Essential equivalence of the general equation for the nonequilibrium reversible-irreversible coupling (GENERIC) and steepest-entropy-ascent models of dissipation for nonequilibrium thermodynamics

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By reformulating the steepest-entropy-ascent (SEA) dynamical model for nonequilibrium thermodynamics in the mathematical language of differential geometry, we compare it with the primitive formulation of the general equation for the nonequilibrium reversible-irreversible coupling (GENERIC) model and discuss the main technical differences of the two approaches. In both dynamical models the description of dissipation is of the "entropy-gradient" type. SEA focuses only on the dissipative, i.e., entropy generating, component of the time evolution, chooses a sub-Riemannian metric tensor as dissipative structure, and uses the local entropy density field as potential. GENERIC emphasizes the coupling between the dissipative and nondissipative components of the time evolution, chooses two compatible degenerate structures (Poisson and degenerate co-Riemannian), and uses the global energy and entropy functionals as potentials. As an illustration, we rewrite the known GENERIC formulation of the Boltzmann equation in terms of the square root of the distribution function adopted by the SEA formulation. We then provide a formal proof that in more general frameworks, whenever all degeneracies in the GENERIC framework are related to conservation laws, the SEA and GENERIC models of the dissipative component of the dynamics are essentially interchangeable, provided of course they assume the same kinematics. As part of the discussion, we note that equipping the dissipative structure of GENERIC with the Leibniz identity makes it automatically SEA on metric leaves.

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I. INTRODUCTION

The basic concepts and applications of equilibrium thermodynamics are among the most consolidated milestones in physics. On the other hand, thermodynamic theories capable of describing nonequilibrium states and their time evolution are still at the forefront of research in physics, fostered by a wide variety of applications and new technologies that are in need of such modeling capability.

Various theories and approaches to nonequilibrium dynamics have been put forward since the pioneering work by Onsager in 1931 [1]. It is not our purpose here to review such huge scientific literature, nor to even acknowledge the many pioneers of this broad topic. Therefore, the reader interested in such reconstructions should not start from our list of references.

The scope of this paper is to compare two quite general geometrical constructions that have evolved independently, with somewhat different purposes, but that turn out to provide almost equivalent—or at least very closely related—dissipative structures that guarantee the compatibility of a nonequilibrium thermodynamics theory with the second law of thermodynamics.

At any level of description, the geometrization of a theory of nonequilibrium (thermo-)dynamics consists in identifying (a) the state space $\mathcal{M}$ assumed for the physical system under study, (b) the structure of this space, (c) the time evolution equation in terms of this structure, (d) the compatibility of dynamics with the statement of the second law of thermodynamics [2], and (e) the symmetry group of the theory, i.e., the group preserving the geometrical structure of $\mathcal{M}$ [3].

Not all existing nonequilibrium thermodynamics theories have been clearly geometrized yet in this sense. However, much progress along these lines has been made and constitutes the background of the present work:

(i) Classical mechanics has been formulated in an abstract (general) setting, in the context of geometric mechanics [4,5]: The natural arenas are symplectic manifolds, and their generalization, i.e., Poisson manifolds.

(ii) Equilibrium thermodynamics has been geometrized in the work by Carathodory [6], the book by Hermann [7], and, for example, the references in Ref. [8].

(iii) Some formulations of nonequilibrium thermodynamics have been reformulated using the important geometric structure of *metriplectic manifolds* (see some history and references in Refs. [9] and [10]).

(iv) In its most renowned presentation, metriplectic dynamics has been called the *general equation for the nonequilibrium reversible-irreversible coupling* (GENERIC) [11], which represents also a generalization in the context of *contact manifolds*.

(v) An apparently less structured approach, SEA dynamics, was proposed in the simplest quantum thermodynamic landscape [12–17] and in a general probabilistic framework [18–22] and recently adapted and generalized for meso- and macroscopic systems in Ref. [23].

In general, a nondissipative evolution is modeled with an antisymmetric tensor, while the dissipative one with a symmetric object. When the latter is a tensor, clearly it may

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be represented by a kind of metric tensor. This is why below we shall associate dissipation with a metric tensor.

Although we shall focus here only on the mathematical formulation, it is worth noting that thermodynamic theories (equilibrium and nonequilibrium) have often been attached very different physical (and philosophical) interpretations. For example:

(a) The Keenan school of thermodynamics has advanced the position that thermodynamics is valid at every scale and that entropy is an intrinsic property of matter which, like energy, builds up from the microscopic level. The SEA geometrical approach originated from probing the extreme consequences of this line of reasoning to seeing how the quantum dynamics should be modified if entropy and dissipation existed even microscopically.

(b) On the other hand, the multiscale dynamics advanced by Grmela sees thermodynamics as "*a meta-theory addressing relations among dynamical theories formulated on different levels of description*" [24]; these relations are expressed in the framework of contact structures [25]. At every scale there is a GENERIC, and in passing from a more detailed level to a less detailed one through "pattern recognition" (or coarse graining [26]) one sees dissipation, even if microscopic dynamics is reversible.

Our scope here is not to elaborate on any of these interpretational issues, nor on the operational definitions and empirical meanings of basic concepts such as energy and entropy. We take the view that, regardless of their interpretation, two theories are identical if their mathematical structures are equivalent.

The paper is structured as follows. In Sec. II we reformulate the SEA and the GENERIC approaches to emphasize their analogies and differences, which we further discuss in Sec. III. In Sec. IV we implement our formalism to the case of the Boltzmann equation. In Sec. V we further elaborate our notation and analysis to establish when and in what sense SEA and GENERIC can be considered equivalent. In Sec. VI we summarize our conclusions.

II. MATHEMATICAL FORMULATION

In this section, we present a mathematical and abstract formulation of the SEA and GENERIC principles that allows a clear comparison between the respective underlying assumptions. To help the reader go through the mathematics and grasp the general meaning without getting sidetracked by the details, we will try to guide the reading as much as possible by adding some nontechnical comments that, albeit strictly unnecessary from the mathematical point of view, are meant to allow a simpler interpretation of the abstract setup.

We will focus on the dynamics. Regarding the kinematics, for both SEA and GENERIC we will assume it to be given. In particular, when in Sec. V we derive relations between the structures of dissipative dynamics in SEA and GENERIC models, we do so under the assumption that the two models adopt the same kinematics. In general, for both SEA and GENERIC, the kinematics is chosen so the state space is a Banach manifold $\mathcal{M}$, i.e., a manifold which—locally—is topologically equivalent to a Banach space.

The time evolution of the state is represented by a curve $\alpha : I \to \mathcal{M}$ ($I \subseteq \mathbb{R}$) on $\mathcal{M}$, and this is an integral curve of a vector field (i.e., the velocity vector is equal to the vector field at each point of the curve). The vector field is composed of two distinguished parts: The first one is a *nondissipative* contribution, X^H, which, depending on the framework, represents Hamiltonian dynamics and/or the local effects of transport due to convective and diffusive fluxes between adjacent elements of a continuum; the second one is a *dissipative* contribution, which models the irreversible aspects of the dynamics (such as the dissipation of mechanical or electrical forms of energy into thermal energy) responsible for the entropy production (the local entropy production in the case of a continuum). In symbols, the time evolution $\alpha(t)$ is an integral curve of the sum of the nondissipative and dissipative vector fields,

$$\dot{\alpha}(t) = X^H_{\alpha(t)} + Y^S_{\alpha(t)}. \tag{1}$$

Our comparison between the SEA and the GENERIC constructions will focus the attention on the dissipative part because this has been the focus of the SEA construction, namely to define the dissipative part Y^S in nonequilibrium frameworks where the nondissipative or transport part X^H is prescribed by other considerations. Instead, the GENERIC construction provides specifications also for X^H.

As we will see below in detail, both the SEA and the GENERIC constructions assume that the dissipative part Y^S of the dynamical equation (1) is directly related to the entropy differential. In the SEA construction, it is related to the projection of the gradient of the local entropy functional onto a linear manifold orthogonal to the gradients of the local functionals representing the conserved properties. In the GENERIC construction we consider in this article (where $\mathcal{M}$ is a metriplectic manifold), it is related to a weaker notion of "gradient."

First, also to establish the notation, we recall some basic notions of differential geometry. The most useful definition of (tangent) vector on a manifold passes through the concept of *derivation*. A *tangent vector* v_p to a point p of the manifold $\mathcal{M}$ is a *derivation* on $C^\infty(\mathcal{M})$; that is, a linear map

$$\begin{aligned} v_p : C^\infty(\mathcal{M}) &\to \mathbb{R} \\ A &\mapsto v_p(A), \end{aligned} \tag{2}$$

which takes any smooth functional A on $\mathcal{M}$, gives a real number $v_p(A)$, and satisfies the *Leibniz rule*

$$v_p(AB) = v_p(A)\, B_p + A_p\, v_p(B) \tag{3}$$

for any functionals A and B, where A_p and B_p denote their values at p. The set of all tangent vectors to p is a vector space, called the *tangent space to* $\mathcal{M}$ *at* p and denoted by $T_p\mathcal{M}$. The disjoint union of all tangent spaces is the *tangent bundle*, denoted by $T\mathcal{M}$. A *vector field* X is a map

$$\begin{aligned} X : \mathcal{M} &\to T\mathcal{M} \\ p &\mapsto X_p, \end{aligned} \tag{4}$$

with the property that $X_p \in T_p\mathcal{M}\ \forall p \in \mathcal{M}$: i.e., it assigns a tangent vector X_p in $T_p\mathcal{M}$ to each point p of $\mathcal{M}$.

By referring to the model space of the manifold, one may express a tangent vector by the linear combination

$$v_p = v_p^k \partial_k, \tag{5}$$

where $\{\partial_k\}$ is a basis of derivations for the tangent space, or—in other words—the partial derivatives with respect to the coordinates. By the same consideration, one is allowed to see $v_p(A)$ as the *directional derivative* of A at p along the tangent vector v_p.

Moreover, one may define the *cotangent space at* p $[T_p^*\mathcal{M} \stackrel{\text{def}}{=} (T_p\mathcal{M})^*]$ as the space of all linear functionals (named *covectors*) on $T_p\mathcal{M}$. The disjoint union of all cotangent spaces is the *cotangent bundle* $T^*\mathcal{M}$. The most important of these linear functionals is the *differential* dA of a smooth functional A on $\mathcal{M}$, which computes the directional derivatives of A at every point p of $\mathcal{M}$ along the tangent vectors to p, i.e., at each point p takes any tangent vector v_p as input and yields the directional derivative $v_p(A)$ as output,

$$dA_p(v_p) = v_p(A). \tag{6}$$

The notion of gradient of a smooth functional requires an additional structure on the manifold. Indeed, it can be defined in an invariant way (i.e., independent of the choice of coordinates) only with respect to a nondegenerate bilinear map on the tangent bundle (or some sub-bundle), which essentially equips the manifold with a metric. The most common case is represented by *(strong) Riemannian manifolds*. These are defined as pairs of a smooth manifold and a (strongly nondegenerate) Riemannian metric tensor field g_p which, at every point p of $\mathcal{M}$, takes as input two vectors in the tangent space $T_p\mathcal{M}$ and yields

$$\begin{aligned} g_p : T_p\mathcal{M} \times T_p\mathcal{M} &\to \mathbb{R} \\ (u_p, v_p) &\mapsto g_p(u_p, v_p) \end{aligned} \tag{7}$$

with $g_p(u_p, v_p) > 0$ for any nonzero u_p and v_p. The property of strong nondegeneracy implies that the vector bundle (linear) map (at every point p) $g_p^\flat : T_p\mathcal{M} \to T_p^*\mathcal{M}$, defined by

$$\left[g_p^\flat(u_p)\right](v_p) = g_p(u_p, v_p) \qquad \forall v_p \in T_p\mathcal{M}, \tag{8}$$

which brings a vector u_p into the covector $g_p^\flat(u_p)$ (i.e., into a linear functional on the tangent space at p), is an isomorphism (often called *musical isomorphism*). Therefore, the inverse map $g_p^\sharp : T_p^*\mathcal{M} \to T_p\mathcal{M}$ is defined, too. We may also define the "inverse" metric tensor, or *cometric tensor*, by

$$g_p(\omega_p, \eta_p) = g_p(g_p^\sharp(\omega_p), g_p^\sharp(\eta_p)). \tag{9}$$

In coordinates and finite dimensions, a physicist would talk about *lowering* and *raising the indexes*:

$$\left(g_p^\flat\right)_{ij} v_p^j = v_{p,i}, \qquad \left(g_p^\sharp\right)^{ij} v_{p,j} = v_p^i, \tag{10}$$

where v^j and v_j are, respectively, the components of a vector and a covector with respect to some chosen basis for the tangent space $T_p\mathcal{M}$ and the cotangent space $T_p^*\mathcal{M}$; $(g_p^\flat)_{ij} = g_{p,ij}$ and $(g_p^\sharp)^{ij} = g_p^{ij}$ are the matrix representations of the maps $g_p^\flat$ and $g_p^\sharp$ with respect to the same bases, and of course $[g_p^{ij}] = [g_{p,ij}]^{-1}$.

One then defines the *gradient* at p of a smooth functional A to be the only vector at p satisfying

$$dA_p(v_p) = g_p(\text{grad}_g\, A|_p, v_p) \quad \forall v_p \in T_p\mathcal{M} \quad \text{and} \quad p \in \mathcal{M}. \tag{11}$$

Uniqueness is guaranteed by the nondegeneracy of the metric field. This may also be restated more explicitly as

$$\text{grad}_g\, A|_p = g_p^\sharp(dA_p). \tag{12}$$

When $\mathcal{M}$ is a vector space V, the tangent space to each point p may be identified with the vector space itself (we write $T_pV \cong V\ \forall p$). Moreover, if the vector space is a Hilbert space $\mathcal{H}$, it is equipped with an inner product, i.e., a nondegenerate bilinear map,

$$\begin{aligned} \langle , \rangle : \mathcal{H} \times \mathcal{H} &\to \mathbb{R} \\ (p, q) &\mapsto \langle p, q \rangle. \end{aligned} \tag{13}$$

If we take the manifold viewpoint, this may also be seen as

$$\begin{aligned} \langle , \rangle : T_p\mathcal{H} \times T_p\mathcal{H} &\to \mathbb{R} \\ (u_p, v_p) &\mapsto \langle u_p, v_p \rangle, \end{aligned} \tag{14}$$

since $T_p\mathcal{H} \cong \mathcal{H}\ \forall p$. Then the particular *gradient* of a functional A at point q, called *variational derivative* of A, is defined implicitly by

$$dA_q(v_q) = \left\langle \left.\frac{\delta A}{\delta p}\right|_q, v_q \right\rangle \quad \forall q \in \mathcal{H} \quad \text{and} \quad v_q \in T_q\mathcal{H}\ (\cong \mathcal{H}). \tag{15}$$

Given the inner product, we may denote by R_p the Riesz isomorphism $R_p : T_p^*\mathcal{H} \to T_p\mathcal{H}$ such that

$$\langle R_p(\omega_p), v_p \rangle = \omega_p(v_p) \quad \forall v_p \in T_p\mathcal{H},\ \forall \omega_p \in T_p^*\mathcal{H}, \tag{16}$$

and hence we may alternatively define the variational derivative explicitly by

$$\left.\frac{\delta A}{\delta p}\right|_q \stackrel{\text{def}}{=} R_q(dA_q). \tag{17}$$

When both structures (an inner product and a metric) are present on a Hilbert space $\mathcal{H}$, we have

$$\text{grad}_g\, A|_p = g_p^\sharp\left[R_p^{-1}\left(\left.\frac{\delta A}{\delta p}\right|_p\right)\right] = \hat{G}_p^{-1}\left(\left.\frac{\delta A}{\delta p}\right|_p\right), \tag{18}$$

where $\hat{G}_p^{-1}$ denotes the inverse of the positive definite and symmetric linear operator $\hat{G} : T_p\mathcal{M} \to T_p\mathcal{M}$ defined by

$$\hat{G}_p(v_p) \stackrel{\text{def}}{=} R_p\left[g_p^\flat(v_p)\right] \quad \forall v_p \in T_p\mathcal{H}. \tag{19}$$

A. Steepest entropy ascent

The SEA principle to model the nonequilibrium dynamics of a thermodynamic system was originally proposed as part of an attempt to design a thermodynamically consistent dynamical law for a unified quantum theory of mechanics and thermodynamics obtained by embedding the second law directly into the set of fundamental postulates [12–16,27–31]. Subsequently, it was extended as a generic modeling tool for probabilistic, constrained maximum-entropy landscapes [18–22,32]. Since in these landscapes the state representative is a probability distribution or its quantum equivalent, the density operator, it seemed natural to define gradients with

respect to the Fisher-Rao metric which is known to exhibit the required invariance features in the absence of additional physical constraints. However, the Fisher metric is not general enough to reproduce the dynamics in other nonequilibrium thermodynamics frameworks. Therefore, an extension of the SEA formulation that adopts a generic metric has been provided in Ref. [23]. In this section we present the structure of such more general formulation. Actually, as part of our effort to cast the construction in the language of differential geometry, we first present a further generalization whereby the state space is not required to be a vector space but may be any (Banach) manifold, and then we present the original formulation where the state manifold is equipped with an inner product so variational derivatives are defined.

The idea behind the SEA construction is to "geometrize" the thermodynamic state space and assume that the part of the local evolution equation that is responsible for irreversible dynamics is in the "direction" of maximal entropy production compatible with the local conservation constraints. The formulation of the SEA principle may be expressed as follows: *The time evolution of the local state is the result of a balance between the effects of transport or Hamiltonian dynamics and the spontaneous and irreversible tendency to advance the local state representative in the direction of maximal entropy production per unit of distance traveled in state space compatible with the conservation constraints* [23].

The mathematical implementation consists in assuming that the dissipative part of the dynamics pushes the states in the direction of the gradient of the restriction of the entropy functional onto the submanifold with constant values of the conserved quantities. Therefore, the dissipative vector field is assumed to point in the direction of maximal directional derivative of the entropy compatible with the conservation constraints.

1. Generalized abstract formulation

Each thermodynamically consistent nonequilibrium theory assumes a level of description for a given physical system (possibly modeled as a continuum) which mathematically amounts to assuming:

(i) a (possibly infinite-dimensional) smooth real Banach manifold $\mathcal{M}$ whose points represent the possible states of the system or, for nonequilibrium states of a continuum, the possible local states at position $\boldsymbol{q}$;

(ii) a set of functionals $c^i : \mathcal{M} \to \mathbb{R}$, which represent the conserved properties of the system or, for a continuum, the local densities of the conserved properties; we denote the submanifold $\{p \in \mathcal{M} : c^i(p) = \text{const}_i\ \forall i\}$ with $\mathcal{M}_{\boldsymbol{c}}$;

(iii) another functional $s : \mathcal{M} \to \mathbb{R}$, which represents the thermodynamic entropy [33–36] of the system or, for a continuum, the local entropy density;

(iv) for each submanifold $\mathcal{M}_{\boldsymbol{c}}$, a (strongly nondegenerate) metric tensor field g which, at every point p of the submanifold $\mathcal{M}_{\boldsymbol{c}(p)}$, takes as input two vectors in the tangent space $T_p\mathcal{M}_{\boldsymbol{c}(p)}$ and yields

$$\begin{aligned} g_p : T_p\mathcal{M}_{\boldsymbol{c}(p)} \times T_p\mathcal{M}_{\boldsymbol{c}(p)} &\to \mathbb{R} \\ (u_p, v_p) &\mapsto g_p(u_p, v_p), \end{aligned} \tag{20}$$

with $g_p(u_p, v_p) > 0$ for any nonzero u_p and v_p, and is such that the map $p \mapsto g_p$ defines a smooth (C^∞) map on $\mathcal{M}$. The condition that defines the space $T_p\mathcal{M}_{\boldsymbol{c}(p)}$ tangent to the constrained submanifold $\mathcal{M}_{\boldsymbol{c}(p)}$ is

$$T_p\mathcal{M}_{\boldsymbol{c}(p)} = \left\{v_p^{\boldsymbol{c}} \in T_p\mathcal{M} : dc_p^i\left(v_p^{\boldsymbol{c}}\right) = 0\ \forall i\right\}. \tag{21}$$

This situation essentially defines a *sub-Riemannian* structure on $\mathcal{M}$. We shall come back to this point in Sec. III B.

The above assumptions allow one to define the gradient with respect to the given metric field g of the smooth functional $s^{\boldsymbol{c}} : \mathcal{M}_{\boldsymbol{c}} \to \mathbb{R}$ defined by the restriction of the functional $s : \mathcal{M} \to \mathbb{R}$ on the submanifold $\mathcal{M}_{\boldsymbol{c}}$ of $\mathcal{M}$ where the conserved functionals c^i are constrained to fixed constant values $\boldsymbol{c}$, i.e., such that

$$v_p^{\boldsymbol{c}} \mapsto ds^{\boldsymbol{c}}\left(v_p^{\boldsymbol{c}}\right) = ds\left(v_p^{\boldsymbol{c}}\right). \tag{22}$$

We can do it either through the following implicit expression [Eq. (11)]: $\text{grad}_g^{\boldsymbol{c}}\, s^{\boldsymbol{c}}|_p$ is the unique vector in $T_p\mathcal{M}_{\boldsymbol{c}(p)}$ such that

$$ds_p^{\boldsymbol{c}}\left(v_p^{\boldsymbol{c}}\right) = g_p\left(\text{grad}_g^{\boldsymbol{c}}\, s^{\boldsymbol{c}}\big|_p, v_p^{\boldsymbol{c}}\right) \qquad \forall v_p^{\boldsymbol{c}} \in T_p\mathcal{M}_{\boldsymbol{c}(p)}, \tag{23}$$

or, explicitly,

$$\text{grad}_g^{\boldsymbol{c}}\, s^{\boldsymbol{c}}\big|_p = g_p^\sharp\left(ds_p^{\boldsymbol{c}}\right). \tag{24}$$

With reference to the time evolution equation (1), the SEA construction focuses only on the dissipative vector field Y^S because its objective is to construct a dynamics in which the entropy functional s is an S-function in the sense defined in Ref. [2] so the maximal entropy states (or, for a continuum, the locally maximal entropy density states) represent the only stable (local) equilibrium states of the system, consistently with the Hatsopoulos-Keenan statement of the second law [37,38]. Instead, the nondissipative vector field X^H in Eq. (1), which represents the reversible components of the system dynamics or, for a continuum, the local net effects of transport of properties between adjacent elements of the continuum, are assumed to be given features of the level of description and coarse graining of the modeling framework in which the SEA construction is to be implemented.

The SEA dynamics is obtained by assuming the dissipative vector field Y^S as follows:

$$Y^S_{\alpha(t)} = \frac{1}{\tau}\,\text{grad}_g^{\boldsymbol{c}[\alpha(t)]}\, s^{\boldsymbol{c}[\alpha(t)]}|_{\alpha(t)} = \frac{1}{\tau} g^\sharp_{\alpha(t)}\left(ds^{\boldsymbol{c}[\alpha(t)]}_{\alpha(t)}\right), \tag{25}$$

where τ is a positive dimensionality constant. Since by definition (23) the vector $\text{grad}_{\boldsymbol{c}}\, s^{\boldsymbol{c}}|_p$ is in $T_p\mathcal{M}_{\boldsymbol{c}(p)}$ and therefore, recalling Eq. (21), is in the kernel of every dc^i, Eq. (25) satisfies automatically the following conservation constraints:

$$dc^i_{\alpha(t)}\left(\dot\alpha(t) - X^H_{\alpha(t)}\right) = dc^i_{\alpha(t)}\left(Y^S_{\alpha(t)}\right) = 0. \tag{26}$$

As discussed in Ref. [23], Eq. (25) can also be viewed as the solution of a maximal entropy production variational problem that in the notation just developed can be expressed as follows:

$$\max_{Y^S}|_p\ ds_p^{\boldsymbol{c}(p)}(Y^S) \text{ subject to } g_p(Y^S, Y^S) = \text{const}. \tag{27}$$

The rate of entropy production can be expressed in the following equivalent forms:

$$\begin{aligned} ds_{\alpha(t)}\left(\dot\alpha(t) - X^H_{\alpha(t)}\right) &= ds_{\alpha(t)}\left(Y^S_{\alpha(t)}\right) \\ &= ds^{\boldsymbol{c}(\alpha(t))}_{\alpha(t)}\left(Y^S_{\alpha(t)}\right) \\ &= g_{\alpha(t)}\left(\text{grad}_g^{\boldsymbol{c}}\, s^{\boldsymbol{c}(\alpha(t))}|_{\alpha(t)}, Y^S_{\alpha(t)}\right) \end{aligned}$$

$$= \frac{1}{\tau}\, g_{\alpha(t)}\big(\operatorname{grad}_g^{\boldsymbol{c}} s^{\boldsymbol{c}(\alpha(t))}|_{\alpha(t)}, \operatorname{grad}_g^{\boldsymbol{c}} s^{\boldsymbol{c}(\alpha(t))}|_{\alpha(t)}\big)$$
$$= \tau\, g_{\alpha(t)}\big(Y^S_{\alpha(t)}, Y^S_{\alpha(t)}\big) \geqslant 0, \tag{28}$$

where the second equality follows from Eq. (26), the third from Eq. (40), the fourth from Eq. (23), the inequality from the positivity of the metric tensor, and the strict equality holds if and only if $Y^S_{\alpha(t)} = 0$. The thermodynamic principle of impossibility of a negative entropy production is thus automatically satisfied.

This thermodynamic consistency feature is very often identified with the second law. However, the second law requires additionally that among the *nondissipative states*, i.e., the states $p_{\rm nd}$ for which $Y^S_{p_{\rm nd}} = 0$, only those that have maximal entropy for the given values of the conserved properties should be stable equilibrium states with respect to a purely dissipative dynamics, i.e., Eq. (1) in which we set $X^H = 0$. In other words, we must also prove that all other nondissipative states that become equilibrium states when we set $X^H = 0$ should be unstable. This nontrivial additional requirement imposes an additional condition onto the properties that must be satisfied by the entropy functional. It is often stated that entropy provides a Lyapunov criterion for the stability of the thermodynamic (local) equilibrium states. However, as discussed in Ref. [2], the rigorous justification of this statement is not trivial and requires that the entropy functional satisfies a weaker criterion than that of being a Lyapunov functional which in Ref. [2] is defined precisely and named the *S*-functional. For the quantum framework, the proof of the conjecture advanced in Ref. [2] that the von Neumann entropy functional $-k_B \operatorname{Tr} \rho \ln \rho$ is indeed an *S*-functional was later found in Ref. [39].

2. *Original inner product formulation*

The original formulations of the SEA constructions in Refs. [12–16,18–23,32] assume that the state manifold $\mathcal{M}$ is equipped with an inner product $\langle\cdot,\cdot\rangle$. As a consequence,

(a) variational derivatives are defined according to Eq. (15);

(b) for shorthand, we denote the variational derivatives of the conserved functionals $c^i : \mathcal{M} \to \mathbb{R}$ with the symbols Ψ^i, i.e.,

$$\Psi^i_p \stackrel{\rm def}{=} \left.\frac{\delta c^i}{\delta p}\right|_p \qquad \forall p \in \mathcal{M}; \tag{29}$$

with the further shorthand symbols $\boldsymbol{c}$ and $\boldsymbol{\Psi}$ to denote the arrays $\boldsymbol{c} = \{c^1, c^2, \dots\}$ and $\boldsymbol{\Psi} = \{\Psi^1, \Psi^2, \dots\}$, and $\operatorname{span}(\boldsymbol{\Psi})$ to denote the linear span of the Ψ^i's;

(c) again for shorthand, we denote the variational derivative of the functional $s : \mathcal{M} \to \mathbb{R}$ with the symbol Φ, i.e.,

$$\Phi_p \stackrel{\rm def}{=} \left.\frac{\delta s}{\delta p}\right|_p \qquad \forall p \in \mathcal{M}. \tag{30}$$

The gradient with respect to the given metric field g of the restriction of the entropy functional $s^{\boldsymbol{c}} : \mathcal{M}_{\boldsymbol{c}} \to \mathbb{R}$ on the submanifold $\mathcal{M}_{\boldsymbol{c}}$ with constant values of the conserved functionals c^i, using Eqs. (12) and (18), can be written explicitly as

$$\operatorname{grad}_g^{\boldsymbol{c}} s^{\boldsymbol{c}}\big|_p = g^\sharp_p\big(ds^{\boldsymbol{c}}_p\big) = \hat{G}^{-1}_p\big(\Phi^{\boldsymbol{c}}_p\big). \tag{31}$$

Moreover, the tangent space $T_p\mathcal{M}$ at any p on $\mathcal{M}$ is viewed as the orthogonal composition $T_p\mathcal{M} = T_p\mathcal{M}_{\boldsymbol{c}(p)} \oplus \operatorname{span}(\boldsymbol{\Psi}_p)$ so any tangent vector can be decomposed as

$$v_p = v^{\boldsymbol{c}}_p + v^{\perp \boldsymbol{c}}_p, \tag{32}$$

with $v^{\boldsymbol{c}}_p$ the component tangent to the submanifold defined by the values at p of the conservation constraints and $v^{\perp\boldsymbol{c}}_p$ the component orthogonal to such submanifold. Indeed, from Eqs. (21) and (15) written for A being one of the conservation constraints, the condition that defines the space $T_p\mathcal{M}_{\boldsymbol{c}(p)}$ tangent to the constrained submanifold (metric leaf) $\mathcal{M}_{\boldsymbol{c}(p)}$ becomes

$$T_p\mathcal{M}_{\boldsymbol{c}(p)} = \big\{v^{\boldsymbol{c}}_p \in T_p\mathcal{M} : dc^i_p\big(v^{\boldsymbol{c}}_p\big) = \big\langle \Psi^i\big|_p, v^{\boldsymbol{c}}_p\big\rangle = 0\ \forall i\big\}, \tag{33}$$

which shows clearly that $T_p\mathcal{M}_{\boldsymbol{c}}$ is the orthogonal complement of the linear span of the Ψ^i's.

Along with decomposition (32), also the differential dF of a smooth functional F on $\mathcal{M}$ is naturally decomposed as

$$dF = dF^{\boldsymbol{c}} + dF^{\perp \boldsymbol{c}}, \tag{34}$$

where $dF^{\boldsymbol{c}}$ computes the directional derivative along the component of the tangent vector that lies in $T_p\mathcal{M}_{\boldsymbol{c}(p)}$ and $dF^{\perp\boldsymbol{c}}$ along the orthogonal component that lies in $\operatorname{span}(\boldsymbol{\Psi}_p)$, i.e.,

$$dF^{\boldsymbol{c}}_p(v_p) = dF\big(v^{\boldsymbol{c}}_p\big) \text{ and } dF^{\perp\boldsymbol{c}}_p(v_p) = dF_p\big(v^{\perp\boldsymbol{c}}_p\big). \tag{35}$$

In particular, when $F = c^i$, definitions (21) and (35) imply the identities $dc^{i,\boldsymbol{c}} = 0$ and $dc^{i,\perp\boldsymbol{c}} = dc^i$, i.e.,

$$dc^{i,\boldsymbol{c}}_p(v_p) = 0 \text{ and } dc^{i,\perp\boldsymbol{c}}_p(v_p) = dc^i_p\big(v^{\perp\boldsymbol{c}}_p\big) = dc^i_p(v_p). \tag{36}$$

Similarly, the decomposition (32) for the vector Φ_p is

$$\Phi_p = \Phi^{\boldsymbol{c}}_p + \Phi^{\perp\boldsymbol{c}}_p. \tag{37}$$

Since $\Phi^{\perp\boldsymbol{c}}_p$ belongs to $\operatorname{span}(\boldsymbol{\Psi}_p)$, there is a set of scalars β^j_p such that

$$\Phi^{\perp\boldsymbol{c}}_p = \hat{P}_{\operatorname{span}(\boldsymbol{\Psi}_p)}(\Phi_p) = \sum_j \beta^j_p\, \Psi^j. \tag{38}$$

Recalling Eq. (15), we readily see that

$$ds^{\perp\boldsymbol{c}}_p(v_p) = \big\langle \Phi^{\perp\boldsymbol{c}}_p, v_p\big\rangle = \sum_j \beta^j_p\, \langle \Psi^j, v_p\rangle = \sum_j \beta^j_p\, dc^j_p(v_p), \tag{39}$$

and, therefore, the constrained differential of s and the constrained variational derivatives are, respectively,

$$ds^{\boldsymbol{c}}_p = ds_p - \sum_j \beta^j_p\, dc^j_p, \tag{40}$$

$$\Phi^{\boldsymbol{c}}_p = \Phi_p - \sum_j \beta^j_p\, \Psi^j_p, \tag{41}$$

where the scalars β^j_p are determined uniquely by the solution of the system of equations that obtains by applying Eq. (40)

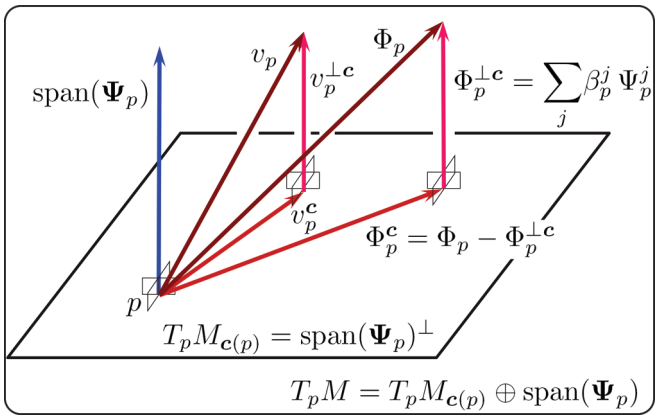

FIG. 1. (Color online) Pictorial representation of the orthogonal decompositions $v_p = v_p^{\boldsymbol{c}} + v_p^{\perp \boldsymbol{c}}$ of a tangent vector and $\Phi_p = \Phi_p^{\boldsymbol{c}} + \Phi_p^{\perp \boldsymbol{c}}$ of the variational derivative of a smooth functional s on $\mathcal{M}$ with respect to the decomposition $T_p\mathcal{M}_{\boldsymbol{c}(p)} \oplus \mathrm{span}(\boldsymbol{\Psi}_p)$ of the tangent space $T_p\mathcal{M}$ at point p on the state manifold $\mathcal{M}$, where $\mathcal{M}_{\boldsymbol{c}(p)}$ is the submanifold with constant values $\boldsymbol{c}(p)$ of a set of smooth functionals $\boldsymbol{c}$ on $\mathcal{M}$ with variational derivatives $\boldsymbol{\Psi}_p$.

to $v_p = \Psi_p^i$ for every i, and noting that $ds_p^{\boldsymbol{c}}(\Psi_p^i) = 0$ (because clearly $\Psi_p^{i,\boldsymbol{c}} = 0$), i.e.,

$$0 = ds_p\big(\Psi_p^i\big) - \sum_j \beta_p^j \, dc_p^j\big(\Psi_p^i\big) \tag{42}$$

or, equivalently, using again Eq. (15),

$$0 = \big\langle \Phi_p, \Psi_p^i \big\rangle - \sum_j \beta_p^j \big\langle \Psi_p^j, \Psi_p^i \big\rangle. \tag{43}$$

Figure 1 represents schematically the construction of the constrained variational derivative $\Phi_{\boldsymbol{c}}$.

The system of equations (43) defining the multipliers β^j can be easily solved, for example, using Cramer's rule. Then, following Refs. [18–23], the β^j's can be written explicitly as ratios of determinants so substitution into Eq. (40) yields the following explicit expression for the constrained differential:

$$ds_p^{\boldsymbol{c}} = \frac{\begin{vmatrix} ds_p & d\tilde{c}_p^1 & \cdots & d\tilde{c}_p^n \\ ds_p\big(\tilde{\Psi}_p^1\big) & d\tilde{c}_p^1\big(\tilde{\Psi}_p^1\big) & \cdots & d\tilde{c}_p^n\big(\tilde{\Psi}_p^1\big) \\ \vdots & \vdots & \ddots & \vdots \\ ds_p\big(\tilde{\Psi}_p^n\big) & d\tilde{c}_p^n\big(\tilde{\Psi}_p^1\big) & \cdots & d\tilde{c}_p^n\big(\tilde{\Psi}_p^n\big) \end{vmatrix}}{\begin{vmatrix} d\tilde{c}_p^1\big(\tilde{\Psi}_p^1\big) & \cdots & d\tilde{c}_p^1\big(\tilde{\Psi}_p^n\big) \\ \vdots & \ddots & \vdots \\ d\tilde{c}_p^n\big(\tilde{\Psi}_p^1\big) & \cdots & d\tilde{c}_p^n\big(\tilde{\Psi}_p^n\big) \end{vmatrix}} \tag{44}$$

and the constrained variational derivative

$$\Phi_p^{\boldsymbol{c}} = \frac{\begin{vmatrix} \Phi_p & \tilde{\Psi}_p^1 & \cdots & \tilde{\Psi}_p^n \\ \big\langle \Phi_p, \tilde{\Psi}_p^1 \big\rangle & \big\langle \tilde{\Psi}_p^1, \tilde{\Psi}_p^1 \big\rangle & \cdots & \big\langle \tilde{\Psi}_p^1, \tilde{\Psi}_p^n \big\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \big\langle \Phi_p, \tilde{\Psi}_p^n \big\rangle & \big\langle \tilde{\Psi}_p^n, \tilde{\Psi}_p^1 \big\rangle & \cdots & \big\langle \tilde{\Psi}_p^n, \tilde{\Psi}_p^n \big\rangle \end{vmatrix}}{\begin{vmatrix} \big\langle \tilde{\Psi}_p^1, \tilde{\Psi}_p^1 \big\rangle & \cdots & \big\langle \tilde{\Psi}_p^1, \tilde{\Psi}_p^n \big\rangle \\ \vdots & \ddots & \vdots \\ \big\langle \tilde{\Psi}_p^n, \tilde{\Psi}_p^1 \big\rangle & \cdots & \big\langle \tilde{\Psi}_p^n, \tilde{\Psi}_p^n \big\rangle \end{vmatrix}}, \tag{45}$$

where we denote by $\tilde{c}^1, \ldots, \tilde{c}^n$ a subset of the c^i's such that the variational derivatives $\tilde{\Psi}_p^1, \ldots, \tilde{\Psi}_p^n$ are linearly independent and form a basis for $\mathrm{span}(\boldsymbol{\Psi}_p)$. By virtue of this choice, the determinant at the denominator is a positive definite Gram determinant. Thus, alternatively, we can write

$$\beta_p^j = \sum_{i=1}^n [\langle \tilde{\boldsymbol{\Psi}}_p, \tilde{\boldsymbol{\Psi}}_p \rangle^{-1}]_{ji} \big\langle \Phi_p, \tilde{\Psi}_p^i \big\rangle, \tag{46}$$

where, of course, $\langle \tilde{\boldsymbol{\Psi}}_p, \tilde{\boldsymbol{\Psi}}_p \rangle^{-1}$ denotes the inverse of matrix $\langle \tilde{\boldsymbol{\Psi}}_p, \tilde{\boldsymbol{\Psi}}_p \rangle$ and $\langle \tilde{\boldsymbol{\Psi}}_p, \tilde{\boldsymbol{\Psi}}_p \rangle$ is a shorthand to indicate the matrix $[\langle \tilde{\Psi}_p^i, \tilde{\Psi}_p^j \rangle]$.

We may also easily construct another set $\overline{c}^1, \ldots, \overline{c}^n$ such that the variational derivatives $\overline{\Psi}_p^1, \ldots, \overline{\Psi}_p^n$ form an orthonormal basis for $\mathrm{span}(\boldsymbol{\Psi}_p)$. In such case, we can write

$$ds_p^{\boldsymbol{c}} = ds_p - \sum_{i=1}^n \big\langle \Phi_p, \overline{\Psi}_p^i \big\rangle \, d\overline{c}_p^i \tag{47}$$

and, for the constrained variational derivative of s,

$$\Phi_p^{\boldsymbol{c}} = \Phi_p - \sum_{i=1}^n \big\langle \Phi_p, \overline{\Psi}_p^i \big\rangle \overline{\Psi}_p^i = \Phi_p - \hat{P}_{\mathrm{span}(\boldsymbol{\Psi}_p)}(\Phi_p), \tag{48}$$

where

$$\begin{aligned} \hat{P}_{\mathrm{span}(\boldsymbol{\Psi}_p)}(\cdot) &= \sum_{i=1}^n \big\langle \, \cdot \, , \overline{\Psi}_p^i \big\rangle \overline{\Psi}_p^i \\ &= \sum_{i=1}^n \sum_{j=1}^n [\langle \tilde{\boldsymbol{\Psi}}_p, \tilde{\boldsymbol{\Psi}}_p \rangle^{-1}]_{ji} \big\langle \, \cdot \, , \tilde{\Psi}_p^i \big\rangle \tilde{\Psi}_p^j \end{aligned} \tag{49}$$

is the operator on $T_p\mathcal{M}$ which projects onto $\mathrm{span}(\boldsymbol{\Psi}_p)$.

The SEA dissipative vector field Y^S becomes

$$\begin{aligned} Y_{\alpha(t)}^S &= \frac{1}{\tau} \, \mathrm{grad}_g^{\boldsymbol{c}} \, s^{\boldsymbol{c}[\alpha(t)]}|_{\alpha(t)} = \frac{1}{\tau} g_{\alpha(t)}^\sharp \big(ds_{\alpha(t)}^{\boldsymbol{c}[\alpha(t)]} \big) \\ &= \frac{1}{\tau} \hat{G}_{\alpha(t)}^{-1} \big(\Phi_{\alpha(t)}^{\boldsymbol{c}[\alpha(t)]} \big), \end{aligned} \tag{50}$$

where τ is a positive dimensionality constant. The conservation constraints are

$$\begin{aligned} dc_{\alpha(t)}^i \big(\dot{\alpha}(t) - X_{\alpha(t)}^H \big) &= dc_{\alpha(t)}^i \big(Y_{\alpha(t)}^S \big) \\ &= \big\langle \Psi_{\alpha(t)}^i, Y_{\alpha(t)}^S \big\rangle = 0. \end{aligned} \tag{51}$$

The various equivalent expressions for ds^c given above show explicitly the SEA construction originally introduced in Refs. [12,16,18] in the quantum thermodynamics framework, whereby the dissipative vector field $Y^S_{\alpha(t)}$ is in the direction of the projection of $\Phi_{\alpha(t)}$ onto the subspace of $T_{\alpha(t)}\mathcal{M}$ orthogonal to all the $\Psi^i|_{\alpha(t)}$'s.

To the list of expressions of the rate of entropy production we can add

$$\begin{aligned} ds_{\alpha(t)}\big(\dot\alpha(t) - X^H_{\alpha(t)}\big) &= ds_{\alpha(t)}\big(Y^S_{\alpha(t)}\big) \\ &= ds_{\alpha(t)}\big(Y^S_{\alpha(t)}\big) - \sum\nolimits_j \beta^j\, dc^j_{\alpha(t)}\big(Y^S_{\alpha(t)}\big) \\ &= \tau\, g_{\alpha(t)}\big(Y^S_{\alpha(t)}, Y^S_{\alpha(t)}\big) = \tau\, \big\langle \hat G_{\alpha(t)}\big(Y^S_{\alpha(t)}\big), Y^S_{\alpha(t)}\big\rangle \geqslant 0. \end{aligned} \tag{52}$$

B. GENERIC

In this section we present the simplest form of the GENERIC construction (see Ref. [11]), the one with the description of entropy production that best resembles the SEA principle.

1. Abstract formulation

We denote by $\mathcal{M}$ the manifold of all possible states γ ($\gamma \in \mathcal{M}$) and build the following structure.

(i) There exist two potentials, a smooth *Hamiltonian functional* $H : \mathcal{M} \to \mathbb{R}$ and a smooth *entropy functional* $S : \mathcal{M} \to \mathbb{R}$, representing—for the chosen level of description—the overall energy and thermodynamic entropy of the system, respectively.

(ii) $\mathcal{M}$ is a (possibly infinite-dimensional) Banach *(co-)metriplectic* manifold, i.e., a manifold carrying two compatible structures as follows.

(iii) A Poisson structure describing the nondissipative part of the dynamics. This is known from geometric mechanics (see, for example, Refs. [4,5]) and consists of a skew-symmetric contravariant 2-tensor field, called the *Poisson tensor field*, which—at every point p of the manifold $\mathcal{M}$—takes two covectors at p as inputs, yields

$$\begin{aligned} P_p : T^*_p\mathcal{M} \times T^*_p\mathcal{M} &\to \mathbb{R} \\ (\omega_p, \eta_p) &\mapsto P_p(\omega_p, \eta_p), \end{aligned} \tag{53}$$

and is such that the map $p \mapsto P_p$ defines a smooth (C^∞) map on $\mathcal{M}$. To this tensor we associate a *Poisson bracket* $\{\cdot,\cdot\} : C^\infty(\mathcal{M}) \times C^\infty(\mathcal{M}) \to C^\infty(\mathcal{M})$ by the assignment:

$$\{A, B\}_p \stackrel{\text{def}}{=} P_p(dA_p, dB_p). \tag{54}$$

The Poisson bracket must satisfy the Jacobi identity

$$\{A,\{B,C\}\} + \{B,\{C,A\}\} + \{C,\{A,B\}\} = 0, \tag{55}$$

which represents a further constraint on the Poisson tensor field P_p. The Poisson tensor also yields the vector bundle (linear) map $P^\sharp_p : T^*_p\mathcal{M} \to T^{**}_p\mathcal{M}$, called the *Poisson operator*, and often assumed to satisfy the condition $P^\sharp_p(T^*_p\mathcal{M}) \subseteq T^{**}_p\mathcal{M} \subseteq T_p\mathcal{M}$, which is needed [40] to guarantee that $P^\sharp_p(dH_p)$ is a vector field. This condition is automatically satisfied whenever the manifold is modeled on a reflexive Banach space or, as a particular case, on a Hilbert space, such as in the Boltzmann equation framework that we discuss as an example in Sec. IV.

Since P_p is assumed to be possibly degenerate, $P^\sharp_p$ is in general noninvertible (it is not a vector-space isomorphism but only a homomorphism). It is noteworthy that condition (55) is imposed so as to implement time-translation invariance of the nondissipative part of the dynamics (integrability condition). We shall see below that GENERIC does not impose an analogous integrability condition on the dissipative part of the dynamics. We further discuss this point in Sec. III B.

(iv) A degenerate co-Riemannian structure (i.e., we have a degenerate *cometric* instead of a nondegenerate metric) describing the dissipative dynamics [41,42]. This consists of a symmetric and non-negative definite contravariant 2-tensor field, called the *friction tensor field*, which—at every point p of the manifold $\mathcal{M}$—takes two covectors at p as inputs, yields

$$\begin{aligned} D_p : T^*_p\mathcal{M} \times T^*_p\mathcal{M} &\to \mathbb{R} \\ (\omega_p, \eta_p) &\mapsto D_p(\omega_p, \eta_p), \end{aligned} \tag{56}$$

and is such that the map $p \mapsto D_p$ defines a smooth (C^∞) map on $\mathcal{M}$.

This tensor equips the set of smooth functionals on $\mathcal{M}$ with the *dissipative bracket* $[\cdot,\cdot] : C^\infty(\mathcal{M}) \times C^\infty(\mathcal{M}) \to C^\infty(\mathcal{M})$ by the assignment:

$$[A, B]_p \stackrel{\text{def}}{=} D_p(dA_p, dB_p). \tag{57}$$

The friction tensor also yields the vector bundle map $D^\sharp_p : T^*_p\mathcal{M} \to T_p\mathcal{M}$, called the *friction operator*, also often assumed to satisfy the condition $D^\sharp(T^*\mathcal{M}) \subseteq T^{**}\mathcal{M} \subseteq T\mathcal{M}$. Also here, since D_p is assumed to be possibly degenerate, $D^\sharp_p$ is in general noninvertible.

With reference to the time evolution equation (1), the GENERIC construction addresses both the nondissipative (Hamiltonian) vector field X^H and the dissipative vector field Y^S.

The Hamiltonian vector field $X^H_{\alpha(t)}$ is assumed to obtain from applying the Poisson operator $P^\sharp$ to the differential of the smooth Hamiltonian functional $H : \mathcal{M} \to \mathbb{R}$,

$$X^H_{\alpha(t)} = P^\sharp_{\alpha(t)}(dH_{\alpha(t)}), \tag{58}$$

while the dissipative vector field $Y^S_{\alpha(t)}$ is assumed to obtain from applying the friction operator $D^\sharp$ to the differential of the smooth entropy functional $S : \mathcal{M} \to \mathbb{R}$,

$$Y^S_{\alpha(t)} = D^\sharp_{\alpha(t)}(dS_{\alpha(t)}), \tag{59}$$

subject to the following supplementary conditions:

(a) The entropy functional S must be chosen among the distinguished functionals (Casimir functionals) of the Poisson structure, i.e., the operator $P^\sharp$ must be such that

$$\begin{aligned} \{S, A\} = P(dS, dA) = dA[P^\sharp(dS)] = 0 \quad \forall A \in C^\infty(\mathcal{M}), \\ \text{or, equivalently,} \quad P^\sharp_{\alpha(t)}(dS_{\alpha(t)}) = 0. \end{aligned} \tag{60}$$

(b) The Hamiltonian functional H must be chosen among the distinguished functionals of the dissipative structure, i.e., the operator $D^\sharp$ must be such that

$$\begin{aligned} [H, A] = D(dH, dA) = dA[D^\sharp(dH)] = 0 \quad \forall A \in C^\infty(\mathcal{M}), \\ \text{or, equivalently,} \quad D^\sharp_{\alpha(t)}(dH_{\alpha(t)}) = 0. \end{aligned} \tag{61}$$

(c) In addition, the other conserved properties of the system are kept constants by the dynamics and, therefore, must be distinguished functionals of both brackets.

As a result of these assumptions, if $\alpha(t)$ satisfies Eq. (1) and A is a smooth functional on $\mathcal{M}$, we calculate the directional derivative of A along the velocity vector $\dot{\alpha}(t)$ in the following way:

$$\begin{aligned}\frac{d}{dt}(A_{\alpha(t)}) &= dA_{\alpha(t)}(\dot{\alpha}(t))\\ &= dA_{\alpha(t)}\big(X^H_{\alpha(t)}\big) + dA_{\alpha(t)}\big(Y^S_{\alpha(t)}\big)\\ &= dA_{\alpha(t)}[P^\sharp_{\alpha(t)}(dH_{\alpha(t)})] + dA_{\alpha(t)}[D^\sharp_{\alpha(t)}(dS_{\alpha(t)})]\\ &= P_{\alpha(t)}(dH_{\alpha(t)},dA_{\alpha(t)}) + D_{\alpha(t)}(dS_{\alpha(t)},dA_{\alpha(t)})\\ &= \{H,A\}_{\alpha(t)} + [S,A]_{\alpha(t)} \end{aligned} \tag{62}$$

or, in more synthetic symbolic notation,

$$\dot{A} = \{H,A\} + [S,A], \tag{63}$$

where, however, we emphasize that $\dot{A}$ denotes neither the total nor the partial derivative of A with respect to time (A is not directly a function of time) but only and precisely what is written above.

From the degeneracy conditions, one easily sees that, for $A = H$,

$$\dot{H} = 0, \tag{64}$$

which reflects the conservation of energy for an isolated system, and, for $A = S$,

$$\dot{S} = [S,S] \geqslant 0, \tag{65}$$

which reflects the principle of entropy nondecrease.

We note in passing that the expression

$$D^\sharp_p(dS_p) \tag{66}$$

is similar in form to Eq. (24). The difference stems from the degeneracy of the tensor field D_p, which prevents us from identifying the expression $D^\sharp_p(dS_p)$ as the gradient vector; this is because the degeneracy prevents a one-to-one correspondence between covectors and vectors. Therefore, we shall refer to $D^\sharp_p(dS_p)$ as the entropy "gradient," in quotation marks. Later, we discuss a supplementary condition [see Eq. (77)] that allows us to associate to it the meaning of a proper *(horizontal) gradient*.

2. *Inner product formulation*

If the manifold is a vector space equipped with an inner product, as in the SEA case, we define variational derivatives according to Eq. (15) and introduce the notation

$$\check{L} \stackrel{\text{def}}{=} P^\sharp R^{-1}, \tag{67}$$

$$\check{M} \stackrel{\text{def}}{=} D^\sharp R^{-1}. \tag{68}$$

We then have, using Eq. (17),

$$X^H_{\alpha(t)} = P^\sharp_{\alpha(t)} R^{-1} R(dH_{\alpha(t)}) = \check{L}|_{\alpha(t)}\left(\frac{\delta H}{\delta p}\bigg|_{\alpha(t)}\right) \tag{69}$$

and

$$Y^S_{\alpha(t)} = D^\sharp_{\alpha(t)} R^{-1} R(dS_{\alpha(t)}) = \check{M}|_{\alpha(t)}\left(\frac{\delta S}{\delta p}\bigg|_{\alpha(t)}\right), \tag{70}$$

and we recover the usual form of the GENERIC,

$$\dot{\alpha}(t) = \check{L}|_{\alpha(t)}\left(\frac{\delta H}{\delta p}\bigg|_{\alpha(t)}\right) + \check{M}|_{\alpha(t)}\left(\frac{\delta S}{\delta p}\bigg|_{\alpha(t)}\right). \tag{71}$$

III. DISCUSSION

The reformulation of the SEA model in the language of differential geometry makes it more easily comparable to the GENERIC model.

First, since in the SEA model the nondissipative or transport part of the dynamics is not rationalized as in GENERIC, but only described case by case, we see that the Poisson structure may be fully imported from GENERIC to SEA without changes. Hence, we shall focus on the dissipative part, analyzing similarities and differences between the two models and highlighting the aspects not completely clear and deserving further analyses.

The following subsections are not meant to be sequential. They can also be read in another order.

A. Original purposes of the two models

In their original article [11], the authors declared the two main purposes of GENERIC:

(1) to reproduce known equations of motion of known physical theories by casting them in a single abstract form and

(2) to suggest new equations for new thermodynamic theories dealing with complex systems.

The goal of the SEA method [23] applied to meso- and macroscopic systems was similar:

(1) to show that a broad selection of known theoretical frameworks for the description of nonequilibrium thermodynamics at various levels of description can all be unified when viewed as implementations of the SEA principle;

(2) to provide rigorous mathematical formalization of the so-called maximum entropy production (MEP) principle, as an attempt to clarifying its meaning, scope, and domain of validity; and

(3) to propose a formalization of known theories which reduces to the linear theories in the proximity of equilibrium, entailing Onsager reciprocity. Hence, showing that such theories are indeed SEA with respect to any metric that at equilibrium reduces to a generalized Onsager conductivity matrix.

However, the original SEA formulation was developed for a very speculative and controversial quantum thermodynamics framework, motivated by the additional fundamental goal to provide a technically consistent connection between a wealth of heuristic discussions about the second law and the arrow of time in the 1970s and 1980s. The attempt consisted in constructing a dynamical theory compatible with the Lyapunov stability requirement suggested by the Hatsopoulos-Keenan statement of the second law of thermodynamics [37,38] whereby the maximum entropy states must be the only equilibrium states of the dynamics that are conditionally stable

in the technical sense defined in Ref. [2], as already discussed above.

B. Differences in the geometric structures

In the GENERIC model, the degeneracy condition (61) imposed on the geometrical structure of the manifold implies that every distinguished functional of the dissipative bracket cannot vary along the dissipative vector field. The entropy "gradient" $D^\sharp(dS)$ is automatically parallel to the level sets of all the distinguished functionals (thus, for example, to the level sets of energy), i.e.,

$$dA(Y^S) = dA[D^\sharp(dS)] = D(dS,dA) = [S,A] = 0, \quad (72)$$

for every distinguished functional A of the dissipative bracket. In other words, the information of constancy of the conserved functionals is contained already in the cometric tensor D.

The SEA model adopts a sub-Riemannian structure [43]. The conserved properties are constant on the submanifolds where purely dissipative time evolution takes place, and the condition (21) defines a *distribution* $\mathcal{D}$ [44] through

$$\mathcal{D}_p = \ker\left(dc_p^1\right) \cap \ker\left(dc_p^2\right) \cap \ldots \cap \ker\left(dc_p^k\right). \quad (73)$$

Since the dc^i's need not necessarily be linearly independent everywhere, the distribution may be *singular*. On this distribution one introduces a metric

$$\begin{aligned} g_p : \mathcal{D}_p \times \mathcal{D}_p &\to \mathbb{R} \\ (u_p, v_p) &\mapsto g_p(u_p, v_p) \end{aligned} \quad (74)$$

with $g_p(u_p,v_p) > 0$ for any nonzero u_p and v_p.

Hereafter, we shall consider finite-dimensional manifolds, because the theorems we will mention are valid for this case. The distribution (73) is *integrable*, i.e., we can find—for each point p—an *integral* submanifold $\mathcal{M}_c$ containing p and such that $T_p\mathcal{M}_c = \mathcal{D}_p$ (see, e.g., Ref. [45]): They are the intersections of the level sets of the conserved functionals. That is why, in Sec. II A 1, we decided to give the "more naive" viewpoint, focusing on the integral submanifolds of the distribution rather than the distribution itself.

The geometric structure of the dissipative dynamics of metriplectic manifolds is also similar to a sub-Riemannian structure, but the distribution $D^\sharp(T^*\mathcal{M})$ is not necessarily integrable.

If, however, we impose the condition

$$\ker(D^\sharp) = \mathrm{span}(\{dc^i\}), \quad (75)$$

we return to the previous situation. This condition means that all the degeneracies in the GENERIC model are related to conservation laws. In this case, as we will see in Sec. V, the SEA and GENERIC formalisms are perfectly equivalent.

The GENERIC model is more similar in spirit to classical mechanics, where the integrals of motion are generally unknown, and finding them is often a great challenge. In the SEA framework, conversely, knowing them is essential for the geometrical construction itself.

A pictorial visualization of the difference between the two constructions can be obtained by introducing in GENERIC the concepts of *symplectic leaves* and *metric leaves*. Symplectic leaves are the submanifolds on which purely Hamiltonian evolution would take place (i.e., assuming the dissipative vector Y^S set identically to zero) [46]. Metric leaves are instead the submanifolds where purely dissipative dynamics would take place (i.e., assuming the nondissipative vector X^H set identically to zero). In the context of GENERIC dynamics, the degeneracy condition (60) implies that symplectic leaves are at constant entropy (and the other distinguished functionals of the Poisson bracket) while the degeneracy condition (61) implies that metric leaves are at constant energy (and the other distinguished functionals of the dissipative bracket). Moreover, for an overall closed and isolated thermodynamic system, the time-independent Hamiltonian functional is a constant of motion and, therefore, both the nondissipative vector X^H and the dissipative vector Y^S lie in a metric leaf. Hence, the GENERIC dynamics cannot leave a particular metric leaf: Each trajectory is effectively constrained on a single metric leaf, as shown in Fig. 2.

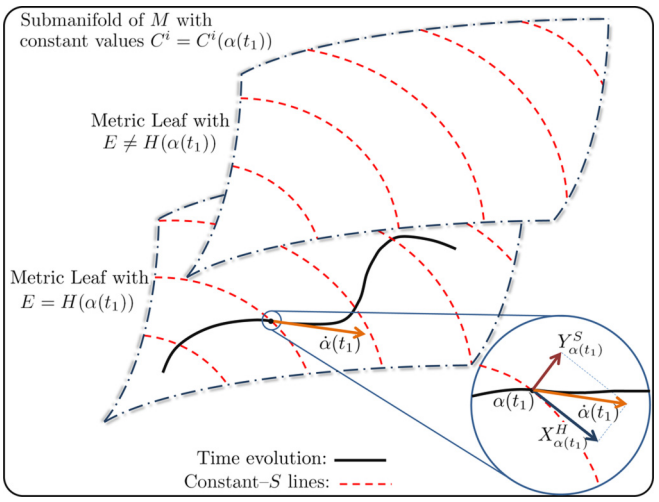

FIG. 2. (Color online) Metric leaves in a manifold: GENERIC dynamics takes place on a single metric leaf.

Figure 3 illustrates the relationship between metric leaves, where GENERIC dynamics (of an overall closed and isolated thermodynamic system) takes place, and symplectic leaves, where purely Hamiltonian dynamics takes place. Metric leaves are surfaces with constant energy, while the symplectic leaves are surfaces with constant entropy (because Hamiltonian dynamics is reversible). As a consequence, the intersection of symplectic leaves on a metric leaf produces isentropic contours and the GENERIC nondissipative vector X^H (for an overall closed and isolated thermodynamic system) is always contained in such an intersection.

In the SEA picture the situation differs for two reasons. The first is that the SEA model is not meant to be restricted to the modeling of overall closed and isolated systems. Therefore, the condition imposed within GENERIC that the vector field X^H must be preserving the overall entropy is not necessarily imposed. Of course, for an isolated system the SEA construction can be made GENERIC by imposing the corresponding degeneracy onto the metric tensor. But the SEA model is meant to apply also for the description of a continuum subjected to general boundary conditions. By assuming a local state description instead of a global one, in terms of the local

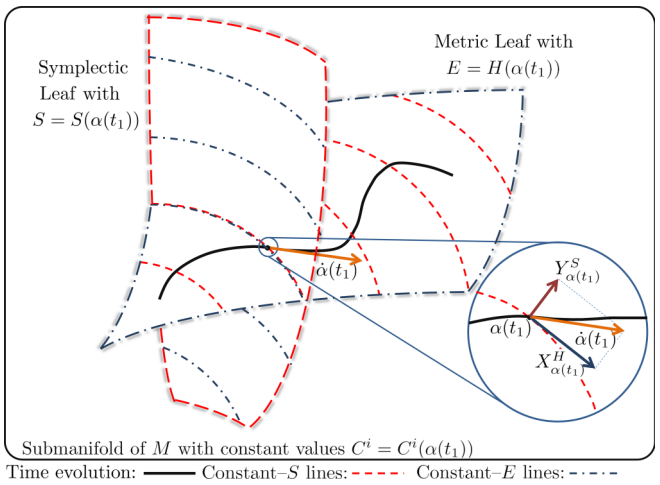

FIG. 3. (Color online) The GENERIC nondissipative vector X^H lies in the intersection of the metric leaf of the time evolution of an isolated system with the symplectic leaf (isentropic surface) being crossed at time t_1 by the time evolution.

entropy density functional $s(\gamma)$ and the local (Lagrangian) entropy flux $\mathbf{J}_S(\gamma)$, it allows one to write the local entropy balance equation in the usual form,

$$\frac{\partial s}{\partial t} + \nabla \cdot \mathbf{J}_S = \Pi_S, \tag{76}$$

where $\nabla \cdot \mathbf{J}_S$ represents the net rate of entropy outflow due to entropy-exchanging interactions between the local element of continuum and its neighbors, and of course it cannot be assumed equal to zero, due to the presence in general of convective and diffusive fluxes of entropy, whereby also its volume integral is in general nonzero. The local entropy production density Π_S (often denoted by σ in nonequilibrium thermodynamics) is controlled by the dissipative vector field Y^S while the transport term $\nabla \cdot \mathbf{J}_S$ is controlled by the nondissipative vector field X^H (which of course controls also the local fluxes of other properties such as mass, momentum, angular momentum, and energy). In order for GENERIC to be extended to include this class of descriptions, the degeneracy condition (60) must be relaxed to properly account for mass, momentum, angular momentum, energy, and entropy fluxes across the boundaries of the system. Some progress in this direction has been already made in Refs. [47,48].

This version of the GENERIC [without imposing Eq. (75)] could be made more similar to the SEA spirit of entropy production maximization by imposing an additional restriction on the GENERIC structure, as we point out below.

As is known from Poisson geometry, where Poisson manifolds foliate into symplectic leaves, a generalized distribution is integrable if and only if it is generated by a family of smooth vector fields and is invariant with respect to their flows. This is the statement of the Stefan-Sussmann theorem [49,50], which is a generalization for singular distributions of the famous Frobenius theorem. In classical mechanics, the condition that assures this integrability is the Jacobi identity, since it forces Hamiltonian flows to be canonical transformations (Poisson maps), that is, to preserve the Poisson structure.

In the GENERIC model, the time evolution of the state does not necessarily preserve the cometric tensor, since dissipative flows themselves are not assumed to preserve the cometric structure. For this reason, the distribution $D^\sharp(T^*\mathcal{M})$ is not integrable.

Instead, we note here that if we additionally endowed the dissipative structure with the *Leibniz identity*

$$[[A,B],C] = [A,[B,C]] + [[A,C],B], \tag{77}$$

which is a generalization of Jacobi identity for non-skew-symmetric brackets [51], we would obtain that dissipative flows preserve the cometric tensor, thus guaranteeing the integrability of the generalized distribution $D^\sharp(T^*\mathcal{M})$ to metric leaves. Then, on metric leaves, we would gain a (nondegenerate) metric, we could calculate distances with it, and we could define gradients by Eq. (11). In this case, we could also interpret GENERIC dynamics as a SEA dynamics on metric leaves.

We may also express this result in general terms as follows. Suppose, for a moment, that there is only dissipative dynamics, so time evolution is confined on a metric leaf in which the degenerate contravariant tensor D is restricted into the nondegenerate one D_L. In this way, we can build the corresponding covariant metric tensor g_L, which acts on vectors as

$$g_L(u,v) = D_L\big(D_L^\flat(u), D_L^\flat(v)\big). \tag{78}$$

In finite dimension, it has matrix $[g_{L,ij}] = [D_L^{ij}]^{-1}$ (for a more rigorous treatment of this procedure for the case of symplectic leaves, see Ref. [40]). Moreover, in the spirit of the variational formulation of the SEA construction, let us consider all unit vectors v at state p [$g_L(v_p, v_p) = 1$] and search for the one that gives the maximal directional derivative of the entropy functional. By definition (11) of gradient of a smooth functional (given the nondegenerate bilinear form g_L) and the Cauchy-Schwarz inequality, we have

$$\begin{aligned} |dS_p(v)|^2 &= |g_L(\operatorname{grad}_L S|_p, v_p)|^2 \\ &\leqslant g_L(\operatorname{grad}_L S|_p, \operatorname{grad}_L S|_p)\, g_L(v_p, v_p) \\ &= \|\operatorname{grad}_L S|_p\|_L^2, \end{aligned} \tag{79}$$

that is, the absolute value of the directional derivative is always smaller than the norm of the gradient vector and reaches its maximum value when

$$v_p = \frac{\operatorname{grad}_L S|_p}{\|\operatorname{grad}_L S|_p\|_L}. \tag{80}$$

The restriction of the total entropy "gradient" $D_p^\sharp(dS_p)$ to the metric leaf is indeed $\operatorname{grad}_L S|_p$, which is sometimes called *horizontal gradient*. Therefore, any nonequilibrium dynamics that can be written in GENERIC form and which satisfies the Leibniz identity (77) is automatically SEA on metric leaves.

However, while the Jacobi identity is a well-known feature of reversible dynamics with deep physical roots in classical mechanics, imposing an analogous condition on the dissipative structure is less founded on physical grounds. For example, we leave it for further investigations to determine whether Eq. (77) is satisfied and whether the time evolution preserves the whole geometric structure in some of the mesoscopic

thermodynamic formulations of dynamics in which the state description is in terms of a maximum entropy family. Such frameworks essentially adopt a kinematics compatible with some version of the maximum entropy formalism (see, e.g., Refs. [52–54]) whereby the nonequilibrium thermodynamic states are assumed to belong to the maximum entropy manifold defined by the local instantaneous values of a given set of mesoscopic properties chosen as the "internal variables" of the system. Typically, this is the set of the constants of the motion augmented by a sufficient number of slowly varying additional properties characterizing some "constraints" (in the sense of Ref. [54]) or some "relevant information that must be included in the analysis" (in the information theory sense; see, e.g., Refs. [55–57]). For example, the recent Ref. [25] assumes a maximum entropy kinematics of this kind and constructs on it a contact-structure-preserving dynamics which effectively combines Hamiltonian and SEA dynamics. Again, Ref. [22] provides another example of maximal-entropy-generation model dynamics for a maximum-entropy discrete-probability-distribution landscape with time-dependent constraints.

C. Relaxation time in SEA

Once the state space has been chosen, namely the manifold where a thermodynamic process occurs, the SEA construction determines in a unique way the local direction of evolution at every point on the manifold and hence the trajectories of time evolution, but in order to do so it requires a choice for the notion of distance between states, i.e., more generally, the choice of a metric field on the tangent space to the submanifold with constant values of the conserved functionals. This choice represents the "modeling knob" that allows the description of different physical behaviors of the system. In other words, systems with identical kinematics and hence identical state spaces may exhibit different nonequilibrium dynamics: When in the same state they evolve differently. It is the metric field g which characterizes the nonequilibrium behavior of the system. As argued in Ref. [23], near equilibrium the metric is directly related to the Onsager matrix of generalized resistances.

It is clear that the rate of evolution along the SEA trajectories is also regulated by the metric, since the velocity of a curve parametrized by time t is the scalar

$$\|\dot{\alpha}(t)\| = \sqrt{g(\dot{\alpha}(t),\dot{\alpha}(t))}, \tag{81}$$

which can be scaled by a constant in the metric tensor.

In the original quantum thermodynamic formulation of the SEA model, a metric (the Fisher-Rao metric) was chosen *ab initio*: This was inspired by the fact that the state is, essentially, a probability measure and the interest was focused on identifying the simplest irreversible dynamics capable of incorporating the second law of thermodynamics. The velocity along the SEA trajectory was scaled by the scalar τ which is allowed to be a functional of the state, i.e., to assume different values along the trajectory in state space. In that simplest context τ represents also the single relaxation time of the physical system being modeled. As shown in Ref. [23, Eq. (87)], τ can be interpreted as an "entropic time" because when time t is measured in units of τ the "speed" along the SEA trajectory is equal to the local rate of entropy increase along the trajectory. Moreover, τ is the Lagrange multiplier of the geometrical constraint in the Lagrangian of the variational formulation of the SEA principle [23, Eq. (72)]. From the modeling point of view, τ is the only knob to scale and control the *strength of the attraction in the SEA direction* along the trajectories of the dynamics.

Here, however, we consider more general physical modeling contexts that include the various frameworks explicitly considered in Ref. [23], such as in complex chemical kinetics or when multiple dissipative kinetic mechanisms give rise even far from equilibrium to Onsager-like couplings (like in thermodiffusion, thermoelectricity, etc.), when isotropy is broken by the presence of phase interfaces or boundaries, or when preferential directions are imposed by externally applied fields. Then the SEA model must account for the multiple relaxation times in effect and this is obtained by assuming a nonisotropic (non Fisher-Rao) local metric tensor field, i.e., the operator $\hat{L} \stackrel{\text{def}}{=} \hat{G}^{-1}/\tau$ introduced in Ref. [23], whose different eigenvalues represent the different local relaxation times up to a common scale factor.

In these more general contexts, the state dependence of the local metric tensor incorporates the information about the different kinetic mechanisms in act and their interplay and fixes the ratios between all pairs of different relaxation times. The entropic time τ could be set to unity and thus absorbed in the metric tensor, but in the present work we prefer to show it explicitly for two reasons. The first is that we wish to maintain a closer formal analogy between the structure of the SEA dissipative vector resulting from Eq. (44) and its equivalent in the original quantum thermodynamics framework. The second reason is to emphasize a somewhat philosophical difference between the GENERIC and SEA approaches.

In fact, the choice considered more "natural" in GENERIC is to embed all the information about the dissipative part of the dynamics inside a single mathematical object, the friction operator. Instead, the "natural" choice in the SEA construction is to single out the three distinct geometrical aspects of the formalism by embedding them in three separate concepts: (1) the foliation of the state space induced by the constants of the motion; (2) the metric field that defines the constrained entropy gradient needed to identify the SEA direction on the corresponding tangent space and, physically, incorporates the information about couplings and relaxation times of the different dissipative mechanisms in play; and (3) the entropic time τ which regulates the speed with which the state evolves along the SEA path in state space.

IV. BOLTZMANN EQUATION

In this section, we illustrate how the two models are implemented in kinetic theory, within the framework of validity of the Boltzmann equation,

$$\begin{aligned}\frac{\partial f(\boldsymbol{r},\boldsymbol{p};t)}{\partial t} &= \left[\frac{\partial \phi(\boldsymbol{r})}{\partial \boldsymbol{r}}\cdot\frac{\partial}{\partial \boldsymbol{p}} - \frac{\boldsymbol{p}}{m}\cdot\frac{\partial}{\partial \boldsymbol{r}}\right] f(\boldsymbol{r},\boldsymbol{p};t) \\ &\quad + \int d^3p_2 \int d^3q_1 \int d^3q_2\, w(\boldsymbol{q}_1,\boldsymbol{q}_2|\boldsymbol{p},\boldsymbol{p}_2) \\ &\quad \times [f(\boldsymbol{r},\boldsymbol{q}_1;t) f(\boldsymbol{r},\boldsymbol{q}_2;t) - f(\boldsymbol{r},\boldsymbol{p};t) f(\boldsymbol{r},\boldsymbol{p}_2;t)],\end{aligned} \tag{82}$$

where $f(\boldsymbol{r},\boldsymbol{p})$ is the one-particle distribution function, $\phi(\boldsymbol{r})$ is the potential of external forces, $w(\boldsymbol{q}_1,\boldsymbol{q}_2|\boldsymbol{p}_1,\boldsymbol{p}_2)$ the transition probability given by

$$\begin{aligned} &w(\boldsymbol{q}_1,\boldsymbol{q}_2|\boldsymbol{p}_1,\boldsymbol{p}_2) \\ &\quad = \delta^{(3)}(\boldsymbol{q}_1+\boldsymbol{q}_2-\boldsymbol{p}_1-\boldsymbol{p}_2) \\ &\qquad \times\delta^{(3)}\big(\boldsymbol{q}_1^2+\boldsymbol{q}_2^2-\boldsymbol{p}_1^2-\boldsymbol{p}_2^2\big)\frac{8}{m}\sigma(\boldsymbol{q}_1,\boldsymbol{q}_2|\boldsymbol{p}_1,\boldsymbol{p}_2), \end{aligned} \tag{83}$$

and σ the differential cross section calculated in the center-of-mass frame. This is the formulation given by Grmela [58] and Öttinger in Ref. [59]. The state space is the infinite-dimensional vector space V of the distribution functions $f(\boldsymbol{r},\boldsymbol{p})$ that are well defined, i.e., non-negative and with finite mean values of the meaningful moments.

At variance with Ref. [59], we choose as suggested in Ref. [23] to reformulate the state description not in terms of the distribution function f but of its square root $\gamma(\boldsymbol{r},\boldsymbol{p})$ so

$$f(\boldsymbol{r},\boldsymbol{p}) = \gamma(\boldsymbol{r},\boldsymbol{p})^2. \tag{84}$$

This is done in order to accomplish three different scopes:

(i) preserving the non-negativity of the distribution function;

(ii) making the gradients of the relevant physical properties belong to a Hilbert space $\mathcal{H}$;

(iii) avoiding the divergence of the entropy gradient outside of the support of $f(\boldsymbol{r},\boldsymbol{p})$ at the expense of an apparent singularity in the equation of motion.

The Boltzmann equation is recovered if the evolution equation for $\gamma(\boldsymbol{r},\boldsymbol{p};t)$ is assumed to be of the form

$$\begin{aligned} &\frac{\partial\gamma(\boldsymbol{r},\boldsymbol{p};t)}{\partial t} \\ &\quad = \left[\frac{\partial\phi(\boldsymbol{r})}{\partial\boldsymbol{r}}\cdot\frac{\partial}{\partial\boldsymbol{p}}-\frac{\boldsymbol{p}}{m}\cdot\frac{\partial}{\partial\boldsymbol{r}}\right]\gamma(\boldsymbol{r},\boldsymbol{p};t) \\ &\qquad + \frac{1}{2\gamma(\boldsymbol{r},\boldsymbol{p},t)}\int d^3q_1\int d^3q_2\int d^3p_2\, w(\boldsymbol{q}_1,\boldsymbol{q}_2|\boldsymbol{p},\boldsymbol{p}_2) \\ &\qquad \times[\gamma(\boldsymbol{r},\boldsymbol{q}_1;t)^2\gamma(\boldsymbol{r},\boldsymbol{q}_2;t)^2-\gamma(\boldsymbol{r},\boldsymbol{p};t)^2\gamma(\boldsymbol{r},\boldsymbol{p}_2;t)^2]. \end{aligned} \tag{85}$$

Equation (85) does present a divergence problem outside of the support of $\gamma(\boldsymbol{r},\boldsymbol{p})$, but this is less problematic because the rates of change of all physical quantities depend on gradients which smooth out the divergence. In other words, they depend on $d\gamma^2/dt$, which is free of this divergence issue.

Each solution of the Boltzmann equation and of its thermodynamically consistent models is a one-parameter family of distribution functions $\alpha : I \to \mathcal{H}$, where

$$\alpha(t) = \gamma(\boldsymbol{r},\boldsymbol{p};t). \tag{86}$$

Thus, the Boltzmann equation and its GENERIC or SEA models take the abstract form of the following differential equation:

$$\dot{\alpha}(t) = X^H_{\alpha(t)} + Y^S_{\alpha(t)}, \tag{87}$$

where the explicit expressions of $X^H_{\alpha(t)}$ and $Y^S_{\alpha(t)}$ differ in the GENERIC and the SEA approach as we have seen in the previous sections in abstract terms and we will see below in specific details for the present framework.

A. GENERIC

For the GENERIC construction, we consider the Hilbert space $\mathcal{H}_{\text{GENERIC}} = L^2(\mathbb{R}^3\times\mathbb{R}^3)$ with inner product

$$\langle x,y\rangle = \int d^3r\int d^3p\, x(\boldsymbol{r},\boldsymbol{p})\, y(\boldsymbol{r},\boldsymbol{p}). \tag{88}$$

The overall mean values of the physical properties are represented by functionals $A[\gamma(\boldsymbol{r},\boldsymbol{p})]$ with associated local field $\tilde{a}(\boldsymbol{r},\boldsymbol{p},\gamma(\boldsymbol{r},\boldsymbol{p}))$ such that $\gamma(\boldsymbol{r},\boldsymbol{p})\,\tilde{a}(\boldsymbol{r},\boldsymbol{p},\gamma(\boldsymbol{r},\boldsymbol{p}))$ belongs to $\mathcal{H}_{\text{GENERIC}}$. As a result, the overall mean value functionals are

$$\begin{aligned} A[\gamma(\boldsymbol{r},\boldsymbol{p})] &= \int d^3r\int d^3p\,\gamma(\boldsymbol{r},\boldsymbol{p})^2\tilde{a}(\boldsymbol{r},\boldsymbol{p},\gamma(\boldsymbol{r},\boldsymbol{p})) \\ &= \langle\gamma,\gamma a\rangle = A \quad \text{with} \quad |A|<\infty. \end{aligned} \tag{89}$$

The normalization condition may be written as $I[\gamma(\boldsymbol{r},\boldsymbol{p})] = \langle\gamma,\gamma\rangle = 1$.

Since $\mathcal{H}_{\text{GENERIC}}$ is a vector space, every tangent space may be identified with the vector space itself, i.e., $T_p\mathcal{H}_{\text{GENERIC}} \cong \mathcal{H}_{\text{GENERIC}}\ \forall p$. The functional derivative has the usual definition, analogous to Eq. (15),

$$\left\langle\left.\frac{\delta A}{\delta\gamma}\right|_{\gamma_0},y\right\rangle = dA_{\gamma_0}(y), \qquad \text{where} \tag{90}$$

$$\gamma_0\in\mathcal{H}_{\text{GENERIC}}, \quad y\in T_{\gamma_0}\mathcal{H}_{\text{GENERIC}}\ (\cong\mathcal{H}_{\text{GENERIC}}). \tag{91}$$

The fundamental properties which generate the dynamical equation in the GENERIC formulation are the overall entropy functional,

$$S[\gamma(\boldsymbol{r},\boldsymbol{p})] = -k_B\int d^3r\int d^3p\,\gamma(\boldsymbol{r},\boldsymbol{p})^2\ln\frac{\gamma(\boldsymbol{r},\boldsymbol{p})^2}{b} = S, \tag{92}$$

where b is a suitable constant with the same dimensions as γ^2, and the overall mean value of the energy, which we write here below the other four collision invariant functionals representing the number of particles and the components of momentum,

$$\begin{aligned} C^0[\gamma(\boldsymbol{r},\boldsymbol{p})] &= \int d^3r\int d^3p\,\gamma(\boldsymbol{r},\boldsymbol{p})^2 = N, \\ C^1[\gamma(\boldsymbol{r},\boldsymbol{p})] &= \int d^3r\int d^3p\, p_x\,\gamma(\boldsymbol{r},\boldsymbol{p})^2 = P_x, \\ C^2[\gamma(\boldsymbol{r},\boldsymbol{p})] &= \int d^3r\int d^3p\, p_y\,\gamma(\boldsymbol{r},\boldsymbol{p})^2 = P_y, \\ C^3[\gamma(\boldsymbol{r},\boldsymbol{p})] &= \int d^3r\int d^3p\, p_z\,\gamma(\boldsymbol{r},\boldsymbol{p})^2 = P_z, \\ C^4[\gamma(\boldsymbol{r},\boldsymbol{p})] &= \int d^3r\int d^3p\left[\frac{\boldsymbol{p}\cdot\boldsymbol{p}}{2m}+\phi(\boldsymbol{r})\right]\gamma(\boldsymbol{r},\boldsymbol{p})^2 = H. \end{aligned} \tag{93}$$

These can be rewritten in compact notation as

$$C^j[\gamma(\boldsymbol{r},\boldsymbol{p})] = \int d^3r\int d^3p\,\psi^j(\boldsymbol{r},\boldsymbol{p})\gamma(\boldsymbol{r},\boldsymbol{p})^2 = C^j, \tag{94}$$

where of course $\psi_0 = 1$, $\psi_1 = p_x$, $\psi_2 = p_y$, $\psi_3 = p_z$, and $\psi_4 = \boldsymbol{p}\cdot\boldsymbol{p}/2m + \phi(\boldsymbol{r})$.

The expressions for the functional derivatives are

$$\left.\frac{\delta S}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})} = -2k_B\gamma(\boldsymbol{r},\boldsymbol{p})\left[\ln\frac{\gamma(\boldsymbol{r},\boldsymbol{p})^2}{b}+1\right], \tag{95}$$

$$\left.\frac{\delta C^j}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})} = 2\gamma(\boldsymbol{r},\boldsymbol{p})\,\psi^j(\boldsymbol{r},\boldsymbol{p}). \tag{96}$$

If the state were chosen to be the distribution function $f(\boldsymbol{r},\boldsymbol{p})$, expression (95) would present a divergence for values of $\boldsymbol{r}$ and $\boldsymbol{p}$ outside the support of the distribution function.

The functionals

$$C^iC^j[\gamma(\boldsymbol{r},\boldsymbol{p})] = \frac{1}{4}\left\langle\left.\frac{\delta C^i}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})},\left.\frac{\delta C^j}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\right\rangle = C^iC^j \tag{97}$$

represent the overall mean values of the collision invariants for $i=0$ or $j=0$ and their overall moments otherwise.

The results in the rest of this subsection are borrowed from Ref. [59], simply recast in terms of $\gamma(\boldsymbol{r},\boldsymbol{p})$ instead of $f(\boldsymbol{r},\boldsymbol{p})$ and written down in full detail.

In the abstract formulation of the GENERIC framework, the evolution equation takes the form

$$\dot\alpha(t) = X^{H,\mathrm{GENERIC}}_{\alpha(t)} + Y^{S,\mathrm{GENERIC}}_{\alpha(t)}, \tag{98}$$

where

$$X^{H,\mathrm{GENERIC}}_{\alpha(t)} = P^\sharp_\gamma|_{\alpha(t)}(dH_{\alpha(t)}) = \breve L_\gamma|_{\alpha(t)}\left(\left.\frac{\delta H}{\delta\gamma}\right|_{\alpha(t)}\right), \tag{99}$$

$$Y^{S,\mathrm{GENERIC}}_{\alpha(t)} = D^\sharp_\gamma|_{\alpha(t)}(dS_{\alpha(t)}) = \breve M_\gamma|_{\alpha(t)}\left(\left.\frac{\delta S}{\delta\gamma}\right|_{\alpha(t)}\right). \tag{100}$$

More explicitly, the evolution equation for $\gamma(\boldsymbol{r},\boldsymbol{p};t)$ is

$$\frac{\partial\gamma(\boldsymbol{r},\boldsymbol{p};t)}{\partial t} = \breve L_\gamma|_{\gamma(\boldsymbol{r},\boldsymbol{p};t)}\left(\left.\frac{\delta H}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p};t)}\right) + \breve M_\gamma|_{\gamma(\boldsymbol{r},\boldsymbol{p};t)}\left(\left.\frac{\delta S}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p};t)}\right). \tag{101}$$

We use the additional subscript γ in $P^\sharp_\gamma|_{\alpha(t)}$, $D^\sharp_\gamma|_{\alpha(t)}$, $\breve L_\gamma|_{\alpha(t)}$, and $\breve M_\gamma|_{\alpha(t)}$ to distinguish these operators from the more standard ones that we give below in terms of $f=\gamma^2$ that we will denote by $P^\sharp_f|_{f(\boldsymbol{r},\boldsymbol{p};t)}$, $D^\sharp_f|_{f(\boldsymbol{r},\boldsymbol{p};t)}$, $\breve L_f|_{\alpha(t)}$, and $\breve M_f|_{\alpha(t)}$.

The Poisson operator at point $\gamma(\boldsymbol{r},\boldsymbol{p})$ is given by

$$\breve L_\gamma|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\left(\left.\frac{\delta A}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\right) = \frac{1}{2\gamma(\boldsymbol{r},\boldsymbol{p})}\left[\frac{\partial}{\partial\boldsymbol{p}}\gamma(\boldsymbol{r},\boldsymbol{p})^2\cdot\frac{\partial}{\partial\boldsymbol{r}} - \frac{\partial}{\partial\boldsymbol{r}}\gamma(\boldsymbol{r},\boldsymbol{p})^2\cdot\frac{\partial}{\partial\boldsymbol{p}}\right]\left[\frac{1}{2\gamma(\boldsymbol{r},\boldsymbol{p})}\left.\frac{\delta A}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\right], \tag{102}$$

and the associated Poisson bracket at point $\gamma(\boldsymbol{r},\boldsymbol{p})$

$$\begin{aligned}
\{A,B\}_{\gamma(\boldsymbol{r},\boldsymbol{p})} &= P_\gamma|_{\gamma(\boldsymbol{r},\boldsymbol{p})}(dA_{\gamma(\boldsymbol{r},\boldsymbol{p})},dB_{\gamma(\boldsymbol{r},\boldsymbol{p})}) = dB_{\gamma(\boldsymbol{r},\boldsymbol{p})}[P^\sharp_\gamma|_{\gamma(\boldsymbol{r},\boldsymbol{p})}(dA_{\gamma(\boldsymbol{r},\boldsymbol{p})})] = \left\langle\left.\frac{\delta B}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})},\breve L_\gamma|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\left(\left.\frac{\delta A}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\right)\right\rangle\\
&= \frac{1}{4}\int d^3r\int d^3p\left[\frac{1}{\gamma(\boldsymbol{r},\boldsymbol{p})}\left.\frac{\delta B}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\right]\left[\frac{\partial}{\partial\boldsymbol{p}}\gamma(\boldsymbol{r},\boldsymbol{p})^2\cdot\frac{\partial}{\partial\boldsymbol{r}} - \frac{\partial}{\partial\boldsymbol{r}}\gamma(\boldsymbol{r},\boldsymbol{p})^2\cdot\frac{\partial}{\partial\boldsymbol{p}}\right]\left[\frac{1}{\gamma(\boldsymbol{r},\boldsymbol{p})}\left.\frac{\delta A}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\right]\\
&= \frac{1}{4}\int d^3r\int d^3p\,\gamma(\boldsymbol{r},\boldsymbol{p})^2\left\{\frac{\partial}{\partial\boldsymbol{r}}\left[\frac{1}{\gamma(\boldsymbol{r},\boldsymbol{p})}\left.\frac{\delta A}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\right]\cdot\frac{\partial}{\partial\boldsymbol{p}}\left[\frac{1}{\gamma(\boldsymbol{r},\boldsymbol{p})}\left.\frac{\delta B}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\right]\right.\\
&\quad\left. - \frac{\partial}{\partial\boldsymbol{p}}\left[\frac{1}{\gamma(\boldsymbol{r},\boldsymbol{p})}\left.\frac{\delta A}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\right]\cdot\frac{\partial}{\partial\boldsymbol{r}}\left[\frac{1}{\gamma(\boldsymbol{r},\boldsymbol{p})}\left.\frac{\delta B}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\right]\right\}\\
&= \int d^3r\int d^3p\,\gamma(\boldsymbol{r},\boldsymbol{p})^2\left\{\frac{\partial}{\partial\boldsymbol{r}}\left[\left.\frac{\delta A}{\delta f}\right|_{f=\gamma(\boldsymbol{r},\boldsymbol{p})^2}\right]\cdot\frac{\partial}{\partial\boldsymbol{p}}\left[\left.\frac{\delta B}{\delta f}\right|_{f=\gamma(\boldsymbol{r},\boldsymbol{p})^2}\right] - \frac{\partial}{\partial\boldsymbol{p}}\left[\left.\frac{\delta A}{\delta f}\right|_{f=\gamma(\boldsymbol{r},\boldsymbol{p})^2}\right]\cdot\frac{\partial}{\partial\boldsymbol{r}}\left[\left.\frac{\delta B}{\delta f}\right|_{f=\gamma(\boldsymbol{r},\boldsymbol{p})^2}\right]\right\}\\
&= \{A,B\}_{f(\boldsymbol{r},\boldsymbol{p})=\gamma(\boldsymbol{r},\boldsymbol{p})^2}.
\end{aligned} \tag{103}$$

The friction operator at point $\gamma(\boldsymbol{r},\boldsymbol{p})$ can be written as follows:

$$\breve M_\gamma|_{\gamma(\boldsymbol{r},\boldsymbol{p};t)}\left(\left.\frac{\delta A}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p};t)}\right) = \int d^3p_1\,\hat M_\gamma[\gamma(\boldsymbol{r},\boldsymbol{p})](\boldsymbol{r},\boldsymbol{p},\boldsymbol{p}_1)\left.\frac{\delta A}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p}_1)}, \tag{104}$$

where

$$\begin{aligned}
\hat M_\gamma[\gamma(\boldsymbol{r},\boldsymbol{p})](\boldsymbol{r},\boldsymbol{p},\boldsymbol{p}_1) &= \frac{1}{4k_B\gamma(\boldsymbol{r},\boldsymbol{p})\gamma(\boldsymbol{r},\boldsymbol{p}_1)}\int d^3q_1\int d^3q_2\int d^3p_2\,w(\boldsymbol{q}_1,\boldsymbol{q}_2|\boldsymbol{p},\boldsymbol{p}_2)[\delta^{(3)}(\boldsymbol{p}-\boldsymbol{p}_1)+\delta^{(3)}(\boldsymbol{p}_2-\boldsymbol{p}_1)\\
&\quad -\delta^{(3)}(\boldsymbol{q}_1-\boldsymbol{p}_1)-\delta^{(3)}(\boldsymbol{q}_2-\boldsymbol{p}_1)]\frac{\gamma(\boldsymbol{r},\boldsymbol{q}_1)^2\gamma(\boldsymbol{r},\boldsymbol{q}_2)^2-\gamma(\boldsymbol{r},\boldsymbol{p})^2\gamma(\boldsymbol{r},\boldsymbol{p}_2)^2}{\ln[\gamma(\boldsymbol{r},\boldsymbol{q}_1)^2\gamma(\boldsymbol{r},\boldsymbol{q}_2)^2]-\ln[\gamma(\boldsymbol{r},\boldsymbol{p})^2\gamma(\boldsymbol{r},\boldsymbol{p}_2)^2]},
\end{aligned} \tag{105}$$

and the associated dissipative bracket at point $\gamma(\boldsymbol{r},\boldsymbol{p})$ reads

$$
\begin{aligned}
[A,B]_{\gamma(\boldsymbol{r},\boldsymbol{p})} &= D_\gamma|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\left(dA_{\gamma(\boldsymbol{r},\boldsymbol{p})},dB_{\gamma(\boldsymbol{r},\boldsymbol{p})}\right) = dB_{\gamma(\boldsymbol{r},\boldsymbol{p})}[D^\sharp_\gamma|_{\gamma(\boldsymbol{r},\boldsymbol{p})}(dA_{\gamma(\boldsymbol{r},\boldsymbol{p})})] = \left\langle \left.\frac{\delta B}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}, \breve{M}_\gamma|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\left(\left.\frac{\delta A}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\right)\right\rangle \\
&= \int d^3r\int d^3p\ \left.\frac{\delta B}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\breve{M}_\gamma|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\left(\left.\frac{\delta A}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\right) = \int d^3r\int d^3p\int d^3p_1\ \left.\frac{\delta B}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\hat{M}_\gamma[\gamma(\boldsymbol{r},\boldsymbol{p})](\boldsymbol{r},\boldsymbol{p},\boldsymbol{p}_1)\ \left.\frac{\delta A}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p}_1)} \\
&= \int d^3r\int d^3p\int d^3p_1\ \left.\frac{\delta B}{\delta f}\right|_{f(\boldsymbol{r},\boldsymbol{p})}\hat{M}_f[f(\boldsymbol{r},\boldsymbol{p})](\boldsymbol{r},\boldsymbol{p},\boldsymbol{p}_1)\ \left.\frac{\delta A}{\delta f}\right|_{f(\boldsymbol{r},\boldsymbol{p}_1)} = \left\langle \left.\frac{\delta B}{\delta f}\right|_{f(\boldsymbol{r},\boldsymbol{p})}, \breve{M}_f|_{f(\boldsymbol{r},\boldsymbol{p})}\left(\left.\frac{\delta A}{\delta f}\right|_{f(\boldsymbol{r},\boldsymbol{p})}\right)\right\rangle \\
&= [A,B]_{f(\boldsymbol{r},\boldsymbol{p})},
\end{aligned}
\tag{106}
$$

where we identify $\hat{M}_f$ as the dissipative "matrix" given in Eq. (12) of Ref. [59],

$$
\begin{aligned}
\hat{M}_f[f(\boldsymbol{r},\boldsymbol{p})](\boldsymbol{r},\boldsymbol{p},\boldsymbol{p}_1) = \frac{1}{k_B}\int d^3q_1\int d^3q_2\int d^3p_2\, w(\boldsymbol{q}_1,\boldsymbol{q}_2|\boldsymbol{p},\boldsymbol{p}_2)[\delta^{(3)}(\boldsymbol{p}-\boldsymbol{p}_1)+\delta^{(3)}(\boldsymbol{p}_2-\boldsymbol{p}_1) \\
-\delta^{(3)}(\boldsymbol{q}_1-\boldsymbol{p}_1)-\delta^{(3)}(\boldsymbol{q}_2-\boldsymbol{p}_1)]\frac{f(\boldsymbol{r},\boldsymbol{q}_1)f(\boldsymbol{r},\boldsymbol{q}_2)-f(\boldsymbol{r},\boldsymbol{p})f(\boldsymbol{r},\boldsymbol{p}_2)}{\ln[f(\boldsymbol{r},\boldsymbol{q}_1)f(\boldsymbol{r},\boldsymbol{q}_2)]-\ln[f(\boldsymbol{r},\boldsymbol{p})f(\boldsymbol{r},\boldsymbol{p}_2)]},
\end{aligned}
\tag{107}
$$

and the corresponding friction operator is

$$
\begin{aligned}
&\breve{M}_f|_{f(\boldsymbol{r},\boldsymbol{p};t)}\left(\left.\frac{\delta A}{\delta f}\right|_{f(\boldsymbol{r},\boldsymbol{p};t)}\right) \\
&\quad = \int d^3p_2\,\hat{M}_f[f(\boldsymbol{r},\boldsymbol{p})](\boldsymbol{r},\boldsymbol{p},\boldsymbol{p}_2)\ \left.\frac{\delta A}{\delta f}\right|_{f(\boldsymbol{r},\boldsymbol{p}_2)}.
\end{aligned}
$$

It is easy but important to verify that the degeneracy requirements

$$
\breve{M}_\gamma|_{\gamma(\boldsymbol{r},\boldsymbol{p};t)}\left(\left.\frac{\delta C^j}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p};t)}\right) = 0 \qquad \forall\, j \tag{108}
$$

are a consequence of the symmetry property (invariance upon exchange of $\boldsymbol{q}_1,\boldsymbol{q}_2$ with $\boldsymbol{p}_1,\boldsymbol{p}_2$) of both the transition probabilities $w(\boldsymbol{q}_1,\boldsymbol{q}_2|\boldsymbol{p}_1,\boldsymbol{p}_2)$ and the positive semidefinite resistance "matrix,"

$$
\begin{aligned}
&\Gamma(\boldsymbol{q}_1,\boldsymbol{q}_2|\boldsymbol{p}_1,\boldsymbol{p}_2) \\
&\quad = \frac{\ln[f(\boldsymbol{r},\boldsymbol{q}_1)f(\boldsymbol{r},\boldsymbol{q}_2)]-\ln[f(\boldsymbol{r},\boldsymbol{p}_1)f(\boldsymbol{r},\boldsymbol{p}_2)]}{f(\boldsymbol{r},\boldsymbol{q}_1)f(\boldsymbol{r},\boldsymbol{q}_2)-f(\boldsymbol{r},\boldsymbol{p})f(\boldsymbol{r},\boldsymbol{p}_1)},
\end{aligned}
\tag{109}
$$

whose form was suggested by the related work in Ref. [60] on chemical kinetics and in the present kinetic theory framework can be interpreted as a resistance matrix due to the collisions from q_1,q_2 to p_1,p_2 and vice versa. Indeed, the entropy production rate can be written as

$$
\begin{aligned}
\Sigma = k_B\int d^3q_1\int d^3q_2\int d^3p_1\int d^3p_2\, w(\boldsymbol{q}_1,\boldsymbol{q}_2|\boldsymbol{p}_1,\boldsymbol{p}_2) \\
\times\Gamma(\boldsymbol{q}_1,\boldsymbol{q}_2|\boldsymbol{p}_1,\boldsymbol{p}_2)[f(\boldsymbol{r},\boldsymbol{q}_1)f(\boldsymbol{r},\boldsymbol{q}_2)-f(\boldsymbol{r},\boldsymbol{p}_1)f(\boldsymbol{r},\boldsymbol{p}_2)]^2.
\end{aligned}
$$

In the case of GENERIC, the effort has been to put the Boltzmann equation in GENERIC form, so the Poisson operator and the friction operator $\hat{M}$ have arisen from this procedure. The friction operators $\hat{M}_\gamma$ and $\hat{M}_f$ given above lead exactly to the collision integral of the Boltzmann equation. In spite of the complexity of such operators, it is hoped that knowing their explicit forms may help identify kinetic models of the Boltzmann collision integral in the same spirit of the BGK model but capable of capturing more features of the collision dynamics and of providing better approximation schemes in the far-non-equilibrium domain. Early attempts along these lines are discussed in Ref. [61].

B. SEA

For the SEA construction, the Hilbert space is $\mathcal{H}_{\rm SEA} = L^2(\mathbb{R}^3)$ with (local) inner product is

$$
(x|y)(\boldsymbol{r}) = \int d^3p\, x(\boldsymbol{r},\boldsymbol{p})\, y(\boldsymbol{r},\boldsymbol{p}), \tag{110}
$$

the local densities of the physical properties are $\boldsymbol{r}$-dependent functionals $a(\boldsymbol{r})[\gamma(\boldsymbol{r},\boldsymbol{p})]$ with associated underlying field $\tilde{a}(\boldsymbol{r},\boldsymbol{p},\gamma(\boldsymbol{r},\boldsymbol{p}))$ such that, for each fixed $\boldsymbol{r}$, $\gamma(\boldsymbol{r},\boldsymbol{p})\,\tilde{a}(\boldsymbol{r},\boldsymbol{p},\gamma(\boldsymbol{r},\boldsymbol{p}))$ belongs to $\mathcal{H}_{\rm SEA}$. As a result, the local density functionals are

$$
\begin{aligned}
a(\boldsymbol{r})[\gamma(\boldsymbol{r},\boldsymbol{p})] &= \int d^3p\,\gamma(\boldsymbol{r},\boldsymbol{p})^2\,\tilde{a}(\boldsymbol{r},\boldsymbol{p},\gamma(\boldsymbol{r},\boldsymbol{p})) \\
&= (\gamma|\gamma a) = a(\boldsymbol{r}) \quad \text{with} \quad |\hat{a}(\boldsymbol{r})|<\infty.
\end{aligned}
\tag{111}
$$

The functional derivative has again the usual definition analogous to Eq. (11), but on $\mathcal{H}_{\rm SEA}$,

$$
\left(\left.\frac{\delta a}{\delta\gamma}\right|_{\gamma_0}\middle| y\right) = da_{\gamma_0}(y) \quad \text{with} \quad \begin{cases}\gamma_0\in\mathcal{H}_{\rm SEA}\\ y\in T_{\gamma_0}\mathcal{H}_{\rm SEA}\ (\cong\mathcal{H}_{\rm SEA})\end{cases}. \tag{112}
$$

Clearly,

$$
\langle A,B\rangle = \int d^3r\ (a|b)(\boldsymbol{r}). \tag{113}
$$

For the SEA formulation the local properties that generate the dynamical equation are the local density and flux fields,

defined as follows:

$$s(\boldsymbol{r})[\gamma(\boldsymbol{r},\boldsymbol{p})] = -k_B \int d^3p\, \gamma(\boldsymbol{r},\boldsymbol{p})^2 \ln \frac{\gamma(\boldsymbol{r},\boldsymbol{p})^2}{b} = s(\boldsymbol{r}),$$
$$c^j(\boldsymbol{r})[\gamma(\boldsymbol{r},\boldsymbol{p})] = \int d^3p\, \psi^j(\boldsymbol{r},\boldsymbol{p})\, \gamma(\boldsymbol{r},\boldsymbol{p})^2 = c^j(\boldsymbol{r}),$$
$$\boldsymbol{J}_{C^j}(\boldsymbol{r})[\gamma(\boldsymbol{r},\boldsymbol{p})] = \int d^3p\, \psi^j(\boldsymbol{r},\boldsymbol{p})\, \frac{\boldsymbol{p}}{m}\, \gamma(\boldsymbol{r},\boldsymbol{p})^2 = \boldsymbol{J}_{C^j}(\boldsymbol{r}). \tag{114}$$

The expressions for the functional derivatives are

$$\left.\frac{\delta s}{\delta \gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})} = -2k_B \gamma(\boldsymbol{r},\boldsymbol{p}) \left[\ln \frac{\gamma(\boldsymbol{r},\boldsymbol{p})^2}{b} + 1\right], \tag{115}$$

$$\left.\frac{\delta c^j}{\delta \gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})} = 2\gamma(\boldsymbol{r},\boldsymbol{p})\, \psi^j(\boldsymbol{r},\boldsymbol{p})\,. \tag{116}$$

We note that the right-hand side of Eqs. (95) and (115) are identical, and this is the same for Eqs. (96) and (116).

Here the functionals

$$c^i c^j[\gamma(\boldsymbol{r},\boldsymbol{p})] = \frac{1}{4}\left(\left.\frac{\delta c^i}{\delta \gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})} \left.\frac{\delta c^j}{\delta \gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}\right) = c^i c^j(\boldsymbol{r}) \tag{117}$$

represent the local mean values of the collision invariants for $i = 0$ or $j = 0$ and the local moments otherwise.

In the abstract formulation of the SEA model, the evolution equation takes the form

$$\dot{\alpha}(t) = X^{H,\mathrm{SEA}}_{\alpha(t)} + Y^{S,\mathrm{SEA}}_{\alpha(t)} \tag{118}$$

where we recall that $\alpha(t) = \gamma(\boldsymbol{r},\boldsymbol{p};t)$. The transport vector field

$$X^{H,\mathrm{SEA}}_{\alpha(t)} = -\frac{\boldsymbol{p}}{m}\cdot\frac{\partial \gamma(\boldsymbol{r},\boldsymbol{p};t)}{\partial \boldsymbol{r}} + \frac{\partial \phi(\boldsymbol{r})}{\partial \boldsymbol{r}}\cdot\frac{\partial \gamma(\boldsymbol{r},\boldsymbol{p};t)}{\partial \boldsymbol{p}} \tag{119}$$

is prescribed and not "derived" as in GENERIC, whereas the dissipative vector field is derived from the gradients of the entropy density and the conserved densities,

$$Y^{S,\mathrm{SEA}}_{\alpha(t)} = \frac{1}{\tau} g^{\sharp}_{\alpha(t)}\left(ds^{\boldsymbol{c}[\alpha(t)]}_{\alpha(t)}\right) = \frac{1}{\tau}\hat{G}^{-1}\left(\left.\frac{\delta s}{\delta \gamma}\right|^{\boldsymbol{c}[\alpha(t)]}_{\alpha(t)}\right). \tag{120}$$

The values of the (Lagrange multipliers) β^j's are found by solving the following system of five algebraic equations [Eq. (43)], $i \in [0,4]$,

$$\sum_{j=0}^{4}\left\langle \left.\frac{\delta c^j}{\delta \gamma}\right|_{\alpha(t)}, \left.\frac{\delta c^i}{\delta \gamma}\right|_{\alpha(t)}\right\rangle \beta^j_{\alpha(t)} = \left\langle \left.\frac{\delta s}{\delta \gamma}\right|_{\alpha(t)}, \left.\frac{\delta c^i}{\delta \gamma}\right|_{\alpha(t)}\right\rangle. \tag{121}$$

The metric tensor g or the equivalent operator $\hat{G}$ that makes the SEA formulation coincide with the full Boltzmann equation can be, in principle, obtained by starting from the expression of the GENERIC friction operator $\breve{M}^{\mathrm{GENERIC}}$ defined by Eqs. (104) and (105), which corresponds to the full Boltzmann collision integral. In fact, in the next section we prove that, given a GENERIC friction operator $\breve{M}$, the metric tensor g identified by Eq. (141) yields the equivalent SEA formulation. In particular, such g is proportional through a scaling dimensionality constant τ to the inverse of the restriction of $\breve{M}$ to $\ker(\breve{M})^{\perp}$. The challenge of deriving the explicit expression of such metric tensor g is left for future work.

The subsequent effort in the SEA philosophy is to find an appropriate metric tensor capable of modeling correctly and efficiently the collision integral of the Boltzmann equation in the same spirit of the traditional kinetic models, such as BGK, ES-BGK, etc., that constitute good approximations near equilibrium, in order to extend their validity to the far-non-equilibrium domain. The problem of identifying criteria for this kind of modeling is still open. Recent numerical results [61] show that the choice of a uniform (Fisher-Rao) metric yields poor models in this framework; more precisely, although near equilibrium it is fully equivalent to the BGK model, in the far-nonequilibrium regime it selects trajectories in state space that diverge from the direction of evolution actually chosen by the full Boltzmann collision integral. It is hoped that the present analysis and perhaps information geometry could provide hints to find a suitable metric for this purpose.

V. EQUIVALENCE OF SEA AND GENERIC (IN MOST FRAMEWORKS)

In this section we show that every SEA model admits a GENERIC form, of course, after making the choice of a kinematics, which is the common starting point. In other words, we prove that we can construct the GENERIC form of any given SEA model. We also prove the converse to be true.

This result holds in the kinetic theory framework of validity of the Boltzmann equation that we considered in the previous section for illustrative purposes. But they are also of much broader validity in that they hold at least for all the frameworks for which the SEA constructions have been made explicit in Ref. [23]. To show such broader validity, below we state the result with explicit reference to the kinetic theory framework but use a more compact notation which points directly to the notation introduced in Ref. [23] in order to unify several different nonequilibrium frameworks and levels of description. In particular, we introduce the following notation, giving a uniform treatment to the symbols used in the section regarding the SEA and GENERIC interpretations of the Boltzmann equation.

Like in the previous sections, we use the same symbol $\gamma(\boldsymbol{r},\boldsymbol{p})$ to denote the states in GENERIC and SEA, even though in SEA the position $\boldsymbol{r}$ is a fixed parameter also for the local functionals. What is important, though, is that the proper functional derivatives in the two frameworks end up being identical functions of $\boldsymbol{r}$ and $\boldsymbol{p}$. Therefore, we denote them by the same symbol. We write the functional derivative of entropy as

$$|\Phi) = \left.\frac{\delta s}{\delta \gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})} = \left.\frac{\delta S}{\delta \gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}, \tag{122}$$

collect a complete set of conserved quantities in the vectors

$$\boldsymbol{c} = \{c^j\}, \qquad \boldsymbol{C} = \{C^j\}, \tag{123}$$

write their functional derivatives as

$$|\boldsymbol{\Psi}) = \left.\frac{\delta \boldsymbol{c}}{\delta \gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})} = \left.\frac{\delta \boldsymbol{C}}{\delta \gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}, \tag{124}$$

and, for simplicity, without loss of generality, assume they are linearly independent [otherwise we drop from sets $\boldsymbol{c}$ and $\boldsymbol{C}$ the conserved quantities that do not have independent functional derivatives, as discussed in Sec. II A 2 after Eq. (43)].

We use the GENERIC friction operator $\breve{M}$ (dropping the apex "GENERIC"), which acts on a vector b on $T_\gamma\mathcal{H}$ according to Eq. (104)

$$\breve{M}|b) = D^\sharp_\gamma(b^*), \tag{125}$$

where b^* is the corresponding covector (the two may be identified thanks to the presence of the inner product). For the SEA operators, we have, for b^c on $T_\gamma\mathcal{H}$,

$$\hat{G}|b^c) = g^\flat_\gamma(b^c), \tag{126}$$

$$\hat{L}|b^c) = \frac{1}{\tau}\hat{G}^{-1}|b^c) = \frac{1}{\tau}g^\sharp_\gamma(b^*), \tag{127}$$

$$(a^c|\hat{G}|b^c) = \left(a^c, g^\flat_\gamma(b^c)\right) = g_\gamma(a^c, b^c). \tag{128}$$

Finally, the dissipative part of the local dynamics, i.e., the part responsible for local entropy generation, like the Boltzmann collision integral in the Boltzmann equation, and the Lagrange multipliers are

$$|\Pi_\gamma) = Y^S_{\alpha(t)}, \tag{129}$$

$$\boldsymbol{\beta} = \left\{\beta^j_{\alpha(t)}\right\}, \tag{130}$$

$$|\boldsymbol{\beta}\cdot\boldsymbol{\Psi}) = \sum_j \beta^j_{\alpha(t)} \left.\frac{\delta c^j}{\delta\gamma}\right|_{\gamma(\boldsymbol{r},\boldsymbol{p})}. \tag{131}$$

Within the GENERIC framework, $|\Pi_\gamma)$ takes the form

$$|\Pi_\gamma) = \breve{M}|\Phi), \tag{132}$$

where $\breve{M}$ is subject to the conditions

$$\breve{M}|\boldsymbol{\Psi}) = 0, \quad \breve{M} \geqslant 0, \quad \text{and} \quad \breve{M} \text{ symmetric}, \tag{133}$$

whereas within the SEA framework it takes the form

$$|\Pi_\gamma) = \hat{L}|\Phi^c) = \hat{L}|\Phi - \boldsymbol{\beta}\cdot\boldsymbol{\Psi}), \tag{134}$$

where $\hat{L}$ is subject to the conditions

$$\hat{L} > 0 \quad \text{symmetric and defined on } \operatorname{span}(\boldsymbol{\Psi})^\perp, \tag{135}$$

and $\boldsymbol{\beta}$ is given by [Eq. (46)]

$$\boldsymbol{\beta} = (\boldsymbol{\Psi}|\boldsymbol{\Psi})^{-1}\cdot(\boldsymbol{\Psi}|\Phi), \tag{136}$$

where $(\boldsymbol{\Psi}|\boldsymbol{\Psi})^{-1}$ denotes the inverse of matrix $(\boldsymbol{\Psi}|\boldsymbol{\Psi})$ with elements $[\langle\Psi^i,\Psi^j\rangle]$.

A. GENERIC form of a SEA model

Now, to prove that every SEA model admits a GENERIC form, we note that we can rewrite Eq. (134) as

$$|\Pi_\gamma) = \hat{L}\hat{P}_{\operatorname{span}(\boldsymbol{\Psi})^\perp}|\Phi). \tag{137}$$

Before we conclude that the operator

$$\breve{M}_{\hat{L},\boldsymbol{\Psi}} = \hat{L}\hat{P}_{\operatorname{span}(\boldsymbol{\Psi})^\perp} \tag{138}$$

provides the GENERIC form (132) of the SEA dynamical equation (134), we must show that $\breve{M}_{\hat{L},\boldsymbol{\Psi}}$ satisfies the requirements stated in Eq. (133). In fact, the first condition is a consequence of $\hat{P}_{\operatorname{span}(\boldsymbol{\Psi})^\perp}|\boldsymbol{\Psi}) = 0$, from which it also follows that $\ker(\breve{M}_{\hat{L},\boldsymbol{\Psi}}) = \operatorname{span}(\boldsymbol{\Psi})$ and when restricted to $\operatorname{span}(\boldsymbol{\Psi})^\perp$ operator $\hat{P}_{\operatorname{span}(\boldsymbol{\Psi})^\perp}$ is the identity and $\breve{M}_{\hat{L},\boldsymbol{\Psi}}$ reduces to $\hat{L}$. The second and third conditions are direct consequences of the symmetry and positive definiteness of $\hat{L}$. To prove even more explicitly that $\breve{M}_{\hat{L},\boldsymbol{\Psi}}$ is positive semidefinite, consider any vector $|b)$ in $T_\gamma\mathcal{H}$ and its decomposition $|b) = |b^c) + |b^{\perp c})$, where $|b^c) = \hat{P}_{\operatorname{span}(\boldsymbol{\Psi})^\perp}|b)$ and $|b^{\perp c}) = |b) - |b^c)$. Then we have $(b|\breve{M}_{\hat{L},\boldsymbol{\Psi}}|b) = (b^c + b^{\perp c}|\hat{L}\hat{P}_{\operatorname{span}(\boldsymbol{\Psi})^\perp}|b^c + b^{\perp c}) = (b^c + b^{\perp c}|\hat{L}|b^c) = (b^c|\hat{L}|b^c) \geqslant 0$ with the equal sign holding only when $|b^c) = 0$, i.e., when $|b)$ lies in the kernel of $\breve{M}_{\hat{L},\boldsymbol{\Psi}}$.

Equation (138) supports explicitly our assertion in Sec. III C that the GENERIC friction operator incorporates both the information about the constants of the motion (it projects onto the local metric leaf orthogonal to their gradients) and the information about the local metric on such leaf: when applied to the entropy gradient it essentially identifies the SEA direction compatible with the local conservation constraints.

This concludes the proof that any SEA formulation can always be put in GENERIC form. Therefore, all the frameworks discussed in Ref. [23], once put into SEA form by choosing the suitable cometric $\hat{L}$, can also be put into GENERIC form (at least as regards the dissipative part) by using the $\breve{M}$ given by Eq. (138) with $\hat{L} = \hat{G}^{-1}/\tau$. In other words, for any operator $\hat{L}$, the operator $\breve{M}$ given in Eq. (138) makes the right-hand side of Eq. (132) become identical to the right-hand side of Eq. (134).

B. SEA form of a GENERIC model

Next we show that also the converse is true, i.e., that any GENERIC formulation can always be put into SEA form provided Eq. (75) holds. To do that, given a GENERIC friction operator $\breve{M}$, we first identify its kernel $\ker(\breve{M})$ and then select as constants of the motion for the SEA formulation a set of state functionals such that their functional derivatives $|\boldsymbol{\Psi})$ form a basis for $\ker(\breve{M})$. This way the dissipative vector fields in both models will conserve the same state functionals. As a result of this choice,

$$\ker(\breve{M}) = \operatorname{span}(\boldsymbol{\Psi}), \tag{139}$$

where $\operatorname{span}(\boldsymbol{\Psi})$ denotes the linear span of the set of vectors $|\boldsymbol{\Psi})$. Clearly, also the following condition holds:

$$\hat{P}_{\ker(\breve{M})} = \hat{P}_{\operatorname{span}(\boldsymbol{\Psi})}. \tag{140}$$

In the framework of the Boltzmann equation, it is well known [62,63] that the kernel of the collision integral coincides with the linear span of the five collision invariants $\psi_0 = 1$, $\psi_1 = p_x$, $\psi_2 = p_y$, $\psi_3 = p_z$, and $\psi_4 = \boldsymbol{p}\cdot\boldsymbol{p}/2m + \phi(\boldsymbol{r})$, i.e., there exist no other linearly independent collision invariants. Since the friction operator given by Eq. (104) and Eq. (105) has been proven to be exactly equivalent to the full Boltzmann collision integral, by applying it to the functional derivatives in Eq. (96), it is easy to verify that the well-known result implies that Eq. (140) holds for $\breve{M}_\gamma$.

To proceed with the proof, let us consider the operator $\hat{L}_{\breve{M}}$ defined by the restriction of $\breve{M}$ on $\ker(\breve{M})^{\perp}$, i.e.,

$$\hat{L}_{\breve{M}}|b^{c}) = \breve{M}|b^{c}) \quad \forall |b^{c}) \in \ker(\breve{M})^{\perp}. \tag{141}$$

In view of the degeneracy requirements $\breve{M}|\mathbf{\Psi}) = 0$, operator $\hat{L}_{\breve{M}}$ is readily shown to convert the SEA equation (134) into the GENERIC equation (132). Indeed,

$$\hat{L}_{\breve{M}}|\Phi^{c}) = \breve{M}|\Phi^{c}) = \breve{M}|\Phi - \boldsymbol{\beta}\cdot\mathbf{\Psi}) = \breve{M}|\Phi). \tag{142}$$

This concludes the proof that we can construct the SEA form of any given GENERIC model.

In order to identify the metric $\hat{G} = \hat{L}^{-1}/\tau$ which makes the Boltzmann equation fit exactly into the SEA form, we would need to identify $\ker(\breve{M}_{\gamma}^{\mathrm{GENERIC}})$ for the dissipative operator $\breve{M}_{\gamma}^{\mathrm{GENERIC}}$ given by Eq. (105). We leave the task of finding the explicit expression of $\hat{P}_{\ker(\breve{M})}$ for future work.

VI. CONCLUSIONS

The main objective of the present paper is the comparison between the SEA dynamical model, initially proposed by Beretta in a quantum thermodynamics framework and recently adapted to meso- and macroscopic systems, and the GENERIC formalism, developed by Grmela and Öttinger. To this end, we reformulated the SEA formalism using the notation of differential geometry similar to that already available for the GENERIC formalism.

Our detailed analysis shows that the two nonequilibrium dynamical models show similar patterns in that both may be considered as belonging to the *maximal-entropy-producing* or the *entropy-gradient* type. In both models the dissipative component of the time evolution of the state of a thermodynamic system is determined by the differential of the entropy functional. In the SEA model it is in the direction of the projection dS^{c} of dS onto the submanifold where the conserved properties are constant. In the GENERIC model it is in the direction of the entropy "gradient" in the metric leaf corresponding to the constant values of the conserved properties (the reason we put gradient between quotation marks is explained at the end of Sec. IIB).

Both structures have been motivated by the search for nonequilibrium thermodynamics formulations that are fully compatible with the second law of thermodynamics. However, specific differences must be pointed out:

(a) The SEA construction focuses only on the dissipative component of the dynamics and describes it by assuming the existence of a sub-Riemannian metric tensor field.

(b) The GENERIC construction tackles with equal emphasis both the nondissipative and the dissipative components of the dynamics and assumes a Poisson structure to describe the nondissipative component and a degenerate co-Riemannian structure to describe the dissipative component.

(c) A SEA model requires the separate specification of (1) a set of time-invariant state functionals $\boldsymbol{c}(p)$ representing constants of the motion or constraints, whose variational derivatives $\mathbf{\Psi}$ determine at every state p the tangent space $T_p\mathcal{M}_{\boldsymbol{c}(p)} = \mathrm{span}(\mathbf{\Psi}_p)^{\perp}$ to the submanifold $\mathcal{M}_{\boldsymbol{c}(p)}$ that contains the dissipative component $Y^{S}_{\alpha(t;p)}$ of the equation of motion, and (2) a metric field $\hat{G}_p$ which for every state p in the state manifold $\mathcal{M}$ defines the geometric notion of distance on the constrained submanifold $\mathcal{M}_{\boldsymbol{c}(p)}$. Physically, the metric tensor $\hat{G}_p$ extends the notion of generalized Onsager resistivity to the far-from-equilibrium domain.

(d) The dissipative part of a GENERIC model requires the specification of a degenerate operator $\breve{M}$ on the space $T_p\mathcal{M}$ tangent to the state manifold $\mathcal{M}$. We have shown that when $\breve{M}$ is constructed so its kernel $\ker(\breve{M})$ coincides with the linear span of the functional derivatives $\mathbf{\Psi}$ of the time-invariant state functionals and its restriction to $\ker(\breve{M})^{\perp}$ is non-negative definite and symmetric, then the model is essentially SEA.

(e) The GENERIC friction operator $\breve{M}$ incorporates both the information about the constants of the motion (it projects onto the local metric leaf orthogonal to their variational derivatives) and the information about the local metric on such leaf. When applied to the entropy variational derivative, it essentially identifies the SEA direction compatible with the conservation constraints. In other words, in the GENERIC formalism the conservation laws are embedded in the degeneracy of the two assumed geometrical structures, while the SEA formalism assumes that the conservation constraints are given explicitly so as to determine the submanifolds where the purely dissipative time evolutions would lie and unfold along the direction of SEA with respect to a metric. The metric represents the couplings and characteristic times of the different dissipative mechanisms in act.

(f) In SEA dynamics, the choice of a nondegenerate metric allows one to univocally define gradients, while in the GENERIC formalism, the choice of a degenerate metric makes it impossible to define a metric and, thus, a gradient, unless a further condition on the dissipative bracket is imposed.

(g) For the description of a continuum, SEA dynamics emerges as a local theory that starts from the local balance equations and implements the assumption of maximal local entropy production density compatible with the local conservation constraints, while the GENERIC formalism emerges as a global theory that implements an entropy gradient dynamics compatible with the global conservation constraints.

Nevertheless, in this paper we show that the descriptions of the dissipative components of the dynamics in the two theories are very closely related, and in some important instances entirely equivalent.

This is the case, for example, of the Boltzmann equation that we work out explicitly in both frameworks not only for illustrative purposes but also to prove the new result that the already-known GENERIC form of the collision integral can also be given a SEA form. The two models have emerged in kinetic theory with different motivations. On one hand, SEA dynamics—which was originally developed [15] as an attempt to understand the fundamental consequences of an attempt to construct a theory of quantum thermodynamics by embedding the second law directly into quantum theory—has been adapted to the framework of kinetic theory with the aim of finding a *simplified* metric to model the collision integral [61] in order to create efficient kinetic models capable of extending to the highly nonequilibrium regime traditional near-equilibrium models such as BGK and ES-BGK. On the other hand, GENERIC, according to one of the two purposes

for which the model was developed by its authors, aims at proving that the Boltzmann equation is a realization of their general abstract dynamics.

Some of the topics considered in the present paper are in need of further ideas or deserve a deeper analysis:

(i) the nondissipative-part formalism that GENERIC borrows from geometric mechanics may be "transferred" to SEA in order to have a more complete model that explicitly considers Hamiltonian dynamics;

(ii) the idea of imposing that the dissipative bracket in GENERIC satisfies the *Leibniz identity* in order to have a nondegenerate metric on the metric leaves could be tested in practical instances by a symbolic algorithm as done for the Jacobi identity in Ref. [64]; and

(iii) as far as open systems are concerned, a parallel could be undertaken between the approach used in Ref. [23] and the mathematical framework of Dirac structures, which the authors of GENERIC claim to play a role in this kind of modeling [26].

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