regular function of (V,E,N) (called a fundamental thermodynamic relation) satisfying the following properties: (S1) a concave function; (S2) $S^{(0)}(\lambda V,\lambda E,\lambda N) = \lambda S^{(0)}(V,N,E)$, where $\lambda \in \mathbb{R}$; (S3) $\frac{\partial S^{(0)}}{\partial E} \geqslant 0$, where $S^{(0)} = 0$ if $(\frac{\partial S^{(0)}}{\partial E})^{-1} = 0$; and (S4) $S^{(0)}$ tends to its maximum allowed by constraints V, N, and E. The two-step procedure described in (2.1)–(2.5) is the standard Legendre transformation. In the examples below we consider the volume V to be fixed (we take it to be equal to 1) and, due to the property (S2), we can take $x_0 = (N,E)$ denoting the number of particles and the energy.

The conjugate variables are $(N^*,E^*) = (-\frac{\mu}{T},\frac{1}{T})$, μ is the chemical potential, and T is the temperature. The property (S2) also implies $\frac{P}{T} = -S^{(0)*}(-\frac{\mu}{T},\frac{1}{T})$, where P is the pressure. Note that pressure, temperature, and chemical potential are defined as the particular derivatives of entropy. Besides the four properties (S1)–(S4) that all entropies $S^{(0)}(N,E)$ possess, the fundamental thermodynamic relations differ for different macroscopic systems. In fact, it is in the fundamental thermodynamic relation where the individual nature of the macroscopic system is expressed in the classical equilibrium thermodynamics. The only way to make the association between macroscopic systems and the fundamental thermodynamic relations, while staying inside the classical equilibrium thermodynamics, is to make experimental observations. Results of such observations are collected in documents known as thermodynamic tables.

2. Equilibrium statistical mechanics: Particle mechanics → equilibrium thermodynamics

In this example we choose Level 1 to be the level of the classical mechanics of particles. We consider it in its Liouville representation [14–16] (i.e., the state variable is the N-particle distribution function rather than position coordinated and momenta of all N particles) and, in addition to fixing the overall volume, we also fix the number of particles. This corresponds, in the setting of the Gibbs equilibrium statistical mechanics [17], to the canonical ensemble. The state variable is thus $x_1 = f_N(1,2,\dots,N)$, where we use the shorthand notation "1" $= (\boldsymbol{r}_1,\boldsymbol{p}_1)$,"2" $= (\boldsymbol{r}_2,\boldsymbol{p}_2),\dots,$"$N$" $= (\boldsymbol{r}_N,\boldsymbol{p}_N)$. By $(\boldsymbol{r}_i,\boldsymbol{p}_i)$ we denote position vectors and momenta of the ith particle. We shall normalize the distribution functions to unity. The number of particles and the volume are fixed.

The entropy on the Liouville level is given by

$$S^{(1\to 0)}(f_N) = -\frac{k_B}{N!}\int d1 \dots \int dN f_N(\ln h^{3N} f_N), \tag{2.8}$$

where h is the Planck constant and distribution functions are normalized,

$$1 = \frac{1}{N!}\int d1 \dots \int dN f_N.$$

This entropy comes, for example, from Eq. (5.3) of Chap. 3 in Ref. [18] or Eq. (7.12) in Ref. [19] when requiring that integral of the distribution function over the phase space is dimensionless and that the summation or integration is carried out over distinct quantum states.

The projection to the level of equilibrium thermodynamics reads

$$\Pi^{(1\to 0)} : f_N \mapsto \left(E = \frac{1}{N!}\int d1 \ldots \int dN H^N f_N, \nu = \frac{1}{N!}\int d1 \ldots \int dN f_N\right), \tag{2.9}$$

where H^N is an N-particle Hamiltonian, e.g.,

$$H^N = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m} + \epsilon(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N). \tag{2.10}$$

The first term in H^N is the kinetic energy of the particles (m is the mass of one particle) and the second term is the potential energy. We note that the individual nature of macroscopic systems is expressed in the mapping $\Pi^{(1\to 0)}$ while the entropy $S^{(1\to 0)}$ is universal. We recall that in the setting of the classical equilibrium thermodynamics the relations are completely reversed, $\Pi^{(0)}$ is universal, and the individual nature is expressed in $S^{(0)}$.

Note that the second component of the projection represents the constraint for maximum entropy when setting $\nu = 1$. The above outlined static reduction based on Lagrange transformation corresponds to maximum entropy under the constraints given by the projection. Hence one needs to add a variable (ν in this case) in order to guarantee this constraint while using the static reduction approach. Also note that volume V and number of particles N act as fixed auxiliary parameters known at both levels.

The first step of the static reduction leads to

$$S^{(0)*}(E^*,\nu^*) = -\frac{k_B}{h^{3N}} Z^N(E^*) \exp[-(\nu^*/k_B + 1)], \tag{2.11}$$

with Z^N being the partition sum

$$Z^N(V,N,E^*) = \frac{1}{N!}\int d1 \ldots \int dN e^{-\frac{1}{k_B}E^* H^N}. \tag{2.12}$$

The second step ends with a fundamental thermodynamic relation

$$S^{(0\leftarrow 1)}(E,\nu) = \nu k_B \ln\left\{\frac{Z^N[(E^*)_{\mathrm{eq}}(E,\nu)]}{\nu h^{3N}}\right\} + E(E^*)_{\mathrm{eq}}(E,\nu), \tag{2.13}$$

where the dependence $(E^*)_{\mathrm{eq}}(E,\nu)$ is given by solving

$$E = -k_B \nu \frac{\partial \ln Z^N(E^*)}{\partial E^*} \tag{2.14}$$

in accordance with the procedure of the static reduction.

Finally, note that the equilibrium distribution function is given by

$$(f_N)_{\mathrm{eq}}(E,\nu) = \frac{\nu}{Z_N[(E^*)_{\mathrm{eq}}(E,\nu)]} \exp\left[-\frac{(E^*)_{\mathrm{eq}}(E,\nu)}{k_B} H_N\right]. \tag{2.15}$$

When setting $\nu = 1$ in the final equations we obtain the fundamental thermodynamic relation and distribution function for the canonical ensemble.

Similarly, the grand-canonical ensemble (with only the volume fixed) and the microcanonical ensemble (with the volume, the number of particles, and the energy fixed) versions of the Gibbs equilibrium statistical mechanics can also be formulated as particular realizations of the static reduction.

3. Boltzmann kinetic theory: One particle kinetic theory → equilibrium thermodynamics

Level 1 is now chosen to be the level of the Boltzmann one-particle kinetic theory [20]. The state variable is the one-particle distribution function: $x_1 = f(\boldsymbol{r},\boldsymbol{p})$, where $\boldsymbol{r}$ and $\boldsymbol{p}$ are the position coordinate and the momentum of one particle, respectively.

Following again Sec. 40 of Ref. [19] or Ref. [7], entropy is given by

$$S^{(1\to 0)}(f) = -k_B \int d\boldsymbol{r} \int d\boldsymbol{p} f(\boldsymbol{r},\boldsymbol{p})\{\ln[h^3 f(\boldsymbol{r},\boldsymbol{p})] - 1\}. \tag{2.16}$$

The projection works as follows:

$$\Pi^{(1\to 0)} : f \mapsto \left[E = \int d\boldsymbol{r} \int d\boldsymbol{p} \frac{\boldsymbol{p}^2}{2m} f(\boldsymbol{r},\boldsymbol{p}), N = \int d\boldsymbol{r} \int d\boldsymbol{p} f(\boldsymbol{r},\boldsymbol{p})\right]. \tag{2.17}$$

The first step of the static reduction leads to

$$S^{(0)*}(V,N,N^*,E^*) = -k_B V \left(\frac{2\pi m k_B}{h^2 E^*}\right)^{3/2} e^{-\frac{N^*}{k_B}}. \tag{2.18}$$

The second step ends with the fundamental thermodynamic relations of ideal gas, the Sackur-Tetrode relation, see, e.g., Ref. [21],

$$S^{(0\leftarrow 1)}(E,V,N) = N k_B \left\{\frac{5}{2} + \ln\left[\frac{V}{N}\left(\frac{4\pi m E}{3 N h^2}\right)^{3/2}\right]\right\}. \tag{2.19}$$

4. Particle mechanics → one-particle kinetic theory

Starting with entropy (2.8), the projection to the level of one-particle kinetic theory is given by

$$f_1(1) = \frac{1}{N!}\int d1 \ldots \int dN \sum_{i=1}^{N} \delta(1-i) f_N(1,\ldots,N), \tag{2.20a}$$

$$\nu = \frac{1}{N!}\int d1 \ldots \int dN f_N(1,\ldots,N). \tag{2.20b}$$

The first step of the reduction leads to

$$S^{(1)*}(f_1^*,\nu^*) = -\frac{k_B e^{-1-\frac{\nu^*}{k_B}}}{h^{3N} N!}\left\{\int d1 \exp\left[-\frac{f_1^*(1)}{k_B}\right]\right\}^N, \tag{2.21}$$

where f_1^* and ν^* are the variables conjugate to f_1 and ν, respectively.

The second step leads to

$$S(f_1,\nu) = -k_B \int d1 f_1(1) \ln[h^3 f_1(1)] - k_B \nu \ln\left(\frac{N!\nu}{\left[\int d1 f_1(1)\right]^N}\right). \tag{2.22}$$

Setting ν equal to 1 and using Stirling formula for approximation of factorials, this entropy becomes

$$S(f_1) = -k_B \int d1\, f_1(1)\{\ln[h^3 f_1(1)] - 1\}, \tag{2.23}$$

which is the standard Boltzmann entropy.

5. *Fluid mechanics: Hydrodynamics → equilibrium thermodynamics*

In the last example we choose Level 1 to be the level of fluid mechanics. This means that the state variable $x_1 = [\rho(\boldsymbol{r}),\boldsymbol{u}(\boldsymbol{r}),e(\boldsymbol{r})]$, where $\boldsymbol{r}$ is the position vector, $\rho(\boldsymbol{r}) = M_{\text{mol}} n(\boldsymbol{r})$ is the local mass per unit volume (M_{mol} is the molar mass), $\boldsymbol{u}(\boldsymbol{r})$ is the momentum field, and $e(\boldsymbol{r})$ is the total local energy per unit volume [i.e., $e(\boldsymbol{r})$ equals the kinetic energy $\frac{\boldsymbol{u}^2}{2\rho}$ plus an internal energy]. If we choose the entropy $S^{(1\to 0)} = \int d\boldsymbol{r} s[\rho(\boldsymbol{r}),\boldsymbol{u}(\boldsymbol{r}),e(\boldsymbol{r})]$ in such a way that $s[\rho(\boldsymbol{r}),\boldsymbol{u}(\boldsymbol{r}),e(\boldsymbol{r})]$ depends locally on $n = \frac{\rho}{M_{\text{mol}}}$ and the internal energy in the same way as at the global equilibrium (this choice is called a *local equilibrium assumption*), then the static reduction gives the global thermodynamic equilibrium relation provided the mapping $\Pi^{(1\to 0)}$ is chosen to be $[\rho(\boldsymbol{r}),\boldsymbol{u}(\boldsymbol{r}),e(\boldsymbol{r})] \mapsto (n_0,e_0) = (\frac{1}{M_{\text{mol}}} \int d\boldsymbol{r} \rho(\boldsymbol{r}), \int d\boldsymbol{r} e(\boldsymbol{r}))$.

6. *Remarks*

As we have seen in the four examples above, in each particular realization of the static reduction we need to choose the state variables x_1, the entropy $S^{(1\to 0)}(x_1)$, and the mapping $\Pi^{(1\to 0)}$, which, at least in the case when Level 0 is the level of the classical equilibrium thermodynamics, includes specification of the energy $E(x_1)$. We make now a few observations about the possible choices.

We begin with the energy $E(x_1)$. There are two distinctly different choices of the energy. First, we choose the state variables x_1 in such a way that the total energy $E(x_1)$ is explicitly included as one of the components of x_1 (see Secs. II A 1 and II A 5). In the second choice, which we made in Secs. II A 2 and II A 3, the state variables do not include the energy itself; the total energy is a function of x_1.

In the setting of the classical equilibrium thermodynamics (see Sec. II A 1), the energy E that is included as one component in the state variables (V,N,E) is directly the energy $E(x_1)$. The mapping Π is thus simply an identity mapping. If we subtract from the total energy the mechanical energy of the macroscopic system as a whole (i.e., the kinetic and the potential energy of the macroscopic system as a whole), then we obtain the internal energy (we shall denote it by the symbol ϵ). Introduction of the internal energy ϵ (whose provenance remains unspecified in the setting of the classical equilibrium thermodynamics but its mechanical nature is recognized by treating it in the same ways as the mechanical energy) is the subject of the so-called first principle of thermodynamics. In the setting of fluid mechanics, presented in Sec. II A 5, it is the local total energy $e(\boldsymbol{r})$ that is one of the components of the state variables $x_1 = [\rho(\boldsymbol{r}),\boldsymbol{u}(\boldsymbol{r}),e(\boldsymbol{r})]$. Consequently, the total energy $E(x_1) = \int d\boldsymbol{r} e(\boldsymbol{r})$. The local internal energy $\epsilon(\boldsymbol{r})$ is related to the local total energy $e(\boldsymbol{r})$ by $e(\boldsymbol{r}) = \frac{\boldsymbol{u}^2(\boldsymbol{r})}{2\rho(\boldsymbol{r})} + \epsilon(\boldsymbol{r})$, where $\frac{\boldsymbol{u}^2(\boldsymbol{r})}{2\rho(\boldsymbol{r})}$ is the local kinetic energy expressed in terms of the remaining components of $x_1 = [\rho(\boldsymbol{r}),\boldsymbol{u}(\boldsymbol{r}),e(\boldsymbol{r})]$. We note, furthermore, that the choice of energy as one of the components of the state variable x_1 is intimately related to the choice of the entropy $S^{(1\to 0)}(x_1)$. This is because the derivative of entropy with respect to energy, having the physical interpretation of the inverse of the absolute temperature, is assumed to be positive and, consequently, the energy $e(\boldsymbol{r})$ as one component of state variables x_1 can be replaced by the entropy $s(\boldsymbol{r})$, where $S^{(1\to 0)} = \int d\boldsymbol{r} s(\boldsymbol{r})$. If this is done, then the relation $E = E(x_1)$, where x_1 includes now $S^{(1\to 0)}$ as one of its components, takes the role of the fundamental thermodynamic relation. Following the terminology of Callen [21], we call the formulation in which the energy is included in state variables the *entropy representation* and the formulation in which the entropy is included in state variables the *energy representation*. These two types of representation of x_1 are also possible in the setting of fluid mechanics if we assume that the positivity of the derivative of entropy with respect to energy holds also locally. We note that if we make such an assumption we are in fact making a weaker version of the local equilibrium assumption. We recall that the local equilibrium assumption requires, in addition, that the local fundamental thermodynamic relation is exactly the same as the global one. For later use we recall relations among derivatives in the two representations (ξ,s) and (ξ,e): $\frac{\partial e}{\partial s} = (\frac{\partial s}{\partial e})^{-1}$; $\frac{\partial \xi}{\partial s} = -\frac{\partial \xi}{\partial e}(\frac{\partial s}{\partial e})^{-1}$.

Now we turn to the specification of $E(x_1)$ that we made in Secs. II A 2 and II A 3. We have assumed there that there is no internal energy (i.e., that there is no energy of unknown provenance). The total energy is assumed to be completely expressed in terms of x_1. This assumption is very clear in the setting of the equilibrium statistical mechanics in Sec. II A 2 since the knowledge of position vectors and momenta of all particles composing macroscopic systems allows us to calculate the complete total energy. There are no details (needed to calculate the total energy) that are ignored. In the context of kinetic theory presented in Sec. II A 3 we obviously ignore many details when we take the one particle distribution function to be the only state variable x_1. However, if we limit ourselves to macroscopic systems composed of completely noninteracting particles, then the one-particle distribution function suffices to express completely the total energy [namely the kinetic energy $\int d\boldsymbol{r} \int d\boldsymbol{v} \frac{\boldsymbol{v}^2}{2m} f(\boldsymbol{r},\boldsymbol{v})$]. The Boltzmann kinetic theory is indeed limited to this kind of macroscopic system. We can now ask the following question. Why do we need entropy in Secs. II A 2 and II A 3 if no detail needed to calculate the total energy is ignored? We answer this question by noting that details are ignored in the time evolution. In the context of the Gibbs equilibrium statistical mechanics the time evolution is in fact almost completely ignored. What remains is only the energy conservation and some kind of "ergodicity-type" hypothesis (whose precise mathematical formulation remains an open problem) according to which averages made in time are the same as some kind of averages made in space of position vectors and momenta of all $\sim 10^{23}$ particles. In the Boltzmann kinetic theory the time evolution is partially ignored. Trajectories of noninteracting particles are rigorously kept but details of the pieces of trajectories traced during collisions (see Sec. III B 1) are ignored.

Finally, we make a comment about the physics that is behind the choice of the state variables x_1. There are in fact three sources of inspiration for choosing x_1. The first one is an insight into the microscopic time evolution and/or theoretical results obtained for it. The second inspiration for complementing a choice already made [we denoted it $(x_1)_0$] by some extra state variables comes from a theoretical investigation of the time evolution of $(x_1)_0$. The extra state variables are found in the vector field generating the time evolution of $(x_1)_0$. We shall see examples of this inspiration in Sec. IV. The third type of inspiration comes from experimental observations. Following this route, we want to select the state variables that are in the closest possible relation to the quantities that are experimentally observed.

III. DYNAMIC REDUCTION: LEVEL 1 → LEVEL 0

In this section we look for the time evolution that makes the reduction discussed in the previous section. This means that we replace the imposition of the entropy maximization (made in the previous section) by introduction of the time evolution on Level 1 that makes the maximization. In the search for the time evolution we can either consider the entropy $S^{(1\to 0)}(x_1)$ as known and look for the corresponding time evolution of x_1 or, inversely, we consider the time evolution of x_1 as known (e.g., from insight and experimental observations) and, by mathematically analyzing it, we identify the corresponding entropy $S^{(1\to 0)}(x_1)$. For instance, the latter approach led Boltzmann to his expression for the entropy (called, in this case, the Boltzmann H-function). In this paper we shall follow the former viewpoint.

There are at least three routes leading to the time evolution on Level 1 during which a given entropy $S^{(1\to 0)}$ reaches its maximum. All three routes lead to the same result; each of them provides, however, its own insight (both physical and mathematical).

On the first route we begin by collecting well-established (i.e., extensively tested with results of experimental observations) mesoscopic dynamical theories and attempt to extract from them a common mathematical structure. This is the route started by Clebsch in Refs. [22] and [23] (by recognizing the Hamiltonian structure of particle mechanics in the nondissipative Euler fluid mechanics) and continuing in Refs. [24–30], with dissipative mesoscopic dynamical theories. The structure of an abstract mesoscopic time-evolution-expressing approach to the level of the classical equilibrium thermodynamics has been called, in Refs. [29,30], GENERIC. It is interesting to note that the archetype GENERIC equation is the Boltzmann kinetic equation [25] that is also historically the first mesoscopic dynamical equation for which the compatibility with the equilibrium thermodynamics has been investigated in Ref. [20].

The second route is based on the mathematical structure identified in the static reduction. The two steps in Sec. II represent essentially Legendre transformations. We then recall that the most natural mathematical environment for Legendre transformations is contact geometry. This is because the contact 1 form specifying the contact geometry is preserved in this type of transformation (such transformations are called contact structure preserving transformations). The suggestion to formulate the classical equilibrium thermodynamics in the setting of contact geometry was put forward first by Hermann in Ref. [31]. In order to extend the static reduction to a dynamic one we then argue as follows. Since the static reduction is a contact-structure-preserving transformation, we suggest that the time evolution making it is a continuous sequence of such transformations. There is a well-known canonical form for such time evolution (see, e.g., Appendix in Ref. [13]). It resembles the canonical form of the Hamiltonian time evolution. Both involve a generating potential. In the case of the Hamiltonian dynamics it is the Hamiltonian (having the physical interpretation of energy) and in the case of the contact dynamics it is a potential called a contact Hamiltonian. The problem to identify the dynamics becomes the problem to identify an appropriate contact Hamiltonian (that, as it turns out, is a sum of two terms, one related to the rate of energy and the other to the rate of entropy—see Refs. [32–35]).

In this paper we shall follow the third route that naturally continues the approach developed in the classical nonequilibrium thermodynamics (e.g., Refs. [5–7]).

A. Dissipation thermodynamics

The third route begins in the same way as the first route. The point of departure is a collection of well-established mesoscopic dynamical theories in which a common structure is searched. The difference is in the size of the collection and in the focus of the search. While the collection of mesoscopic theories from which the GENERIC structure has been extracted is very large (it includes, among others, fluid mechanics and kinetic theory) the basis from which the classical nonequilibrium thermodynamics has emerged is essentially only fluid mechanics. Kinetic theory (and, related to it, Grad's hierarchy [36]) serves as a microscopic theory generating fluid mechanics and its extensions rather than a mesoscopic theory that itself is a particular realization of the abstract nonequilibrium thermodynamics. As for the structure emerging in the investigation, the first observation made on both routes is that the vector fields generating the time evolution in mesoscopic theories are a sum of two parts. One generates the time evolution that leaves the entropy unchanged and the other makes it to grow. The former is called a *nondissipative vector field* and the latter the *dissipative vector field*. After this observation is made, the focus on the first route is put onto the nondissipative part (its Hamiltonian structure is recognized) and the focus on the third route is on the dissipative part. A closer look at the dissipative vector fields reveals that they involve certain quantities that have been called in nonequilibrium thermodynamics *dissipative fluxes*. We shall denote them, following the traditional notation, by use of the symbol $\boldsymbol{J} = (J_1, J_2, \ldots, J_K)$. For example, in the context of the classical fluid mechanics, they are the Fourier heat flux and the Navier-Stokes momentum flux. Following the abstraction made in the classical nonequilibrium thermodynamics [5–8], we regard the dissipative fluxes $\boldsymbol{J}$ simply as new state variables. Their relation to x_1 and to its time evolution will be discussed later in Sec. III B in what is called *constitutive relations*. The state space whose elements are $\boldsymbol{J}$ will be denoted by $M_1^{(J)}$ [i.e., $\boldsymbol{J} \in M_1^{(J)}$].

Now we turn to reductions introduced in the previous section. We make a static reduction of $M_1^{(J)}$ to another space $M_0^{(J)}$. The role that the entropy plays in the reduction of M_1 to M_0 is taken by a new potential that we shall denote by the symbol Θ and call a *dissipation potential* [8,37–39]. Contrary to the entropy, we require Θ to be convex and thus the reduction is made by minimizing the dissipation potential (instead of maximizing the entropy as was done in the previous section). The other properties of Θ depend on the choice of $M_0^{(J)}$. We begin our investigation with the reduction to states at which no dissipation takes place. At such states the dissipative fluxes are absent. This means that we begin by choosing $M_0^{(J)}$ to be composed of only one element, namely $(0,0,\ldots,0)$. Consequently, we require the dissipation potential $\Theta(\boldsymbol{J})$ to satisfy the following properties:

(i) $\Theta(0) = 0$,

(ii) Θ reaches its minimum at $\boldsymbol{J} = 0$,

(iii) Θ is a convex function of $\boldsymbol{J}$ in a neighborhood of $\boldsymbol{J} = 0$. (3.1)

The conjugates of $\boldsymbol{J}$ with respect to Θ will be denoted by $\boldsymbol{X}$, i.e.,

$$\boldsymbol{X} = \Theta_{\boldsymbol{J}} \tag{3.2}$$

and called *dissipative forces*. We use hereafter the shorthand notation in which the symbol placed in the subscript position denotes a derivative with respect to the quantity represented by the symbol, i.e., $\frac{\partial\Theta}{\partial \boldsymbol{J}} = \Theta_{\boldsymbol{J}}$. Still another comment regarding the notation used in this section is in order. In the previous section we used the star in the superscript position to denote the conjugate variable. We shall keep this notation uniquely for the conjugation with respect to entropy. In Sec. IV we shall adopt $\boldsymbol{J}$ into the state variables x_1 and, consequently, the entropy S will also depend on $\boldsymbol{J}$. We shall then have $\boldsymbol{J}^* = \frac{\partial S}{\partial \boldsymbol{J}}$. By using the symbol $\boldsymbol{X}$ to denote the conjugate of $\boldsymbol{J}$ with respect to the potential Θ we keep the notation established in nonequilibrium thermodynamics.

As in the previous section, we make the static reduction by use of Legendre transformations. The potential involved in the transformations is now the dissipation potential Θ. In particular, the Legendre transformation of $\Theta(\boldsymbol{J})$ corresponding to a complete replacement of $\boldsymbol{J}$ with their conjugates $\boldsymbol{X}$ will be denoted by the symbol $\Xi(\boldsymbol{X})$; i.e., $\Xi(\boldsymbol{X}) = -\Theta[\tilde{\boldsymbol{J}}(\boldsymbol{X})] + \langle \boldsymbol{X}, \tilde{\boldsymbol{J}}(\boldsymbol{X})\rangle$, where $\tilde{\boldsymbol{J}}(\boldsymbol{X})$ is a solution to $\boldsymbol{X} = \Theta_{\boldsymbol{J}}$.

From the relation $\tilde{\boldsymbol{J}} = \Xi_{\boldsymbol{X}}$ we obtain

$$\frac{\partial \tilde{J}_i}{\partial X_k} = \frac{\partial \tilde{J}_k}{\partial X_i}. \tag{3.3}$$

We note that this relation is in fact the Maxwell relation (2.7) in dissipation thermodynamics. Both the Maxwell relation (2.7) and the Maxwell relation (3.3) in dissipation thermodynamics are direct consequences the conjugation operation. The potential that provides the passage between state variables and their conjugates is the entropy in the equilibrium thermodynamics and the dissipation potential [related by (3.11) to the entropy production] in the dissipation thermodynamics. In the particular case of the quadratic dissipation potential

$$\Xi(\boldsymbol{X}) = \tfrac{1}{2}\langle \boldsymbol{X}, \boldsymbol{\Lambda}\boldsymbol{X}\rangle \tag{3.4}$$

the relations (3.1) and (3.3) become the classical Onsager reciprocity relation [5,40]:

$$\tilde{\boldsymbol{J}} = \boldsymbol{\Lambda}\boldsymbol{X}, \tag{3.5}$$

where $\boldsymbol{\Lambda}$ is a symmetric and positive definite linear operator. We call therefore the relation (3.3) a *Maxwell-Onsager relation*.

B. Constitutive relations, dissipative dynamics

Our next task is to relate the static thermodynamics in the space $M_1^{(J)}$ (developed in Sec. III A) to the time evolution taking place on Level 1 and to describe its dynamic reduction to Level 0. We shall achieve this goal with the following two relations. First, it is a relation between $(\boldsymbol{J},\boldsymbol{X})$ and (x_1,x_1^*) and, second, it is an equation governing the time evolution of x_1 involving the dissipation potential.

The constitutive relation is

$$\boldsymbol{X} = \Gamma x_1^*, \tag{3.6}$$

where Γ is required to be such that the equality

$$\langle x_1^*, \Xi_{x_1^*}\rangle = \langle \boldsymbol{X}, \Xi_{\boldsymbol{X}}\rangle \tag{3.7}$$

holds so entropy production can be written in terms of $\boldsymbol{x}^*$ or $\boldsymbol{X}$ equivalently.

As we consider dissipative dynamics only, the equation governing the time evolution of x_1 is assumed to have the form

$$\dot{x}_1 = \chi(x_1)\frac{\partial \Xi}{\partial x_1^*}, \tag{3.8}$$

where $\chi : M_1 \to \mathbb{R}^+$ remains an unspecified function. Its most important property is that $\chi(x_1) > 0$. Note, however, that χ is usually equal to unity.

In the terminology established in nonequilibrium thermodynamics, the relation (3.6) together with the time evolution equation (3.8) constitute a *constitutive relation*.

Before investigating consequences of the constitutive relation we shall comment about the geometrical interpretation of (3.8). The conjugate state variable $x_1^* = \frac{\partial S^{(1\to 0)}(x_1)}{\partial x_1}$ is a covector. In order to transform it into a vector generating the time evolution (i.e., into the right-hand side of the time evolution equation) we have to use some kind of a geometrical structure in the state space M_1. We note that in the particular case of the quadratic potential $\Xi(\boldsymbol{X}) = \frac{1}{2}\langle \boldsymbol{X}, \boldsymbol{\Lambda}\boldsymbol{X}\rangle$ and Γ being a linear operator, the time evolution equation (3.8) takes the form

$$\dot{x}_1 = \Gamma^T \boldsymbol{\Lambda}\Gamma x_1^*. \tag{3.9}$$

In this equation we can now interpret $\Gamma^T\boldsymbol{\Lambda}\Gamma$ as a metric tensor. In this case the geometrical structure in M_1 is thus the Riemannian structure. In the particular case of the quadratic dissipation potential, its introduction is thus equivalent to equipping M_1 with the Riemannian structure. We therefore regard the introduction of a general dissipation potential Ξ as introduction of a *generalized Riemannian geometry* into the state space M_1. The passage from a covector x_1^* to a vector is made in the Riemannian geometry by $x_1^* \to \Gamma^T\boldsymbol{\Lambda}\Gamma x_1^*$ and in the generalized Riemannian geometry by $x_1^* \to \Xi_{x_1^*}$.

We can now prove four consequences of the constitutive relation (3.6) and (3.8). The particular form (3.9) of the linear Onsager time evolution has been noted, by attempting to extract a common structure from several well-established mesoscopic time evolutions, in Ref. [41].

Next we note that (3.6) and (3.8) imply

$$\dot{S}^{(1\to 0)} = \langle x_1^*, \Xi_{x_1^*}\rangle = \langle \boldsymbol{X}, \Xi_{\boldsymbol{X}}\rangle \geqslant 0. \tag{3.10}$$

The last inequality is a consequence of the properties (3.1). We call therefore (in accordance with the traditional terminology [6,8])

$$\sigma = \langle \boldsymbol{X}, \boldsymbol{J}\rangle = \langle \boldsymbol{X}, \Xi_{\boldsymbol{X}}\rangle \geqslant 0 \tag{3.11}$$

an *entropy production*.

The third consequence of the constitutive relation (3.6) and (3.8) is an implication of the Lyapunov theorem in which (3.10) is used. Provided the time evolution generated by (3.8) preserves $\Pi^{(1\to 0)}(x_1)$, the property (3.10) allows us to consider the thermodynamic potential (2.1) as a Lyapunov function corresponding to the approach $x_1 \to x_0$ as $t \to \infty$. We see therefore that the time evolution of x_1 governed by (3.10) indeed makes the reduction of Level 1 to Level 0. The conservation of $\Pi^{(1\to 0)}(x_1)$ (which, at least in the case when Level 0 is the level of the classical equilibrium thermodynamics, includes conservation of the energy) can always be guaranteed by an appropriate degeneracy of the dissipation potential Ξ. We shall see examples in Sec. III B 1.

The fourth implication of the constitutive relation (3.6) and (3.8) is a new version of the Maxwell-Onsager relation (3.3). By taking into account (3.6) and (3.8) in the relation (3.3) we arrive at

$$\frac{\partial(\dot{x_1})_i}{\partial(x_1^*)_k} = \frac{\partial(\dot{x_1})_k}{\partial(x_1^*)_i}, \tag{3.12}$$

where x_1 is a K-dimensional vector $x_1 = [(x_1)_1, \ldots, (x_1)_K]$; similarly, we write also x_1^*.

1. Examples

Particular realizations of the abstract formulation of dissipation thermodynamics and constitutive relations in familiar settings help to reveal its physical content.

a. Simple relaxation. In the first example we simply take $\Gamma =$ identity operator. If, in addition, we limit ourselves to the quadratic dissipation potential $\Xi(\boldsymbol{X}) = \frac{1}{2}\langle \boldsymbol{X}, \boldsymbol{\Lambda X}\rangle$, then the time evolution equation (3.8) is simply $\dot{x_1} = \boldsymbol{\Lambda} x_1^*$.

b. Fourier heat conduction. In the next example we turn to fluid mechanics. For the sake of brevity, we limit ourselves only to heat transfer so we choose $x_1 = e(\boldsymbol{r})$. Following Fourier, we take $\Gamma = \nabla = (\frac{\partial}{\partial r_1}, \frac{\partial}{\partial r_2}, \frac{\partial}{\partial r_3})$. If we again consider only the quadratic dissipation potential, (3.6) is the Fourier constitutive relation and (3.8) has the form $\frac{\partial e}{\partial t} = -\nabla(\lambda \nabla e^*)$.

c. Chemical kinetics. In the third example we consider the mass-action-law time evolution arising in chemical kinetics. In this context the state variables $x_1 = \boldsymbol{n} = (n_1, \ldots, n_p)$ are numbers of moles of p species $\mathbb{A}_1, \ldots, \mathbb{A}_p$ undergoing q chemical reactions: $\alpha_1^{(j)}\mathbb{A}_1 + \cdots + \alpha_p^{(j)}\mathbb{A}_p \rightleftarrows \beta_1^{(j)}\mathbb{A}_1 + \cdots + \beta_p^{(j)}\mathbb{A}_p$, $j = 1, \ldots, q$. We define stoichiometric coefficients $\gamma_i^{(j)} = \beta_i^{(j)} - \alpha_i^{(j)}$; $j = 1, \ldots, q$; $i = 1, \ldots, p$, and stoichiometric matrix $\boldsymbol{\gamma}$ with the rows $(\gamma_1^{(j)}, \ldots, \gamma_p^{(j)})$; $j = 1, \ldots, q$. The constitutive relation (3.6) and (3.8) becomes in this setting $\boldsymbol{X} = \boldsymbol{\gamma}\boldsymbol{n}^*$, where $\boldsymbol{X} = (X^{(1)}, \ldots, X^{(q)})$ are chemical affinities of q chemical reactions and $\boldsymbol{n}^* = (n_1^*, \ldots, n_p^*)$ are chemical potentials of p species. The time evolution equation (3.8) is now $\dot{\boldsymbol{n}} = \Xi_{\boldsymbol{n}^*} = \boldsymbol{\gamma}^T\boldsymbol{J}$, where $\boldsymbol{J} = \Xi_{\boldsymbol{X}}$. It can be directly verified that this time evolution equation is indeed the Guldberg-Waage mass-action-law dynamics provided $\Gamma = \boldsymbol{\gamma}$, the dissipation potential $\Xi = \sum_{l=1}^{q} W^{(l)}(\boldsymbol{n})[e^{\frac{1}{2}X^{(l)}} + e^{-\frac{1}{2}X^{(l)}} - 2]$, where $[W^{(1)}(\boldsymbol{n}), \ldots, W^{(q)}(\boldsymbol{n})]$ are related to rate coefficients (for the explicit form of this relation see Ref. [42]), and the entropy that equals $-\sum_{i=1}^{p}(n_i \ln n_i + Q_i n_i)$, where $(Q_1, \ldots, Q_p)$ are constants.

We have thus proven that the well-established mass-action-law dynamics is another particular realization of the general formulation developed above in this section. But what new information does this reformulation of the familiar mass-action-law time evolution equations bring to the chemical kinetics itself? We note three new results.

By casting the mass-action-law time evolution equations to the form of (3.8), we have a proven approach, as $t \to \infty$, for the state of chemical equilibrium at which all chemical affinities $[X^{(1)}, \ldots, X^{(q)}]$ disappear.

(i) The mass-action-law in the form (3.6) and (3.8) is a generalization of the original Guldberg-Waage dynamics in the sense that the relation between the numbers of moles and chemical potentials remains in (3.6) and (3.8) unspecified.

(ii) The formulation (3.6) and (3.8) of the mass-action-law dynamics has been used in Ref. [42] to extend it (by including fluctuations) and to couple it to mechanics in Refs. [43,44].

(iii) Finally, the formulation (3.6) and (3.8) reveals Maxwell-Onsager reciprocity relations (3.3) and (3.12) among extents of the reactions $\boldsymbol{J}$ and affinities $\boldsymbol{X}$ or, alternatively, if the Maxwell-Onsager relations are formulated in the form of (3.12), then it reveals relations among rates of the numbers of moles and chemical potentials. Such relations are absolutely invisible in the standard chemical kinetics. In order to see more clearly the relations (3.3) in the context of chemical kinetics, we write them explicitly for the special case of two reactions {i.e., $q = 2$, $\boldsymbol{X} = [X^{(1)}, X^{(2)}]$ and $\boldsymbol{J} = [J^{(1)}, J^{(2)}]$}:

$$\begin{aligned}
\left[\frac{\partial X^{(1)}}{\partial J^{(2)}}\right]_{J^{(1)}} &= \left[\frac{\partial X^{(2)}}{\partial J^{(1)}}\right]_{J^{(2)}}\\
\left[\frac{\partial J^{(1)}}{\partial X^{(2)}}\right]_{X^{(1)}} &= \left[\frac{\partial J^{(2)}}{\partial X^{(1)}}\right]_{X^{(2)}}\\
\left[\frac{\partial J^{(1)}}{\partial J^{(2)}}\right]_{X^{(1)}} &= -\left[\frac{\partial X^{(2)}}{\partial X^{(1)}}\right]_{J^{(2)}}\\
\left[\frac{\partial J^{(2)}}{\partial J^{(1)}}\right]_{X^{(2)}} &= -\left[\frac{\partial X^{(1)}}{\partial X^{(2)}}\right]_{J^{(1)}}.
\end{aligned} \tag{3.13}$$

We emphasize that the law of mass action is outside of Classical Irreversible Thermodynamics (CIT), see [7], and relations (3.13) hold even outside the the regime of CIT. Moreover, relations (3.13) reduce in CIT to a single relation (that is in accordance with Onsager reciprocal relations, see Ref. [45] for full discussion of the reciprocal relations within GENERIC). Relations (3.13) hold universally for any two coupled chemical reactions with any number of interacting species and any relation between $\boldsymbol{n}$ and chemical potentials $\boldsymbol{n}^*$ [i.e., for any entropy $S(\boldsymbol{n})$].

d. Boltzmann collision term. Dissipation in the Boltzmann kinetic equation is brought about by ignoring details of particle trajectories traced during collisions. The ignorance involves: (i) limitation to only binary collisions, (ii) that binary collisions are assumed to take place at one point in the position space (this means that only momenta of colliding particles change during collisions), (iii) that values of momenta of two outgoing particles are constrained only by requiring conservation of the kinetic energy and the momentum during the collision, and (iv) that there are no paired and higher-order correlations in the distribution of the particles. This viewpoint of binary collisions allows us to consider them as chemical reactions $\mathbb{V}+\mathbb{V}_1 \leftrightarrows \mathbb{V}'+\mathbb{V}'_1$, where $\mathbb{V}$ denotes the species labeled by momentum $\boldsymbol{p}$, and similarly then for the species labeled by the momentum $\boldsymbol{p}_1$ of the companion particle and the species labeled by the outgoing momenta $\boldsymbol{p}'$ and $\boldsymbol{p}'_1$.

By applying chemical kinetics reviewed in the previous illustration we obtain: $\boldsymbol{X}(\boldsymbol{r},\boldsymbol{p},\boldsymbol{p}_1,\boldsymbol{p}',\boldsymbol{p}'_1) = \Gamma f^*(\boldsymbol{r},\boldsymbol{p}) = -f^*(\boldsymbol{r},\boldsymbol{p}) - f^*(\boldsymbol{r},\boldsymbol{p}_1) + f^*(\boldsymbol{r},\boldsymbol{p}') + f^*(\boldsymbol{r},\boldsymbol{p}'_1)$, $\Xi = \int d\boldsymbol{p} \int d\boldsymbol{p}_1 \int d\boldsymbol{p}' \int d\boldsymbol{p}'_1 W(f;\boldsymbol{p},\boldsymbol{p}_1,\boldsymbol{p}',\boldsymbol{p}'_1)(e^{\frac{1}{2}X}+e^{-\frac{1}{2}X}-2)$, where the following properties are satisfied: (i) W differs from zero and is positive only if $\boldsymbol{p}+\boldsymbol{p}_1 = \boldsymbol{p}'+\boldsymbol{p}'_1$ and $p^2+p_1^2 = (p')^2+(p')_1^2$ and (ii) there is symmetry with respect to the exchanges $\boldsymbol{p} \leftrightarrows \boldsymbol{p}_1$ and $(\boldsymbol{p},\boldsymbol{p}_1) \leftrightarrows (\boldsymbol{p}',\boldsymbol{p}'_1)$. Requirement (i) is the degeneracy condition guaranteeing conservation of the momentum and energy (we recall that the only energy in the Boltzmann kinetic theory is the kinetic energy) and requirement (ii) guarantees (3.7). By a direct verification (see Ref. [33]) we prove that the time evolution equation (3.8) is the Boltzmann kinetic equation without the term $-\frac{\partial(\frac{\boldsymbol{p}}{m}f)}{\partial \boldsymbol{r}}$, i.e., the equation $\frac{\partial f(\boldsymbol{r},\boldsymbol{p})}{\partial t} = \int d\boldsymbol{p}_1 \int d\boldsymbol{p}' \int d\boldsymbol{p}'_1 W^{(B)}(f;\boldsymbol{p},\boldsymbol{p}_1,\boldsymbol{p}',\boldsymbol{p}'_1) \times [f(\boldsymbol{r},\boldsymbol{p}')f(\boldsymbol{r},\boldsymbol{p}'_1) - f(\boldsymbol{r},\boldsymbol{p})f(\boldsymbol{r},\boldsymbol{p}_1)]$, provided the entropy $S^{(1\to 0)}(f)$ is the Boltzmann entropy introduced in Sec. II A 3 and $W^{(B)}$ is related to W appearing in the dissipation potential Ξ by $W^{(B)}(f;\boldsymbol{p},\boldsymbol{p}_1,\boldsymbol{p}',\boldsymbol{p}'_1) = \frac{1}{2}W(f;\boldsymbol{p},\boldsymbol{p}_1,\boldsymbol{p}',\boldsymbol{p}'_1)[f(\boldsymbol{r},\boldsymbol{p})f(\boldsymbol{r},\boldsymbol{p}_1)f(\boldsymbol{r},\boldsymbol{p}')f(\boldsymbol{r},\boldsymbol{v}'_1)]^{-\frac{1}{2}}$.

C. Nondissipative dynamics that is compatible with the dissipative dynamics

The main focus in our search for the time evolution of x_1 has been on its role in reducing Level 1 to Level 0. So far, we have identified the time evolution during which the entropy is raised (called a dissipative time evolution) which then, with the help of the Lyapunov theorem, implies the reduction. Without entering into delicate mathematical details of investigation of the reduction time evolution (see, e.g., Ref. [46]), we recognize that we also have to include inthe time evolution during which the entropy remains unchanged (called nondissipative time evolutions). We shall see then in Sec. III D that the well-established mesoscopic dynamics (notably the one described by the Boltzmann kinetic equation) are indeed combinations of both dissipative and nondissipative dynamics.

In this section we thus turn to the nondissipative dynamics during which the entropy, which has emerged in the dissipative dynamics, remains constant. Such nondissipative dynamics is then called a nondissipative dynamics that is compatible with the dissipative dynamics. For the energy preserving dynamics we require, in addition, that the nondissipative time evolution leaves the energy $E(x_1)$ unchanged. We shall follow two routes: The first is described in Sec. III C 1 and the second in Sec. III C 2.

1. Hamiltonian dynamics

On the first route, we take inspiration from the particular case when Level 1 is chosen to be the level of the classical mechanics of particles. This means that the state variables are $x_1 = (1,2,\ldots,N)$ (we use the notation introduced in Sec. II A 2) and the time evolution is Hamiltonian. We recall that the Hamiltonian time evolution is generated by a potential $E(x_1)$ that is Hamiltonian and has the physical interpretation of energy. The time evolution equations are

$$\dot{x}_1 = LE_{x_1}, \tag{3.14}$$

where L is the Poisson bivector transforming the covector E_{x_1} into a vector. We call L a Poisson bivector if

$$\{A,B\} = \langle A_{x_1}, LB_{x_1}\rangle \tag{3.15}$$

is a Poisson bracket. By $\langle,\rangle$ we denote the scalar product in the state space M_1, and A and B are real valued functions of x_1. We recall that we use the notation $A_{x_1} = \frac{\partial A}{\partial x_1}$, where $\frac{\partial}{\partial x_1}$ denotes the ordinary partial derivative if the state space M_1 is finite dimensional and the Volterra functional derivative if M_1 is infinite dimensional. We recall that $\{A,B\}$ is a Poisson bracket if $\{A,B\} = -\{B,A\}$ and the Jacobi identity $\{A,\{B,C\}\}+\{B,\{C,A\}\}+\{C,\{A,B\}\}=0$ holds. We note that the time evolution generated by (3.14) preserves the energy (since $\dot{E} = \{E,E\} = 0$). The Poisson bracket (3.15) corresponding to the state variables $x_1 = (1,2,\ldots,N)$ is given by $\{A,B\} = \sum_{i=1}^N (A_{\boldsymbol{r}_i}B_{\boldsymbol{p}_i} - B_{\boldsymbol{r}_i}A_{\boldsymbol{p}_i})$.

Summing up, in order to specify the Hamiltonian time evolution of x_1 we need a potential $E(x_1)$ that has the physical interpretation of energy and Poisson bivector L transforming the gradient of energy into a vector field. If we want to relate the time evolution (3.14) to the dissipative dynamics we need more. In particular, we need to incorporate into the time evolution the entropy $S^{(1\to 0)}(x_1)$ that generates the dissipative time evolution. The way we shall relate (3.14) to the entropy is by requiring that the entropy remains unchanged during the time evolution. We note that this will be the case if the Poisson bivector L is appropriately degenerate in the sense that $\{A,S^{(1\to 0)}\} = 0$ for all A. Then, indeed, as it follows from (3.14), $\dot{S}^{(1\to 0)} = \{S^{(1\to 0)},E\} = 0$. We recall the terminology established in Hamiltonian dynamics (see, e.g., Ref. [47]). A function C satisfying $\{A,C\} = 0$ for all A is called a Casimir. We thus require that the entropy $S^{(1\to 0)}(x_1)$ is a Casimir of the Poisson bivector L. Our problem now is to find L with such a property.

As we are still confined to the classical mechanics of particles, we begin the search with the state variables $x_1 = (1,2,\ldots,N)$. The Poisson bracket is nondegenerate and its only Casimir is a constant. We thus see that with the choice $x_1 = (1,2,\ldots,N)$ of state variables we cannot combine the Hamiltonian time evolution with the dissipative dynamics.

We pass therefore to the Liouville representation in which $x_1 = f_N(1,2,\ldots,N)$ is the N-particle distribution function. In this representation the Poisson bracket (3.15) is given by (see Ref. [47])

$$\{A,B\} = \langle A_{x_1}, LB_{x_1}\rangle = \int d1 \ldots \int dN f_N \sum_{i=1}^{N} \times \left(\frac{\partial A_{f_N}}{\partial \boldsymbol{r}_i}\frac{\partial B_{f_N}}{\partial \boldsymbol{p}_i} - \frac{\partial B_{f_N}}{\partial \boldsymbol{r}_i}\frac{\partial A_{f_N}}{\partial \boldsymbol{p}_i} \right). \tag{3.16}$$

This Poisson bracket is indeed degenerate. It is easy to verify that any function $C(f_N) = \int d1 \ldots \int dN c(f_N)$, where c is $\mathbb{R} \to \mathbb{R}$ function $f_N \mapsto c$ is a Casimir of the bracket (3.16). In particular, thus the Gibbs entropy introduced in Sec. II A 2 is a Casimir and, consequently, the Gibbs entropy remains unchanged during the Hamiltonian time evolution generated by (3.14) with the Poisson bracket (3.16). The observation that we have made above about Casimirs of (3.16) implies also that the entropy is not singled out by the requirement of degeneracy. It is the dissipative time evolution that introduces the entropy.

If we now choose Level 1 to be a general mesoscopic level, then we still assume that the fully microscopic Hamiltonian time evolution (3.14) remains inherited in at least a part of the mesoscopic time evolution. We shall call it a nondissipative part of the time evolution. We shall indeed see below that many well-established mesoscopic time evolution equations are a combination of (3.8) and (3.14). The compatibility of (3.14) with (3.8) requires degeneracy of the Poisson bracket. The entropy, which emerges in the dissipative part of the time evolution, has to be a Casimir of the bracket (3.15).

As an illustration, we note that the free flow term $-\text{div}[f(\boldsymbol{r},\boldsymbol{p})\frac{\boldsymbol{p}}{m}]$ in the Boltzmann equation has indeed the form (3.14) with the Poisson bracket (3.16) in which $N = 1$ and the energy $E(f) = \int d\boldsymbol{r} \int d\boldsymbol{p} f(\boldsymbol{r},\boldsymbol{p})\frac{p^2}{2m}$.

Another illustration is provided by Euler fluid mechanics [48]. We take $x_1 = [\rho(\boldsymbol{r}),s(\boldsymbol{r}),\boldsymbol{u}(\boldsymbol{r})]$. If we compare these state variables with those in Sec. II A 5, then we see that we are replacing the energy field $e(\boldsymbol{r})$ with the entropy field $s(\boldsymbol{r})$ (see the comments made in Sec. II A 6). If the local entropy $s(\boldsymbol{r}) = s(\rho,\boldsymbol{u},e;\boldsymbol{r})$ appearing in Sec. II A 5) is such that $\frac{\partial s(\boldsymbol{r})}{\partial e(\boldsymbol{r})} > 0$ [which is indeed the case since $\frac{\partial s(\boldsymbol{r})}{\partial e(\boldsymbol{r})}$ has the physical interpretation of the inverse of the local absolute temperature], then the transformation $[\rho(\boldsymbol{r}),e(\boldsymbol{r}),\boldsymbol{u}(\boldsymbol{r})] \to [\rho(\boldsymbol{r}),s(\boldsymbol{r}),\boldsymbol{u}(\boldsymbol{r})]$ is one to one and we can indeed make such a replacement. We can directly verify that the Euler fluid mechanics equations

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &= -\partial_i(\rho E_{u_i}) \\
\frac{\partial s}{\partial t} &= -\partial_i(s E_{u_i}) \\
\frac{\partial u_i}{\partial t} &= -\partial_j(u_i E_{u_j}) - \rho(\boldsymbol{r})\partial_i E_{\rho(\boldsymbol{r})} \\
&\quad - s(\boldsymbol{r})\partial_i E_{s(\boldsymbol{r})} - u_k(\boldsymbol{r})\partial_i E_{u_k(\boldsymbol{r})}
\end{aligned} \tag{3.17}$$

are indeed a particular realization of (3.14) with the Poisson bracket (see Refs. [23,47])

$$\begin{aligned}
\{A,B\} = \int d\boldsymbol{r}[&\rho(\partial_i(A_\rho)B_{u_i} - \partial_i(B_\rho)A_{u_i}) \\
&+ s(\partial_i(A_s)B_{u_i} - \partial_i(B_s)A_{u_i}) \\
&+ u_j(\partial_i(A_{u_j})B_{u_i} - \partial_i(B_{u_j})A_{u_i})]
\end{aligned} \tag{3.18}$$

and the energy $E = \int e(\boldsymbol{r})$, where $e(\boldsymbol{r}) = e(\rho,s,\boldsymbol{u};\boldsymbol{r})$ is the image of $s(\boldsymbol{r}) = s(\rho,e,\boldsymbol{u};\boldsymbol{r})$, appearing in Sec. II A 5 under the transformation $[\rho(\boldsymbol{r}),e(\boldsymbol{r}),\boldsymbol{u}(\boldsymbol{r})] \to [\rho(\boldsymbol{r}),s(\boldsymbol{r}),\boldsymbol{u}(\boldsymbol{r})]$. The last equation in (3.17) can be put into the form of the local conservation law $\frac{\partial u_i}{\partial t} = -\partial_j(u_i E_{u_j}) - \partial_i p$ provided $p(\boldsymbol{r}) = -e(\boldsymbol{r}) + \rho(\boldsymbol{r})E_{\rho(\boldsymbol{r})} + s(\boldsymbol{r})E_{s(\boldsymbol{r})} + \boldsymbol{u}(\boldsymbol{r})E_{\boldsymbol{u}(\boldsymbol{r})}$. But this is the equilibrium thermodynamic relation related the pressure to the entropy. In the above equation we use the summation convention and the shorthand notation $\partial_i = \frac{\partial}{\partial r_i}$.

2. *Godunov dynamics*

On the second route we let ourselves to be motivated by the Euler fluid mechanics [48]. The state variables are chosen to be all fields (i.e., functions of the position coordinate $\boldsymbol{r}$) and the time evolution equations are local conservation laws. This means that $x_1 = \boldsymbol{q}(\boldsymbol{r}) = [q_1(\boldsymbol{r}),\ldots,q_N(\boldsymbol{r})]$ and

$$\frac{\partial \boldsymbol{q}}{\partial t} = -\text{div}\,\boldsymbol{Q}(\boldsymbol{q}), \tag{3.19}$$

where $\boldsymbol{Q} = (Q_1,\ldots,Q_N)$ are fluxes. If we assume that one of the fields included in $\boldsymbol{q}(\boldsymbol{r})$ is the local energy $e(\boldsymbol{r})$, then the time evolution generated by (3.19) is also energy preserving [indeed, the total energy $E = \int d\boldsymbol{r} e(\boldsymbol{r})$ is preserved].

Now we proceed to entropy conservation. In this setting we shall say that the time evolution generated by (3.19) is entropy preserving if there exists a field $s(\boldsymbol{r})$ that is a pointwise function of $\boldsymbol{q}(\boldsymbol{r})$ and its time evolution induced by (3.19) is another local conservation law

$$\frac{\partial s}{\partial t} = -\text{div}\,\boldsymbol{Q}^{(s)}, \tag{3.20}$$

where $\boldsymbol{Q}^{(s)}$ is the flux corresponding to the field $s(\boldsymbol{r})$. Godunov has noted (see Refs. [49–52]; the proof is made by a direct verification) that the time evolution generated by (3.19) is entropy preserving if (3.19) can be cast in the form

$$\frac{\partial \boldsymbol{q}^*}{\partial t} = -\text{div}\,\boldsymbol{Q}^*, \tag{3.21}$$

where $\boldsymbol{q}^* = \frac{\partial \tilde{s}}{\partial \boldsymbol{q}}$ and $\boldsymbol{Q}^* = \frac{\partial \tilde{\mathcal{S}}}{\partial \boldsymbol{q}}$; $\tilde{s}(\boldsymbol{r})$ is pointwise and a concave function of $\boldsymbol{q}(\boldsymbol{r})$, and $\tilde{\mathcal{S}}(\boldsymbol{r}) = [(\tilde{\mathcal{S}})_1(\boldsymbol{r}),(\tilde{\mathcal{S}})_2(\boldsymbol{r}),(\tilde{\mathcal{S}})_3(\boldsymbol{r})]$ is a pointwise vector function of $\boldsymbol{q}(\boldsymbol{r})$. The field $s(\boldsymbol{r})$, whose time evolution is governed by the local conservation law (3.20), is given by $s(\boldsymbol{r}) = -\tilde{s}(\boldsymbol{r}) + \langle \boldsymbol{q}^*,\boldsymbol{q}\rangle(\boldsymbol{r})$ and the flux $\boldsymbol{Q}^{(s)}$ by $\boldsymbol{Q}^{(s)} = -\tilde{\mathcal{S}} + \langle \boldsymbol{Q}^*,\boldsymbol{q}\rangle(\boldsymbol{r})$. We use the following notation: $\langle \boldsymbol{q}^*,\boldsymbol{q}\rangle(\boldsymbol{r}) = q_1^*(\boldsymbol{r})q_1(\boldsymbol{r}) + \cdots + q_N^*(\boldsymbol{r})q_N(\boldsymbol{r})$ and $(\langle \boldsymbol{Q}^*,\boldsymbol{q}\rangle)_i(\boldsymbol{r}) = (Q_1^*)_i(\boldsymbol{r})q_1(\boldsymbol{r}) + \cdots + (Q_N^*)_i(\boldsymbol{r})q_N(\boldsymbol{r})$; $i = 1,2,3$. Consequently, the total entropy $S^{(1\to 0)}$ that is preserved during the time evolution governed by (3.21) is $S^{(1\to 0)} = \int d\boldsymbol{r} s(\boldsymbol{r})$.

As an illustration, we note that the equations governing the time evolution of the classical Euler fluid mechanics have indeed the form (3.19) of local conservation laws with $\boldsymbol{q}(\boldsymbol{r})$ given in Sec. II A 5. Moreover, the time evolution of the local entropy is governed by (3.20) [and thus the time evolution equations of the classical Euler fluid mechanics can be put into the Godunov form (3.21)], provided the local scalar pressure arising in the fluxes $\boldsymbol{Q}(\boldsymbol{r})$ is related to the local entropy in the same way as at the equilibrium thermodynamics (i.e., we make the local equilibrium assumption).

We have seen in Sec. III C 1 that the Euler fluid mechanics equations also represent the Hamiltonian dynamics that is compatible with the dissipative dynamics involving the local equilibrium entropy. The Euler fluid dynamics is thus both Hamilton and Godunov. The question of how these two types of dynamics relate in general remains unanswered.

D. GENERIC dynamics

We now combine the dissipative and the nondissipative dynamics introduced in Secs. III B and III C 1. We begin by noting that both are generated by a potential. In the dissipative dynamics it is the entropy $S^{(1\to 0)}(x_1)$ and in the nodissipative dynamics it is the energy $E(x_1)$. The gradient of entropy x_1^* (a covector) is transformed in dissipative dynamics into a vector by the dissipation potential [which we regard as a generalized Riemannian structure; see the text in Sec. III B that follows Eq. (3.8)] and the gradient of energy $E(x_1)$ is transformed into a vector in nondissipative dynamics by the Poisson bivector L. We now need to know how the energy behaves in the dissipative dynamics and how the entropy behaves in the nondissipative dynamics. If the energy is included in $\Pi^{(1\to 0)}(x_1)$, then the energy remains inactive (i.e., it does not change) in the dissipative time evolution. This property is guaranteed by degeneracy of the dissipation potential Ξ (i.e., degeneracy of the generalized Riemannian structure). In the nondissipative dynamics it is, on the other hand, the entropy that remains inactive. This property is guaranteed by degeneracy of the Poisson bivector L (or, equivalently, by requiring that the entropy is a Casimir of the Poisson bracket corresponding to L).

The degeneracies of L and Ξ that we have just recalled allow us to combine the entropy and the energy into one potential, $\Phi^{(1\to 0)}(x_1,x_0^*)$, introduced in (2.1) and called a thermodynamic potential, and use only this single potential to generate both dissipative and nondissipative dynamics. We thus write the combination of the dissipative and nondissipative time evolution equation in the form

$$\dot{x}_1 = \frac{1}{e_0^*} L x_1^\dagger - \Xi_{x_1^\dagger}, \tag{3.22}$$

where L is a Poisson bivector. The superscript dagger denotes conjugation with respect to $\Phi^{(1\to 0)}(x_1,x_0^*)$, i.e., $x_1^\dagger = \frac{\partial \Phi^{(1\to 0)}(x_1,x_0^*)}{\partial x_1}$.

We make six comments.

Comment 1. We note that the time evolution generated by (3.22) manifestly describes the approach Level 1 → Level 0 that we discussed in the static reduction in Sec. II. Indeed, as $t \to \infty$, solutions to (3.22) approach $(x_0^*)_{\mathrm{eq}}(x_0)$ that are solutions of (2.2). The explicit presence of the parameters belonging to Level 0 in (3.22) displays manifestly the required degeneracies of the dissipative and nondissipative time evolution equations introduced in Secs. III B and III C and also displays the fact that this dynamics addresses two levels, namely Level 1 and Level 0.

Comment 2. A brief history of (3.22) was reviewed at the beginning of Sec. III. We recall that (3.22) was called GENERIC in Refs. [29,30] and that two monographs [53,54] and, more recently, a review article [33] have been written about equations such as (3.22). However, the search for alternative, and possibly more appropriate from both the mathematical and the physical points of view, formulations continues. As for the nondissipative term [the first term on the right-hand side of (3.22)], we mention in particular the Godunov dynamics recalled in Sec. III C 2 and the investigation reported in Ref. [55]. Regarding the dissipative (the second) term on the right-hand side of (3.22), there are even more variations that have been suggested. We recall that the formulation (3.22) with dissipation potential is the same as the one introduced in Ref. [29]. Similar but not equivalent formulations have been suggested in Refs. [56,57]. In this paper we are contributing to the clarification of the physical content of the dissipation potential by relating it to the classical results of nonequilibrium thermodynamics reported in Refs. [5–8] and by deriving its consequences (3.13) in the specific context of chemical kinetics.

Comment 3. From the geometrical point of view, (3.22) is a vector field generated by one potential, namely the thermodynamic potential $\Phi^{(1\to 0)}(x_1,x_0^*)$, and involving two geometrical structures transforming covectors (e.g., gradients of a potential) into vectors. One such structure is the Poisson structure playing this role in the Hamiltonian mechanics. If we limit ourselves only to this type of dynamics, then the Poisson structure is preserved during the time evolution (this is a direct consequence of the Jacobi identity). The second structure is a generalized Riemannian structure (i.e., the dissipation potential Ξ) playing this role in the gradient dynamics. Neither of these two structures are preserved in the GENERIC time evolution generated by (3.22). It would be much more satisfactory from the geometrical point of view to reformulate (3.22) into a form in which there is only one geometrical structure that has the following two properties: (i) It transforms gradients of two different potentials into vector fields representing both dissipative and nondissipative dynamics and (ii) it is preserved during the time evolution. In such reformulation the difference between dissipative and nondissipative part of the vector field is not in the geometrical structure [as it is in (3.22)] but in generating potentials.

It turns out [32–35] that such a reformulation is indeed possible in the setting of contact geometry. In addition to its geometrical appeal, it also has a physical appeal. The time evolution (3.22) formulated in the setting of contact geometry becomes a continuous sequence of Legendre transformations that are an infinitesimal version of the Legendre transformations making the static reductions in Sec. II.

Comment 4. We have combined in (3.22) the dissipative and nondissipative time evolution by simply adding the vector fields generating them. This simple addition of two different vector fields has, however, very complex consequences on trajectories generated by the resulting vector field. Let us recall, for instance, the situation in the particular case of the Boltzmann kinetic equation. The Boltzmann vector field is a sum of the Hamiltonian part and the dissipative part that is the Boltzmann collision term described in Sec. III B 1.

In the absence of the Hamiltonian part, the collision term in the vector field drives $f(\boldsymbol{r},\boldsymbol{p})$ to local Maxwellian distributions [obtained as a solution to $\boldsymbol{X}(\boldsymbol{r},\boldsymbol{p},\boldsymbol{p}_1,\boldsymbol{p}',\boldsymbol{p}'_1) = -f^*(\boldsymbol{r},\boldsymbol{p}) - f^*(\boldsymbol{r},\boldsymbol{p}_1) + f^*(\boldsymbol{r},\boldsymbol{p}') + f^*(\boldsymbol{r},\boldsymbol{p}'_1) = 0$] that form a submanifold of M_1. The submanifold, which we denote $\mathcal{M}_{\text{loc}M} \subset M_1$, is an image of a mapping $[\rho(\boldsymbol{r}),\boldsymbol{p}(\boldsymbol{r}),e(\boldsymbol{r})] \hookrightarrow M_1$. The exact form of the mapping (see, e.g., Ref. [36]) is not important for the argument below.

In the absence of the collision term, the Hamiltonian part of the vector field is solved by $f(\boldsymbol{r},\boldsymbol{p}) \to f(\boldsymbol{r} - \frac{\boldsymbol{p}}{m}t,\boldsymbol{p})$, where $f(\boldsymbol{r},\boldsymbol{p})$ is the distribution function at the initial time $t = 0$ and the entropy remains unchanged during the time evolution.

If both the Hamiltonian and the collision terms are present (i.e., if we consider the complete Boltzmann kinetic equation), then $f(\boldsymbol{r},\boldsymbol{p},t)$ tends to the total equilibrium manifold $\mathcal{M}_{\text{tot}M} \subset \mathcal{M}_{\text{loc}M} \subset M_1$ at which $[\rho(\boldsymbol{r}),\boldsymbol{p}(\boldsymbol{r}),e(\boldsymbol{r})]$ are independent of $\boldsymbol{r}$. This means that the Hamiltonian vector field, that by itself does not cause any dissipation, brings about an additional dissipation if added to the dissipative collision-generated vector field. The proof of this statement, initiated by Grad in Ref. [36] and brought into full generality by Villani in Ref. [46], is an example of beautiful mathematics involved in an analysis of solutions of equations of GENERIC type (3.22) (see also Ref. [58]).

Comment 5. The Jacobi identity plays an important role in Hamiltonian mechanics. It guarantees that the Poisson structure of M_1, defined by L, is preserved during the time evolution (indeed, the Jacobi identity guarantees that $\frac{d}{dt}\{A,B\} = \{\frac{dA}{dt},B\} + \{A,\frac{dB}{dt}\} = \{\{A,E\},B\} + \{A,\{B,E\}\} = \{\{A,B\},E\}$). Its role in GENERIC dynamics is obviously much less important. In the presence of the dissipative part, the Poisson structure is not preserved in GENERIC dynamics irrespective of L satisfying or not satisfying the Jacobi identity. The properties of the bivector L that also continue to be very important in GENERIC dynamics are its antisymmetry and its degeneracy. This observation has also been made in the contact structure formulation of GENERIC (see Refs. [32–35]).

Comment 6. If the dissipation potential $\Xi(x_1,x_1^*)$ is chosen to be quadratic [i.e., $\Xi(x_1,x_1^*) = \frac{1}{2}\langle x_1^*,\boldsymbol{\Lambda}(x_1)x_1^*\rangle$ with $\boldsymbol{\Lambda}(x_1) \geqslant 0$; see (3.4)], then the dissipative part of the vector field becomes

$$\dot{x_1} = [\boldsymbol{\Lambda}(x_1)x_1^*]_{x_1^*=S_{x_1}}. \tag{3.23}$$

There are, however, many well-established dissipative time evolutions (including the one arising in chemical kinetics and the Boltzmann collision dynamics, both discussed in Sec. III B 1), that cannot be cast into this form. There is therefore a general agreement that the dissipation time evolution equation (3.23) is not sufficiently general and has to be modified. There are at least two ways to make this modification. First, by replacing (3.23) with (3.8), which uses the dissipation potential, and, second, by replacing (3.23) with

$$\begin{aligned}\dot{x_1} &= [\boldsymbol{\Lambda}(x_1,x_1^*)x_1^*]_{x_1^*=S_{x_1}}\\ \boldsymbol{\Lambda}(x_1,x_1^*) &\geqslant 0.\end{aligned} \tag{3.24}$$

There is no general agreement regarding which of these two methods is preferred. Below, we shall recall the arguments in favor of the dissipation potential formulation. We shall then also mention arguments favoring (3.24) and argue against them.

1. Arguments in favor of the dissipation potential

(1) The time evolution (3.23) represents gradient dynamics. The vector field [i.e., the right-hand side of (3.23)] is a gradient of the potential $S(x_1)$ (i.e., a covector) transformed into a vector by the Riemannian structure represented by the matrix $\boldsymbol{\Lambda}(x_1)$. The dissipation potential formulation (3.8) still keeps the geometrical interpretation of a generalization of the gradient dynamics. The transformation of a covector into a vector is not made in (3.8) by a Riemannian structure but by making a gradient of another potential, namely the dissipation potential. On the other hand, the formulation (3.24) has no geometrical interpretation that would relate it to the gradient dynamics.

(2) The dissipation potential is an essential ingredient of dissipation thermodynamics that has always been a part of the classical nonequilibrium thermodynamics. We have shown its relation to the dissipative time evolution in Sec. III A. In addition, the dissipative time evolution was presented in the form of (3.8) in Refs. [37,59].

(3) Recently, the formulation (3.8) has arisen in an attempt to arrive at a mesoscopic time evolution from the microscopic particle dynamics, see Bruce Turkington's paper [3], and also in an attempt to extend Onsager's derivation of the Onsager reciprocity relations to the far-from-equilibrium nonlinear regime in Ref. [60].

(4) The Maxwell-Onsager relations (3.13) hold only if the chemical kinetics is generated by the dissipation potential. These (and those that are similar to them) relations represent thus a concrete tool to prove or disprove experimentally the dissipation potential formulation of chemical kinetics.

2. Arguments against the dissipation potential and our answers to them

(1) The dissipation potential formulation (3.8) excludes an antisymmetric Casimir-type contribution (not producing entropy and not being a part of the Hamiltonian dynamics) to the time evolution. Such a contribution is, on the other hand, allowed in the time evolution generated by (3.23) or (3.24). Our answer to this objection is presented in Ref. [45]. Essentially, we argue that the Casimir-type terms can always be seen as remnants of a reduction made from extended (in the sense discussed in the next section) formulations as the antisymmetric coupling should be given by the Hamiltonian part of the evolution.

(2) The time evolution (3.24) is clearly more general than the time evolution equation (3.8) [note that if we equate the right-hand sides of (3.8) and (3.24), then the symmetry of the second derivative of the dissipation potential represents a restriction on the matrix $\boldsymbol{\Lambda}(x_1,x_1^*)$]. In principle (see Ref. [61]), it is therefore possible to identify a dissipative time evolution that is experimentally proven to exist and that can be formulated in the form (3.24) but cannot be formulated

in the form (3.8). While, of course, we cannot exclude this possibility, we consider the experimental observations needed for such a proof as very difficult, if not impossible, to realize.

(3) Some attempts to derive mesoscopic dynamics from the microscopic particle dynamics indicate a preference for the formulation (3.24) (e.g., Kleeman's paper [4]). To answer this objection we recall that any path from the microscopic to a mesoscopic dynamics is just one of essentially infinitely many paths that all involve many types of steps in which some details, judged as unimportant, are ignored. If one path indicates some features of the mesoscopic dynamics, then another one may indicate a different feature. Indeed, the path followed by Turkington in Ref. [3] indicates that the mesoscopic dissipative dynamics has the form (3.8). As admitted in Kleeman's paper [4], further research should be conducted to fully compare the Kleeman's and Turkington's approaches, and compatibility between Kleeman's approach and GENERIC with dissipation potential should be thus further studied. Moreover, the preference for the dissipative bracket in Ref. [4] is established within the weak-noise limit, where the irreversible evolution is linearized. Therefore, one should not regard that preference as a decisive argument for choosing a dissipation bracket instead of a dissipation potential.

IV. EXTENSION: LEVEL 1 → LEVEL 2

So far, we have looked from Level 1 toward a more macroscopic Level 0. In this section we look in the opposite direction toward a more microscopic level that we shall call Level 2. The reason for this new interest may be, for example, the finding that our experimental observations on Level 1 appear to be impossible to reproduce and/or that they do not agree with Level 1 theoretical predictions. As an example, we recall a need for more details in both experimental and theoretical fluid mechanics when the fluids of interest become the polymeric fluids arising in the processing of plastic materials. Where shall we find the pertinent extra details? There are several sources of inspiration for the enlargement of the state space M_1. We mention three but we shall follow only the third one.

The archetype example of the first source of inspiration for choosing extra state variables is the above-mentioned extension of the classical fluid mechanics motivated by its failure to explain polymeric fluids. The pertinent details in this example are identified by turning to the microscopic constituents of the fluids. Some of their characteristics then become the extra state variables that, in combination with x_1, become state variables x_2 in the extended state space M_2. Specifically, in polymeric fluids, we model the complex polymeric macromolecules as, for example, dumbbells and include their mechanical characteristics (as, e.g., extension and orientation) into the set of the state variables used in classical fluid mechanics (see Ref. [62]).

The second inspiration is based on the way the experimental observations are made and on the form in which the results appear. Let the experimental observations be limited to those that constitute the experimental basis of Level 1. Moreover, let the results of the measurements be found, strictly speaking, impossible to reproduce since the results appear to fluctuate. The occurrence of fluctuations may be due to an increase in the precision of the measurements and/or due to the fact that some details ignored in Level 1 begein to play an important role in the situations under investigation. The problem now is to use the extra information provided by an analysis of fluctuations to introduce a new, more microscopic, Level 2, on which the results of extended (i.e., Level 2) experimental observations would not fluctuate (or would still fluctuate but with a diminished intensity). One way to achieve this goal was presented in Ref. [63].

The third inspiration comes from dissipation thermodynamics. In Sec. III A we introduced its static version and, subsequently, in Sec. III B, we implemented it into the time evolution in M_1. Now we shall develop its dynamic version (i.e., we step up to a more microscopic Level 2 on which $\boldsymbol{J}$ or quantities related to it play the role of independent state variables) and then we shall combine the time evolution arising in it with the time evolution in M_1. From the physical point of view, the essence of this approach to extensions is an introduction of additional inertia into the time evolution in M_1. The vector field (or a part of it) generating the time evolution on Level 1 is taken as an independent state variable and a new time evolution equation is constructed for it. The first examples of this type of extension were presented in research of heat transfer [64] and in the fluid mechanics that was viewed as a theory reduced from the Boltzmann equation (Grad's hierarchy introduced in Ref. [36]; see also Refs. [9–12]). In the rest of this paper we explore the extrainertia extensions in the light of the reduction theory developed in the previous sections and work out some examples.

We begin by introducing a new state space M_2 as a Cartesian product of M_1 and $M_1^{(J)}$ [i.e., $M_2 = M_1 \times M_1^{(J)}; (x_1,\boldsymbol{J}) \in M_2$]. As we did in the two previous sections in the investigation of reductions, we shall also make a distinction between static and dynamic versions in the investigation of extensions.

First, we turn to the static extension. We make it by extending the entropy $S^{(1\to 0)}(x_1)$ into a new entropy $S^{(2\to 0)}(x_1,\boldsymbol{J})$ defined in the space M_2. We make the extension by

$$S^{(2\to 0)}(x_1,\boldsymbol{J}) = S^{(1\to 0)}(x_1) - K\,\Theta(\boldsymbol{J}), \tag{4.1}$$

where K is a phenomenological coefficient having the physical dimension of time.

Having extended the entropy from M_1 to M_2 we now reduce it back to M_1. By making the Legendre transformation in $\boldsymbol{J}$ we arrive at

$$S^{(1\to 0)}(x_1) + K\,\Xi(\boldsymbol{X}). \tag{4.2}$$

In the absence of constraints, the reduced entropy $S^{(2\leftarrow 1)} = S^{(1\to 0)}(x_1) + K[\Xi(\boldsymbol{X})]_{\boldsymbol{X}=0} = S^{(1\to 0)}(x_1)$ is thus [due to the properties (3.1) of the dissipation potential] the original entropy in the space M_1. If, on the other hand, we impose the constitutive relation (3.6), we arrive at

$$S^{(2\leftarrow 1)} = S^{(1\to 0)}(x_1) + K[\Xi(\boldsymbol{X})]_{\boldsymbol{X}=\Gamma x_1^*}, \tag{4.3}$$

which is a new entropy in the space M_1. We note that this new entropy involves quantities appearing in the dissipative time evolution that takes place in M_1.

Now we turn to the dynamic version of the above static extension and reduction. Our objective is to construct an equation governing the time evolution of $x_2 = (x_1,\boldsymbol{J})$ and thus establish a new level of description that we call Level 2. The time evolution in M_2 is required to be compatible with Level 0 and Level 1 in the following sense.

Requirement of the compatibility with Level 0. The time evolution in M_2 reduces Level 2 to Level 0. This means that the equation governing the time evolution of x_2 possesses the structure identified in Sec. III (in which Level 1 is now replaced by Level 2).

Requirement of the compatibility with Level 1. The approach $x_2 \to x_0$ proceeds in two stages. In the first stage, called a *fast time evolution*, $x_2 \to x_1$ and Level 1 (with the time evolution taking place on it) is recovered. In the second stage, called a *slow time evolution*, the original time evolution in M_1 makes the passage $x_1 \to x_0$.

First, we shall formulate Level 2 dynamics in a simple finite dimensional setting. Next, we make it more explicit in the context of heat transfer.

A. Toy illustration

The three levels, called Level 0, Level 1, and Level 2, are introduced as follows.

1. *Level 0*

The state space M_0 is a one-dimensional space with elements $x_0 = e_0$, where e_0 has the physical interpretation of energy. The fundamental thermodynamic relation is $S^{(0)}(e_0)$.

2. *Level 1*

The state space M_1 is a two-dimensional space with elements $x_1 = (q,e)$. The quantity e is the same as in Level 0 and the physical interpretation of q is left unspecified (it could be a scalar characterizing the internal structure, for instance, a free volume). The fundamental thermodynamic relation is $S^{(1\to 0)}(q,e)$, and the mapping $M_1 \to M_0$ is given by $\Pi^{(1\to 0)} : (q,e) \mapsto e_0$.

Now we introduce time evolution into M_1. We assume that the time evolution is only dissipative and that the energy e is conserved. Moreover, if we choose $X = q^*$, then the time evolution (3.8) becomes

$$\frac{d}{dt}\begin{pmatrix} q \\ e \end{pmatrix} = \begin{pmatrix} \Xi_{q^*} \\ 0 \end{pmatrix} \tag{4.4}$$

in the entropy representation and

$$\frac{d}{dt}\begin{pmatrix} q \\ s \end{pmatrix} = \begin{pmatrix} \Xi_{q^*} \\ q^*\Xi_{q^*} \end{pmatrix} \tag{4.5}$$

in the energy representation.

From these time evolution equations we then obtain $S^{(0\leftarrow 1)}(e) = [S^{(1\to 0)}]_{q^*=0}$, that is, the fundamental thermodynamic relation in M_0 implied by the fundamental thermodynamic relation $S^{(1\to 0)}(q,e)$ in M_1.

3. *Level 2*

The state space M_2 is a three-dimensional space with coordinates $x_2 = (p,q,e)$. The quantities q and e are the same as in M_1, the physical interpretation of the new quantity p can be deduced from the time evolution equations introduced below. The extension of Level 1 to Level 2 is made by adopting a new state variable p. The mappings $\Pi^{(2\to 0)}$ and $\Pi^{(2\to 1)}$ are given by $(p,q,e) \mapsto e$ and $(p,q,e) \mapsto (q,e)$, respectively, and the fundamental thermodynamic relation is $S^{(2\to 0)}(p,q,e)$.

Now we introduce the time evolution into M_2 that is compatible with Level 0 and Level 1. We prove below that one such time evolution is governed by

$$\frac{d}{dt}\begin{pmatrix} p \\ q \\ e \end{pmatrix} = \begin{pmatrix} 0 & -1 & \frac{q^*}{e^*} \\ 1 & 0 & -\frac{p^*}{e^*} \\ -\frac{q^*}{e^*} & \frac{p^*}{e^*} & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} + \begin{pmatrix} \Theta_{p^*} \\ 0 \\ 0 \end{pmatrix}. \tag{4.6}$$

Note that, typically, q is an even variable while p is an odd variable with respect to the time-reversal transformation, see, e.g., Ref. [45]. Therefore, evolution of q is reversible while evolution of p contains both reversible and irreversible parts.

4. *Compatibility of Level 2 with Level 1 and Level 0*

First, we prove that (4.6) is indeed a particular realization of the GENERIC equation (3.22). In order to see that, we have to show that the first term on the right-hand side of (4.6) is Hamiltonian. We note that energy in the entropy representation is simply $E(p,q,e) = e$ and thus its gradient is indeed the vector $(0,0,1)^T$. Next, we have to prove that the matrix that multiplies the vector $(0,0,1)^T$ is a Poisson bivector L. To prove it, we pass from the entropy representation to the energy representation [i.e., from the state variables (p,q,e) to (p,q,s)] by use of the transformation $p = p, q = q, s = s(p,q,e)$. This transformation between two representations is one to one since $e^* = s_e > 0$. Under this transformation the matrix that multiplies the vector $(0,0,1)^T$ in (4.6) transforms into $\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$. This transformed matrix is indeed a Poisson bivector (Jacobi identity and antisymmetry are clearly fulfilled) and thus also the matrix that multiplies the vector $(0,0,1)^T$ in (4.6) is a Poisson bivector (because the transformation between two representations is one to one). In the energy representation we also clearly see that the entropy $S^{(2\to 0)}(p,q,e) = s(p,q,e)$ is a Casimir of the Poisson bracket corresponding to it.

Now we turn our attention to the second term on the right-hand side of (4.6). This term is the same as the second term on the right-hand side of (3.22) provided Θ is a dissipation potential satisfying the properties (3.1). We have thus proven that (4.6) is indeed a particular representation of the GENERIC equation (3.22).

Next we turn to the compatibility of the Level 2 dynamics (4.6) with the Level 1 dynamics (4.4). Let $S^{(2\to 0)}$ and Θ be chosen in such a way that p, which has been adopted on Level 2 as an extra state variable, evolves faster than q (we recall that e does not evolve at all). We limit ourselves to the stage in the time evolution in which p has already reached its stationary value that is determined, as we see in the first equation in (4.6), by

$$\frac{1}{e^*}q^* + \Theta_{p^*} = 0. \tag{4.7}$$

In this stationary state, p becomes completely enslaved to q and remains in this relation to q for the rest of the time evolution. This means that after reaching the stationary state [obtained as a solution to (4.7)] p evolves in time only due to the time evolution of q.

Equation (4.7) can be rewritten as

$$\frac{\partial}{\partial p^*}\left[-\Theta(p^*) + q^*\left(-\frac{p^*}{e^*}\right)\right] = 0, \tag{4.8}$$

which yields a function $\tilde{p}^*(q^*)$. Note that the term q^* should be interpreted as a force while the term $(-\frac{p^*}{e^*})$ is the corresponding flux which is identified as the right-hand side of the evolution equation for q. When function $\tilde{p}^*(q^*)$ is plugged back into this last expression, a new dissipation potential Ξ is obtained, which is a Legendre transformation of the original dissipation potential Θ [with respect to the variable p^* when taking into account Eq (4.7)],

$$\Xi(q^*) = -\Theta[\tilde{p}^*(q^*)] - q^*\frac{\tilde{p}^*(q*)}{e^*}. \tag{4.9}$$

Moreover, derivative of this new dissipation potential with respect to q^* is given simply by

$$\Xi_{q^*} = -\frac{\tilde{p}^*(q^*)}{e^*}. \tag{4.10}$$

This completes the Legendre transformation analogously to the procedure presented in Sec. III A.

For example, if the dissipation potential on Level 2 is quadratic, i.e.,

$$\Theta(p^*) = \tfrac{1}{2}\Lambda(p^*)^2, \tag{4.11}$$

the relaxed value of p^* becomes

$$\tilde{p}^*(q^*) = -\frac{1}{\Lambda}\frac{q^*}{e^*} \tag{4.12}$$

and the dissipation potential on Level 1 is equal to

$$\Xi(q^*) = \frac{1}{2}\frac{1}{\Lambda}\left(\frac{q^*}{e^*}\right)^2. \tag{4.13}$$

When function $\tilde{p}^*$ is plugged back into evolution equations (4.6), the equations become

$$\frac{d}{dt}\begin{pmatrix} p \\ q \\ e \end{pmatrix} = \begin{pmatrix} 0 \\ \Xi_{q^*} \\ 0 \end{pmatrix}. \tag{4.14}$$

That means that the Legendre transformation of the dissipation potential on Level 2, Θ, to the dissipation potential on Level 1, Ξ, changes the evolution equations on Level 2, Eq. (4.6), to evolution where p has already relaxed and q evolves only irreversibly (in contrast to evolution of q on Level 2, which was reversible).

As for the compatibility of Level 2 with Level 0, this property of solutions to (4.6) now follows simply from the compatibility of Level 2 with Level 1 (proven in the previous paragraph) and from the compatibility of Level 1 with Level 0 that we have proven on Level 1.

Before proceeding to a more detailed investigation of the approach of Level 2 to Level 1, we make an important observation about (4.6). Let us look at (4.6) through the eyes of the standard viewpoint of extensions. This means that our point of departure is the equation governing the time evolution of q, namely the second equation in (4.6) (i.e., $\frac{dq}{dt} = -\frac{1}{e^*}p^*$). Instead of specifying the flux p^* arising on its right-hand side (in other words, instead of providing a constitutive relation for the flux p^*) we adopt it as a new state variable and propose an equation governing its time evolution. Subsequently, by requiring the compatibility of the total time evolution with equilibrium thermodynamics (i.e., Level 0) and the original Level 1 time evolution, we specify, or at lest restrict the choice of, the extra time evolution equation. We can indeed regard the genesis of (4.6) in this way but with one important difference. The state variable that we have adopted as an independent state variable is not the flux itself but its conjugate. We see clearly that the recipe for extension is not to take the flux and make it a new state variable but to take a flux and make its conjugate a new state variable. This important feature of extensions has been missed in their initial investigations [9–12] because Grad's hierarchy [36], which has served as a prototype of extensions, does not display this feature due to its very narrow limitation of ideal gases.

How do we interpret these two levels of description physically? Consider a ball on a billiard table. If one only considers the *position* of the ball, one makes observations on Level 1, where q and energy constitute the state variables. Evolution on this level of description is irreversible and thus it is only observed that the ball tends to stop its motion.

If, on the other hand, one considers also the *momentum* of the ball, one makes a more detailed observation, and the evolution is partly reversible (given by the Poisson bracket) and partly irreversible (given by the dissipation potential Θ, which describes friction between the ball and the table). This more detailed level of description is nothing more than classical Newtonian mechanics.

Consider now that there is a smooth pit in the center of the billiard table. The ball eventually stops in the pit due to gravity, but before that happens it rolls around the pit or even a little away from the pit and then back. Entropy on Level 1 reaches its maximum when the ball is in the pit. But as the ball may even go away from the pit for some period of time, the entropy may be even decrease for a period of time. An observer on Level 1 would refer to this phenomenon as fluctuations.

On the other hand, an observer measuring also momentum of the ball, i.e., on Level 2, would not see any fluctuations since he or she would simply integrate Newton's laws to predict the trajectory of the ball precisely. Fluctuations thus can be regarded as an invitation to a higher level of description, where they become predictable, and what seems to be irreversible on a less-detailed level of description may become reversible on a more detailed level.

5. *Fast time evolution*

We continue by putting the approach of Level 2 into Level 1. We want to make the time evolution (we have already given it a name, we called it a fast time evolution) into the GENERIC form (3.22). In other words, we look for a particular realization of (3.22), generating the fast time evolution to make the reduction $M_2 \to M_1$.

We summarize what we already know about the fast time evolution. First, we know that the states approached as $t \to \infty$ are solutions to (2.2). Second, we note that in this particular example of the fast time evolution there is no Hamiltonian part (at least near equilibrium, where variables with the same parity are coupled by the dissipation potential, see Ref. [45]). We therefore concentrate on the dissipative part and look for the thermodynamic potential $\Phi^{(2\to 1)}(p,q,e)$ that generates it. The problem of identification of the fast time evolution is in fact a problem of separating the time evolution equations (4.6) into two uncoupled equations, one governing the fast time evolution of p in which (q,e) appear as parameters and the other equation that is Eq. (4.4) governing the slow time evolution of q. If the time evolution equations (4.6) were linear, then such a separation would represent block diagonalization. A detailed analysis of the solutions to (4.6) that would be needed to solve the separation problem [note that such an analysis would first require us to provide a more detailed specification of the quantities in (4.6) (like the entropy $S^{(2\to 0)}(p,q,e)$ and the dissipation potential Θ] will not be made in this paper. Instead, we only suggest one possible fast time evolution and verify that it possesses the essential property that we require from it, namely that it leads to states that are solutions to (2.2).

The time evolution equation that we propose for the fast time evolution is

$$\frac{dp}{dt} = -\Lambda^{(2\to 1)}\Phi_p^{(2\to 1)}(p,q,e), \tag{4.15}$$

where

$$\Phi^{(2\to 1)}(p,q,e) = -S^{(2\to 0)}(p,q,e) - \Xi_{q^*}p \tag{4.16}$$

and$\Lambda^{(2\to 1)}$ is a positive constant,

We see immediately that (4.15) is indeed a particular realization of (3.22). Note that the dissipation potential in this particular realization of (3.22) is the quadratic potential $\frac{1}{2}\Lambda^{(2\to 1)}(p^*)^2$, where a star denotes the conjugate with respect to $\Phi^{(2\to 1)}$. We also see that solutions to (4.15) approach, as $t\to\infty$, solutions to $\Phi_p^{(2\to 1)}(p,q,e)=0$ and that the equation $\Phi_p^{(2\to 1)}(p,q,e)=0$ is the same as Eq. (2.2). Consequently, we have proven that solutions to (4.15) approach the stationary state determined by (2.2).

Next, we recall that if we regard the GENERIC equation (3.22) as an equation representing reduction to Level 0, then the potential $\Phi^{(2\to 0)}(p,q,e)$ that generates it becomes the fundamental thermodynamic relation on Level 0 if it is evaluated at the state reached as $t\to\infty$, which is the state obtained as a solution to $\Phi_p^{(2\to 0)}(p,q,e)=0$; $\Phi_q^{(2\to 0)}(p,q,e)=0$. We shall thus interpret $[\Phi^{(2\to 1)}(p,q,e)]_{\Phi_p^{(2\to 1)}(p,q,e)=0}$ as the fundamental thermodynamic relation on Level 1 implied by its compatibility with both Level 0 and Level 2. In accordance with the terminology introduced in Sec. II we denote this fundamental relation by the symbol $S^{(1\leftarrow 2)}(q,e)$. In order to express this relation more explicitly, we realize that $[\Phi^{(2\to 1)}(p,q,e)]_{\Phi_p^{(2\to 1)}(p,q,e)=0}$ is a Legendre transformation of $S^{(2\to 0)}(p,q,e)$ in the p variable [in accordance with the notation introduced in Sec. II, we denote it $S^{(2\to 0)*}(p^*,q,e)$] that is evaluated at $p^* = -\Xi_{q^*}$. Consequently [compare with (4.3)],

$$S^{(1\leftarrow 2)}(q,e) = [S^{(2\to 0)*}(p^*,q,e)]_{p^*=-\Xi_{q^*}}. \tag{4.17}$$

This fundamental thermodynamic relation involves quantities belonging to both Level 2 and Level 0. It is in particular the entropy $S^{(2\to 0)}(p,q,e)$, addressing the compatibility of Level 2 with Level 0, and the dissipation potential Θ (or, alternatively, Ξ) emerging in the dissipative part of the time evolution on Level 2.

B. Heat transfer

Let us now invert the extension proposed in the preceding example to show how a method of reduction from a higher (more microscopic) level of description works. Namely, it is the purpose of this section to illustrate the reduction from the level of Maxwell-Cattaneo heat transfer (Level 2), where state variables are $\boldsymbol{x}_2 = [\boldsymbol{w}(\boldsymbol{r}),s(\boldsymbol{r})]$ ($\boldsymbol{w}$ being a vector field odd with respect to time-reversal transformation [45]), to Fourier (Level 1), where state variables are $x_1 = s(\boldsymbol{r})$.

The Poisson bracket on Level 2 is, see Ref. [65],

$$\begin{aligned}\{A,B\} &= \int d\boldsymbol{r}s(\partial_i A_s B_{w_i} - \partial_i B_s A_{w_i})\\ &\quad + \int d\boldsymbol{r}w_i(\partial_j A_{w_i} B_{w_j} - \partial_j B_{w_i} A_{w_j}),\end{aligned} \tag{4.18}$$

where A_{w_i} stands for $(\frac{\partial A}{\partial w_i})_s$. In the entropy representation, where state variables are $e(\boldsymbol{r})$ and $\boldsymbol{w}(\boldsymbol{r})$, the Poisson bracket of a functional A and energy

$$E = \int d\boldsymbol{r}e(\boldsymbol{r}) \tag{4.19}$$

becomes

$$\begin{aligned}&\{A,E\}\\ &\quad = \int d\boldsymbol{r}A_{w_i}\left[-s(\boldsymbol{w},e)\partial_i\frac{1}{e^*} + \partial_j\left(w_i\frac{w_j^*}{e^*}\right) + w_j\partial_i\left(\frac{w_j^*}{e^*}\right)\right]\\ &\qquad + \int d\boldsymbol{r}A_e\left\{\partial_i\left[s\frac{w_i^*}{(e^*)^2}\right] - \partial_j\left[w_i\frac{w_i^*w_j^*}{(e^*)^2}\right]\right\}.\end{aligned} \tag{4.20}$$

See, for example, Ref. [21] or Ref. [19] to see how one can pass between the two representations. Note that the conjugate variables were identified with the corresponding derivatives of entropy.

The dissipation potential is specified as

$$\Theta(e,e^*,\boldsymbol{w}^*) = \frac{1}{2}\int d\boldsymbol{r}\Lambda(e,e^*)(\boldsymbol{w}^*)^2, \tag{4.21}$$

where $\Lambda(e,e^*)$ is a yet-unspecified function of e and e^*. Evolution equations are then recovered from $\dot{A} = \langle A_{\boldsymbol{x}_2},\dot{\boldsymbol{x}}_2\rangle = \int d\boldsymbol{r}A_{w_i}\dot{w}_i + A_e\dot{e}$, in particular,

$$\frac{\partial w_i}{\partial t} = -s\partial_i\frac{1}{e^*} + \partial_j\left(w_i\frac{w_j^*}{e^*}\right) + w_j\partial_i\left(\frac{w_j^*}{e^*}\right) + \Theta_{w_i^*}, \tag{4.22a}$$

$$\frac{\partial e}{\partial t} = \partial_i\left[s\frac{w_i^*}{(e^*)^2}\right] - \partial_j\left[w_i\frac{w_i^*w_j^*}{(e^*)^2}\right]. \tag{4.22b}$$

The Legendre transformation introduced in Sec. III A works on Θ as follows:

$$\frac{\partial}{\partial \boldsymbol{w}^*}\left(-\Theta(e,e^*,\boldsymbol{w}^*) + \int d\boldsymbol{r}\, \underbrace{e^*}_{X_e} \underbrace{\left\{\partial_i\left[s\frac{w_i^*}{(e^*)^2}\right] - \partial_j\left[w_i\frac{w_i^* w_j^*}{(e^*)^2}\right]\right\}}_{J_e}\right) = 0, \tag{4.23}$$

where the force is given simply by conjugate to e and the flux is identified as the right-hand side of the evolution equation for e. Equation (4.23) can be rewritten as

$$\left[\Lambda\delta_{ij} + \left(\partial_i\frac{1}{e^*}\right)w_j + \left(\partial_j\frac{1}{e^*}\right)w_i\right]\tilde{w}_j^*(e^*) = s\partial_i\frac{1}{e^*}. \tag{4.24}$$

Entropy on the Maxwell-Cattaneo level is usually defined as

$$S^{(2\to 0)} = \int d\boldsymbol{r} s^{(1\to 0)}[e(\boldsymbol{r})] - \frac{1}{2}\beta\boldsymbol{w}(\boldsymbol{r})^2, \tag{4.25}$$

see Ref. [65]. The static reduction has been shown to be compatible with simple maximization of entropy with constraints. Therefore, the static reduction from the Maxwell-Cattaneo level with entropy (4.25) and projection $\Pi(\boldsymbol{w},e) = e$ eventually leads to

$$\boldsymbol{w} = 0 \quad \text{everywhere} \tag{4.26}$$

on Level 1. This way Eq. (4.24) simplifies to

$$\tilde{\boldsymbol{w}}^*(e^*) = \frac{1}{\Lambda(e,e^*)}s^{(1\to 0)}\partial_i\frac{1}{e^*} \tag{4.27}$$

and, when plugging this condition and (4.26) into the evolution equation for $\boldsymbol{w}$, Eq. (4.22a), one obtains that variable $\boldsymbol{w}$ no longer evolves on Level 1, i.e., the time derivative is equal to zero.

Plugging Eq. (4.27) and Eq. (4.26) back into Eq. (4.23) leads to a new dissipation potential:

$$\Xi(e^*) = \frac{1}{2}\int d\boldsymbol{r}\frac{[s^{(1\to 0)}(e)]^2}{\Lambda}\left(\nabla\frac{1}{e^*}\right)^2, \tag{4.28}$$

the derivative of which is

$$\begin{aligned}\Xi_{e^*} = \nabla\left\{\frac{[s^{(1\to 0)}(e)]^2}{\Lambda(e,e^*)(e^*)^2}\nabla\frac{1}{e^*}\right\} - \frac{[s^{(1\to 0)}(e)]^2}{2\Lambda^2(e,e^*)(e^*)^8}\frac{\partial}{\partial e^*}\\ \times[\Lambda(e,e^*)(e^*)^4](\nabla e^*)^2.\end{aligned} \tag{4.29}$$

To fulfill the degeneracy that energy (4.19) is conserved during the evolution prescribed by this dissipation potential, it is necessary to require that

$$\Lambda(e,e^*) = \frac{\Lambda_0(e)}{(e^*)^4}, \tag{4.30}$$

where $\Lambda_0(e)$ is an arbitrary positive function. This relation resembles the Stefan-Boltzmann law where energy density of a photon gas is also proportional to the fourth power of temperature. It should be noted, however, that this does not restrict the final dependence of the measured heat conductivity since the dependence of Λ_0 on e still provides enough generality for the conductivity to be a general function of temperature. In summary, the Legendre transformation provides a new dissipation potential on the lower level of description.[1]

When condition (4.30) is satisfied, the last term in Eq. (4.29) disappears and the evolution equations on Level 1 become

$$\frac{\partial w_i}{\partial t} = 0, \tag{4.31}$$

$$\frac{\partial e}{\partial t} = \Xi_{e^*} = \nabla\left\{\frac{[s^{(1\to 0)}(e)]^2(e^*)^2}{\Lambda_0(e)}\nabla\frac{1}{e^*}\right\}, \tag{4.32}$$

which is the standard Fourier heat conduction when $[s^{(1\to 0)}]_e$ is substituted for e^*. Note that these equations are precisely those equations obtained from (4.22) when relations (4.27) and (4.26) are plugged into it. The advantage of the formulation in terms of dissipation potential Ξ is that it is demonstrated that the GENERIC structure is respected by the reduction from Level 2 to Level 1.

Interestingly, conservation of energy on Level 1, which is expressed by the degeneracy of dissipation potential Ξ, restricts dissipation potential Θ, which lives on Level 2, to some extent. In other words, the Poisson bracket has to be related to Θ in such a way that the dissipation potential constructed by the Legendre transformation, Ξ, satisfies the required degeneracy.

In summary, starting with Maxwell-Cattaneo heat transfer (Level 2), one can formulate evolution on Level 1 (Fourier heat transfer) by use of a simple Legendre transformation. Indeed, Legendre transformation in the sense of the dissipative thermodynamics of dissipation potential on Level 2 leads to the dissipation potential on Level 1. Evolution of variable e, which is reversible on Level 2, becomes irreversible on Level 1. Moreover, the structure of GENERIC is respected by this reduction.

Before ending this example we put the results obtained above into the context of some other results obtained for the Cattaneo heat conduction. Joseph and Preziosi [66] provide an extensive review of the problem of heat waves, and many properties of the Maxwell-Cattaneo equation are demonstrated. The reduction to Fourier heat conduction is done by either setting certain parameters to particular values (e.g., relaxation time to zero) or by choosing an appropriate relaxation memory kernel.

Although indeed such reductions provide efficient passages to more macroscopic forms of particular equations, they lack a common structure which could be used for other physical problems. From the thermodynamic point of view, an example of such a structure can be the GENERIC equation (or the contact geometric reformulation), where the principle of

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[1] Note that the new dissipation potential is indeed convex in the sense that $\langle e^*, \Xi_{e^*}\rangle \geqslant 0$, as can be verified easily.

maximum entropy is extensively used during the reductions. In summary, the advantage of our treatment of the reduction from Maxwell-Cattaneo to Fourier is that a unifying thermodynamic structure is proposed that provides the passage between levels of description.

Note, however, that we do not have the ambition to derive any general and unique method of reductions. Rather, we propose a new method of reduction, the generality and elegance of which is provided by the GENERIC equation, and a particular realization of which is demonstrated on the passage from Maxwell-Cattaneo to Fourier. The advantage of the method to previously developed methods, see, e.g., Ref. [67], is, for example, that no neglect of higher-order terms is needed. Still, we do not claim that the method be the only one possible.

Instead, we are trying to identify a multiscale structure that is compatible with GENERIC (with a dissipation potential formulation) so one could change levels of description in a thermodynamically sound way. Additionally, we do not provide a generalization of nonequlibrium thermodynamics nor it is a new thermodynamic framework. We look for new relationships and applications within a general, well-defined, and studied nonequilibrium thermodynamics.

Kalospiros *et al.* [68] describe heat transfer within the so-called one-generator formalism [53], where the Hamiltonian structure is not recongnized. A more general treatment of heat transfer can be found in Ref. [65], where the Hamiltonian structure of heat transfer is found and particular approaches to heat transfer are shown to be realizations of the GENERIC equation. In Ref. [68] the reduction is carried out by again setting certain parameters to particular values, which can be an efficient but not general method. In summary, the description of heat transfer in the present manuscript is based on a more general framework of the GENERIC equation than the treatment in Ref. [68], and the reduction is carried out by use of a thermodynamic procedure that transcends the particular application to heat transfer.

V. CONCLUDING REMARKS

Complex macroscopic systems (as, for instance, the systems studied in biology) cannot be investigated on a single level of description. There is a need for a more abstract theory that could be applied on different levels and that would also include a structure addressing relations among the levels. We consider the classical nonequilibrium thermodynamics as a nucleus from which the more abstract multilevel theory unfolds. In this paper we continue the development in this direction that began in Refs. [33–35] and references cited therein. Our attention is focused in this paper in particular on the dissipation thermodynamics developed in Refs. [5,6,8]) and extended thermodynamics developed in Refs. [9–12,36].

An abstract formulation of these two branches of nonequilibrium thermodynamics is then shown to provide a unified setting for several well-established mesoscopic theories. Moreover, some of the results obtained in the abstract theory become new results in the specific mesoscopic theories. The mesoscopic theories serving as examples in this paper include Gibbs equilibrium statistical mechanics, Boltzmann kinetic theory, chemical kinetics, and Fourier and Maxwell-Cattaneo heat transfer. The new results obtained in the examples include reciprocity relations among extents of reactions and affinities in chemical kinetics (3.13) and a systematic reduction from the Maxwell-Cattaneo heat transfer to the standard Fourier heat transfer.

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APPENDIX: SIMPLE MAXIMIZATION OF ENTROPY

The purpose of this section is to show that the final result of the static reduction introduced in Sec. II is compatible with simple maximization of entropy with constraints given by variables x_0.

Let us, therefore, start with the final result of the static reduction, entropy $S^{(0\leftarrow 1)}$, and go backwards so the relation to entropy $S^{(1\rightarrow 0)}$ is revealed explicitly. Using Eq. (2.4), entropy on Level 0 becomes

$$\begin{aligned} S^{(0\leftarrow 1)}(x_0) &= -S^{(0)\star}[(x_0^\star)_{\rm eq}(x_0)] + \langle (x_0^\star)_{\rm eq}(x_0), x_0\rangle \\ &= S^{(1\rightarrow 0)}\{(x_1)_{\rm eq}[(x_0^\star)_{\rm eq}(x_0)]\} \\ &\quad - \langle (x_0^\star)_{\rm eq}(x_0), \Pi\{(x_1)_{\rm eq}[(x_0^\star)_{\rm eq}(x_0)]\} - x_0\rangle. \end{aligned} \tag{A1}$$

Plugging Eqs. (2.3) and (2.4) into Eq. (2.5) leads to

$$\left.\frac{\partial}{\partial x_0^\star}\right|_{(x_0^\star)_{\rm eq}(x_0)} (-S^{(1\rightarrow 0)}[(x_1)_{\rm eq}(x_0^\star)] + \langle x_0^\star, \Pi[(x_1)_{\rm eq}(x_0^\star)]\rangle) = x_0. \tag{A2}$$

The derivative of the first term can be rewritten as

$$\begin{aligned} &\left.\frac{\partial}{\partial x_0^\star}\right|_{(x_0^\star)_{\rm eq}(x_0)} S^{(1\rightarrow 0)}[(x_1)_{\rm eq}(x_0^\star)] \\ &= \left.\frac{\partial S^{(1\rightarrow 0)}}{\partial x_1}\right|_{(x_1)_{\rm eq}[(x_0^\star)_{\rm eq}(x_0)]} \left.\frac{\partial (x_1)_{\rm eq}}{\partial x_0^\star}\right|_{(x_0^\star)_{\rm eq}(x_0)} \\ &\overset{\text{Eq. (II.2)}}{=} \left\langle (x_0^\star)_{\rm eq}(x_0), \left.\frac{\partial \Pi}{\partial x_1}\right|_{(x_1)_{\rm eq}[(x_0^\star)_{\rm eq}(x_0)]} \left.\frac{\partial (x_1)_{\rm eq}}{\partial x_0^\star}\right|_{(x_0^\star)_{\rm eq}(x_0)}\right\rangle. \end{aligned} \tag{A3}$$

Plugging this last equation into Eq. (A2) finally leads to

$$\Pi[(x_1)_{\rm eq}(x_0^\star)_{\rm eq}(x_0)] = x_0, \tag{A4}$$

and the entropy on Level 0 implied by Level 1, Eq. (A1), becomes

$$S^{(0\leftarrow 1)}(x_0) = S^{(1\to 0)}\{(x_1)_{\rm eq}[(x_0^\star)_{\rm eq}(x_0)]\}. \tag{A5}$$

To show that this indeed is the result that can be obtained by simple maximization of entropy $S^{(1\to 0)}$ with constraints given by the projection Π, it is sufficient to show that the point at which that entropy is evaluated is the same in both procedures.

Simple maximization of entropy $S^{(1\to 0)}$ leads to

$$S^{(0\leftarrow 1)}_{\rm MaxEnt}(x_0) = S^{(1\to 0)}[(x_1)_{\rm MaxEnt}(x_0)], \tag{A6}$$

where $(x_1)_{\rm MaxEnt}(x_0)$ is the solution to

$$\frac{\partial}{\partial x_1}\bigg|_{(x_1)_{\rm MaxEnt}(x_0)} (S^{(1\to 0)} - \langle (x_0^\star)_{\rm MaxEnt}(x_0), \Pi(x_1)\rangle) = 0, \tag{A7}$$

$$\Pi[(x_1)_{\rm MaxEnt}(x_0)] = x_0. \tag{A8}$$

From Eqs. (2.5) and (A4) it follows, moreover, that

$$(x_1)_{\rm MaxEnt}(x_0) = (x_1)_{\rm eq}[(x_0^\star)_{\rm eq}(x_0)] \quad \text{and} \tag{A9a}$$

$$(x_0^\star)_{\rm MaxEnt}(x_0) = (x_0^\star)_{\rm eq}(x_0). \tag{A9b}$$

Comparing Eq. (A5) to Eq. (A6) with (A9) then leads to the conclusion that the entropy on Level 0 implied by Level 1 by the static reduction, $S^{(0\leftarrow 1)}$, is the same entropy that can be obtained by simple maximization of entropy $S^{(1\to 0)}$ with the constraint that the the image of projection Π is constant, $S^{(0\leftarrow 1)}_{\rm MaxEnt}(x_0)$. The static reduction thus indeed can be regarded as a procedure of entropy maximization, but the full static reduction, as presented in Sec. II, provides more information about the passage from Level 1 to Level 2 as functions $\Phi^{(0)\star}$ and $S^{(0)\star}$ are revealed. Moreover, the formulation of the static reduction in terms of Legendre transformations is useful in the contact-geometric formulation of thermodynamics [35].

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