By reformulating the Steepest-Entropy-Ascent (SEA) dynamical model for non-equilibrium thermodynamics in the mathematical language of Differential Geometry, we compare it with the primitive formulation of the 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 onto the irreversible component of the time evolution, chooses a (non-degenerate) Riemannian metric tensor as dissipative structure, and uses the local entropy density field as potential. GENERIC emphasizes the coupling between the reversible and irreversible 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 compare the implementations of two models in the framework of Kinetic Theory and prove that the known GENERIC formulation of the Boltzmann Equation is SEA. We then provide a formal proof that in more general frameworks, whenever the GENERIC structure is equipped with an inner product, the SEA and GENERIC models of the irreversible 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.

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 non-equilibrium 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 non-equilibrium 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 non-equilibrium thermodynamics theory with the second law of thermodynamics.

At any level of description, the geometrization of a theory of non-equilibrium (thermo)dynamics consists in identifying: (a) the state space $M$ 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 $M$ [3].

Not all existing non-equilibrium thermodynamic 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:

- 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.
- Equilibrium Thermodynamics has been geometrized in the work by Carathéodory [6], the book by Hermann [7], and – for example – the references in [8].
- Some formulations of Non-equilibrium Thermodynamics have been reformulated using the important geometric structure of metriplectic manifolds (see some history and references in [9] and [10]).
- In its most renowned presentation, metriplectic dynamics has been called General Equation for the Non-Equilibrium Reversible-Irreversible Coupling (GENERIC) [11], which represents also a generalization in the context of contact manifolds.
- An apparently simpler and less structured approach (Steepest-Entropy-Ascent dynamics) was proposed in a quantum thermodynamic landscape [12], and recently adapted and generalized for meso- and macroscopic systems in [13].
In general, a reversible evolution is modeled with an antisymmetric tensor, while the irreversible one with a symmetric object. When the latter is a tensor, clearly it may 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 non-equilibrium) have often been attached very different physical (and philosophical) interpretations. For example:

- 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.

- 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” [13]; these relations are expressed in the framework of contact structures [19]. 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 [16]) 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 interpretations, two theories are identical if their mathematical structures are equivalent.

The paper is structured as follows. In Section II we reformulate the SEA and the GENERIC approaches so as to emphasize their analogies and differences, which we further discuss in Section III. In Section IV we implement our formalism to the case of the Boltzmann Equation. In Section V we further elaborate our notation and analysis so as to establish when and in what sense SEA and GENERIC can be considered equivalent. In Section VII 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 non-technical 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 kinetics, for both SEA and GENERIC we will assume it to be given. In particular, when in Section V we will derive relations between the structures of dissipative dynamics in SEA and GENERIC models, we will do under the assumption that the two models adopt the same kinetics. In general, for both SEA and GENERIC, the kinetics is chosen so that the state space is a Banach manifold $M$, i.e., a manifold which locally is topologically equivalent to a Banach space.

The time evolution of the state is represented by a curve $\alpha : I \to M (I \subseteq \mathbb{R})$ on $M$, and this is an integral curve of a vector field (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 reversible 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 reversible and dissipative vector fields,

$$\dot{\alpha}(t) = X^H_{\alpha(t)} + Y^S_{\alpha(t)}.$$  \hspace{1cm} (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 $Y^S$ 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 $M$ is a metriplectic manifold), it is related to a weaker notion of ‘gradient’.

First of all, 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 $M$ is a derivation on $C^\infty(M)$; that is, a linear map

$$v_p : C^\infty(M) \to \mathbb{R} \quad F \mapsto v_p(F),$$  \hspace{1cm} (2)
which takes any smooth functional $F$ on $M$, gives a real number $v_p(F)$ and satisfies the Leibniz rule

$$v_p(FG) = v_p(F)G_p + F_p v_p(G)$$

(3)

for any functionals $F$ and $G$, where $F_p$ and $G_p$ denote their values at $p$. The set of all tangent vectors to $p$ is a vector space, called the tangent space to $M$ at $p$ and denoted by $T_pM$. The disjoint union of all tangent spaces is the tangent bundle, denoted by $TM$. A vector field $X$ is a map

$$X : M \rightarrow TM$$

$$p \mapsto X_p,$$

(4)

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

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

$$v_p = v^k p \partial_k,$$

(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 $v_p(F)$ as the directional derivative of $F$ at $p$ along the tangent vector $v_p$.

Moreover, one may define the cotangent space at $p$ $(T^*_pM \overset{\text{def}}{=} (T_pM)^*)$ as the space of all linear functionals (named covectors) on $T_pM$. The disjoint union of all cotangent spaces is the cotangent bundle $T^*M$. The most important of these linear functionals is the differential $dF$ of a smooth functional $F$ on $M$, which computes the directional derivatives of $F$ at every point $p$ of $M$ 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 $v_p(F)$ as output,

$$dF_p(v_p) = v_p(F)$$

(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 non-degenerate bilinear map on the tangent bundle, which essentially equips the manifold with a metric.

For example, with respect to an inner product $\langle \cdot, \cdot \rangle$ (which is a non-degenerate bilinear map), the gradient of a functional $F$ at point $p$ may be defined implicitly by

$$dF_p(v_p) = \langle \text{grad} F_p, v_p \rangle \quad \forall v_p \in T_pM.$$  

(7)

The main difference between SEA and the dissipative part of GENERIC stems from the technical nature of the bilinear form adopted to define gradients.

A. Steepest Entropy Ascent

The Steepest Entropy Ascent (SEA) principle to model the non-equilibrium dynamics of a thermodynamic system was originally proposed in Intrinsic Quantum Thermodynamics \[12, 17–23\], subsequently extended to probabilistic, constrained maximum entropy landscapes \[24–26\]. 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 non-equilibrium thermodynamics frameworks. Therefore, an extension of the SEA formulation that adopts a generic metric has been provided in \[13\]. 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 present a further generalization whereby the state space is no longer required to be a vector space but may be any (Banach) manifold.

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 \[13\].

The mathematical implementation consists in assuming that the dissipative part of the dynamics pushes the states in the direction of the projection of the entropy gradient onto the linear manifold orthogonal to the gradients 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 orthogonality to the gradients of all the conserved quantities.

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

- a (possibly infinite-dimensional) smooth real Banach manifold $M$ whose points represent the possible states of the system or, for nonequilibrium states of a continuum, the possible local states at position $q$;
- a set of functionals $c^i : M \rightarrow \mathbb{R}$, which represent the conserved properties of the system or, for a continuum, the local densities of the conserved properties;
- another functional $s : M \rightarrow \mathbb{R}$, which represents the thermodynamic entropy \[27\] of the system or, for a continuum, the local entropy density;
• a (strongly non-degenerate) Riemannian metric tensor field \( g \) which, at every point \( p \) of the manifold \( M \), takes as input two vectors in the tangent space \( T_p M \), yields
\[
g_p : T_p M \times T_p M \rightarrow \mathbb{R}
\]
(8)
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 \((C^\infty)\) map on \( M \).

The property of strong non-degeneracy implies that the vector bundle (linear) map (at every point \( p \)) \( \hat{g}_p : T_p M \rightarrow T^*_p M \)
\[
\hat{g}_p = g_p(\cdot, u_p) \quad \forall u_p \in T_p M ,
\]
(9)
which brings a vector \( u_p \) into the covector \( g_p^\dagger(u_p) \) (i.e., into a linear functional on the tangent space at \( p \)), is an isomorphism (often called musical isomorphism). Therefore, the inverse map \( g_p^\dagger : T^*_p M \rightarrow T_p M \) is defined too. In coordinates and finite dimensions, a physicist would talk about lowering and raising the indexes:

\[
(g^\dagger_p)^{ij} v^p_i = v^p_j \quad \forall v^p_j \in T_p M ,
\]
(10)
where \( v^p_i \) and \( v^p_j \) are respectively the components of a vector and a covector with respect to some chosen basis for the tangent space \( T_p M \) and the cotangent space \( T^*_p M \); \((g_p^\dagger)^{ij} = g_p^{ij}\) and \((g_p^\dagger)^{ij} = g_p^{ij}\) are the matrix representations of the maps \( g_p^\dagger \) and \( g_p \) with respect to the same bases, and of course \((g_p^{ij}) = (g_p^{ij})^{-1}\). We may also define the ‘inverse’ metric tensor, or co-metric tensor by:

\[
g_p(\omega_p, \eta_p) = g_p(g_p^\dagger(\omega_p), g_p^\dagger(\eta_p)) .
\]
(11)

We are thus ready to define the gradient of a smooth functional \( a : M \rightarrow \mathbb{R} \) with respect to the metric field \( g \). We can do it either through the following implicit expression (Eq. (7)):

\[
da_p(v_p) = g_p(\text{grad } a|_p, v_p) \quad \forall v_p \in T_p M ;
\]
(12)
or, explicitly,

\[
\text{grad } a|_p = g_p^\dagger(da_p) .
\]
(13)

With reference to the time evolution equation (1), the SEA construction focuses only with 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 that 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 [31][32]. Instead, the non-dissipative vector field \( X^H \) in Eq. (4), 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

\[
Y^S_{\alpha(t)} = \frac{1}{\tau} \left( \text{grad } s_{\alpha(t)} - \sum_j \beta^j_{\alpha(t)} \text{grad } c|_{\alpha(t)} \right)
\]
(14)
where \( \tau \) is a positive dimensionality constant and the \( \beta^j \)'s are multipliers defined by the system of equations obtained by inserting Eq. (14) into the following conservation constraints

\[
dc^a_{\alpha(t)} \left( \dot{a}_t - X^H_{\alpha(t)} \right) = dc^a_{\alpha(t)} \left( Y^S_{\alpha(t)} \right)
\]

\[
= g_{\alpha(t)}(\text{grad } c|_{\alpha(t)}, Y^S_{\alpha(t)}) = 0 ,
\]
(15)
which implies that the dissipative vector field \( Y^S \) must be orthogonal to the gradients of the functionals representing the conserved properties.

The resulting system, which defines the \( \beta^j \)'s implicitly, is

\[
\sum_j g_{\alpha(t)}(\text{grad } c|_{\alpha(t)}, \text{grad } c|_{\alpha(t)}) \beta^j_{\alpha(t)} \quad \forall i ;
\]
(16)
or, in terms of the co-metric tensor \( g \),

\[
\sum_j g_{\alpha(t)}(dc^i|_{\alpha(t)}, dc^j|_{\alpha(t)}) \beta^j_{\alpha(t)} \quad \forall i ;
\]
(17)
This system of equations can be easily solved, for example using Cramer’s rule. Then, the \( \beta^j \)'s can be written explicitly as ratios of determinants so that substitution into Eq. (14) yields the following explicit expression for the dissipative vector field \( Y^S \) (for compactness of notation, we drop the subscripts \( \alpha(t) \))

\[
Y^S = \frac{1}{\tau} \begin{vmatrix}
g(\xi^1, \text{grad } s) & g(\xi^1, \xi^1) & \cdots & g(\xi^1, \xi^n) \\
g(\xi^n, \text{grad } s) & g(\xi^n, \xi^1) & \cdots & g(\xi^n, \xi^n) \\
\vdots & \vdots & \ddots & \vdots \\
g(\xi^1, \xi^1) & \cdots & g(\xi^1, \xi^n) & g(\xi^n, \xi^1) & \cdots & g(\xi^n, \xi^n)
\end{vmatrix}
\]
(18)
where the linearly independent vectors $\xi^1, \ldots, \xi^n$ are any basis (not necessarily orthonormal) for the linear span of the set of gradient vectors $\{\text{grad} \ c^i|_{\alpha(t)}\}$ for all the conserved functionals. The determinant at the denominator is a non-negative definite Gram determinant by virtue of the assumed strict positivity of the metric tensor field $g$ (and the linear independence of the set $\{\xi^i\}$). We may choose the set $\{\xi^i\}$ to coincide with the set of gradient vectors $\{\text{grad} \ c^i|_{\alpha(t)}\}$ if they are linearly independent, otherwise we may take a subset in which we removed those that are linearly dependent on the others. We may also easily construct an orthonormal basis $\xi^1, \ldots, \xi^n$ for the linear span of the set of the $\text{grad} \ c^i|_{\alpha(t)}$’s, so that $g(\xi^i, \xi^j) = \delta_{ij}$ and, therefore, we can write

$$
\tau Y^S_{\alpha(t)} = \text{grad} \ s|_{\alpha(t)} - \sum_{i=1}^{n} g_{\alpha(t)}(\xi^i, \text{grad} \ s|_{\alpha(t)}) \xi^i_{\alpha(t)} = \left[ \hat{I} - \hat{P}_{\text{span} \{\text{grad} \ c^i|_{\alpha(t)}\}} \right] \text{grad} \ s|_{\alpha(t)}
$$

(19)

where $\hat{I}$ denotes the identity operator on $T_{\alpha(t)}M$ and $\hat{P}_{\text{span} \{\text{grad} \ c^i|_{\alpha(t)}\}}$ the projection operator onto the linear span of the gradient vectors for all the conserved functionals.

Among the various equivalent expressions for $Y^S_{\alpha(t)}$, given above, Eq. (19) shows explicitly the SEA construction originally introduced in [20, 26] in the quantum thermodynamics framework, whereby the dissipative vector field $Y^S_{\alpha(t)}$ is in the direction of the projection of $\text{grad} \ s|_{\alpha(t)}$ onto the subspace of $T_{\alpha(t)}M$ orthogonal to all the $\text{grad} \ c^i|_{\alpha(t)}$’s. Figure 1 represents schematically the construction in the simplest case where for illustrative purposes we assume only one conserved property $c^1 = e$, the energy, we denote the only multiplier by $\beta^e$ and we assume that $X^H_{\alpha(t)}$ is orthogonal to both $\text{grad} \ e|_{\alpha(t)}$ and $\text{grad} \ s|_{\alpha(t)}$.

The rate of entropy production can be expressed as follows, where again in the intermediate steps we drop the subscripts $\alpha(t)$ for compactness of notation,

$$
d s_{\alpha(t)} \left( \dot{\alpha}(t) - X^H_{\alpha(t)} \right) = d s_{\alpha(t)} \left( Y^S_{\alpha(t)} \right) = g_{\alpha(t)}(\text{grad} \ s|_{\alpha(t)}, Y^S_{\alpha(t)}) = \frac{1}{\tau} g(\text{grad} \ s, \text{grad} \ s - \sum_j \beta^j \text{grad} \ c^j) = \frac{1}{\tau} g(\text{grad} \ s - \sum_j \beta^j \text{grad} \ c^j, \text{grad} \ s - \sum_j \beta^j \text{grad} \ c^j) = \tau g_{\alpha(t)}(Y^S_{\alpha(t)}, Y^S_{\alpha(t)}) \geq 0 ,
$$

(20)

where the fourth equality follows from Eq. (16), 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 non-dissipative states, i.e., the states $p_{\text{dad}}$ for which $Y^S_{\alpha(t)} = 0$, 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 non-dissipative states, which become equilibrium states when we set $X^H = 0$, should be unstable. This non-trivial 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 [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 [2] is defined precisely and named S-functional. For the quantum framework, the proof of the conjecture advanced in [2] that the von Neumann entropy functional $-k_B \text{Tr} \rho \ln \rho$ is indeed an S-functional was later found in [33].

**B. GENERIC**

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

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

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

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

- A Poisson structure describing the reversible part of the dynamics. This is known from Geometric Mechanics (see, for example, [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 $M$ – takes two covectors at $p$ as inputs, yields

$$P_p: T_p^*M \times T_p^*M \to \mathbb{R}$$

$$(\omega_p, \eta_p) \mapsto P_p(\omega_p, \eta_p) \ ,$$

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

$$\{A, B\}_p \overset{\text{def}}{=} P_p(\text{d}A_p, \text{d}B_p) \ .$$

The Poisson bracket must satisfy the Jacobi identity

$$\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0 \ , \quad (23)$$

which represents a further constraint on the Poisson tensor field $P_p$. The Poisson tensor also yields the Poisson operator $P_p$ on $\mathcal{F}(\mathcal{H}_M)$, which is called Poisson operator, and often assumed to satisfy the condition $P_p(T_p^*M) \subseteq T_p^*M \subseteq T_pM$, which is needed [34] to guarantee that $P_p(\text{d}H_p)$ 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 Section [1]. Since $P_p$ is assumed to be possibly degenerate, $P_p$ is in general non-invertible (it is not a vector-space isomorphism, but only a homomorphism).

It is noteworthy that condition [23] is imposed so as to implement time-translation invariance of the reversible part of the dynamics (integrability condition). We shall see below that GENERIC does not impose an analogous integrability condition on the irreversible part of the dynamics. We further discuss this point in Section [11]

- A degenerate co-Riemannian structure (i.e., we have a degenerate co-metric instead of a non-degenerate metric) describing the irreversible dynamics [35]. 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 $M$ – takes two covectors at $p$ as inputs, yields

$$D_p: T_p^*M \times T_p^*M \to \mathbb{R}$$

$$(\omega_p, \eta_p) \mapsto D_p(\omega_p, \eta_p) \ ,$$

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

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

$$[A, B]_p \overset{\text{def}}{=} D_p(\text{d}A_p, \text{d}B_p) \ .$$

The friction tensor also yields the vector bundle map $D_p: T_p^*M \to T_pM$, called friction operator, also often assumed to satisfy the condition $D_p(T_p^*M) \subseteq T_p^*M \subseteq TM$. Also here, since $D_p$ is assumed to be possibly degenerate, $D_p$ is in general non-invertible.

With reference to the time evolution equation [1], the GENERIC construction addresses both the non-dissipative (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 $H: M \to \mathbb{R}$,

$$X^H_{\alpha(t)} = P^\sharp_{\alpha(t)}(\text{d}H_{\alpha(t)}) \ ,$$

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 $S: M \to \mathbb{R}$,

$$Y^S_{\alpha(t)} = D^\sharp_{\alpha(t)}(\text{d}S_{\alpha(t)}) \ ,$$

subject to the following supplementary conditions.

- 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

$$\{S, A\} = P(\text{d}S, \text{d}A) = \text{d}A( P^\sharp(\text{d}S)) = 0 \quad \forall A \in C^\infty(M) \ , \quad \text{or, equivalently, } \ P^\sharp_{\alpha(t)}(\text{d}S_{\alpha(t)}) = 0. \quad (28)$$

- 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

$$[H, A] = D(\text{d}H, \text{d}A) = \text{d}A( D^\sharp(\text{d}H)) = 0 \quad \forall A \in C^\infty(M) \ , \quad \text{or, equivalently, } \ D^\sharp_{\alpha(t)}(\text{d}H_{\alpha(t)}) = 0. \quad (29)$$

- Also 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 $M$, we calculate the directional derivative of $A$ along the velocity vector $\dot{\alpha}(t)$
in the following way:
\[
\frac{d}{dt}(A_\alpha(t)) = dA_\alpha(t)(\dot{\alpha}(t)) = \\
= dA_\alpha(t)(X^H_\alpha(t) + P^\circ_{\alpha(t)}(dH_\alpha(t))) + dA_\alpha(t)(D^g_{\alpha(t)}(dS_\alpha(t))) \\
= P_{\alpha(t)}(dH_\alpha(t), dA_\alpha(t)) + D_{\alpha(t)}(dS_\alpha(t), dA_\alpha(t)) \\
= \{H, A\}_\alpha + [S, A]_\alpha(t) \\
\]
(30)
or, in more synthetic symbolic notation,
\[
\dot{A} = \{H, A\} + [S, A] \\
\]
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 \(A = H\),
\[
\dot{H} = 0 \\
\]
which reflects the conservation of energy for an isolated system; and, for \(A = S\),
\[
\dot{S} = [S, S] \geq 0 \\
\]
which reflects the principle of entropy non-decrease.

We note in passing that the expression
\[
D^g_p(dS_p) \\
\]
(34)
is similar in form to Eq. (33). The difference stems from the degeneracy of the tensor field \(D_p\), which prevents us from identifying the expression \(D^g_p(dS_p)\) as the gradient vector; this is because the degeneracy prevents a one-to-one correspondence between covectors and vectors. Therefore, we shall refer to \(D^g_p(dS_p)\) as the entropy “gradient”, in quotation marks. Later, we discuss a supplementary condition (see Eq. (36)) that allows us to associate to it the meaning of a proper (horizontal) gradient.

### III. DISCUSSION

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

First of all, since in the SEA model the reversible 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;
2. to suggest new equations for new thermodynamic theories dealing with complex systems.

The goal of the SEA method [13] applied to meso- and macroscopic systems was similar:

1. to show that a broad selection of known theoretical frameworks for the description of non-equilibrium 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;
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 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 70’s and 80’s. 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 [31] [32] 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 (29) 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” \(D^g(dS)\) is automatically parallel to the level sets of all the distinguished functionals (thus, for example, to the level set of the energy), i.e.,
\[
dA(Y^S) = dA(D^g(dS)) = D(dS, dA) = [S, A] = 0 \\
\]
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 co-metric tensor $D$.

Instead, the SEA model is built on a Riemannian manifold and, consequently, there cannot be preliminary assumptions on the functionals representing the conserved properties, i.e., that they are distinguished functionals of some structure. As a consequence, in the SEA method the conservations must be imposed explicitly.

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) \[37\]. Metric leaves are instead the submanifolds where purely dissipative dynamics would take place (i.e., assuming the reversible vector $X^H$ set identically to zero).

In the context of GENERIC dynamics, the degeneracy condition \[28\] implies that symplectic leaves are at constant entropy (and the other distinguished functionals of the Poisson bracket) while the degeneracy condition \[29\] 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 reversible 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 pictorially in Figure 2.

In the SEA picture the situation is different 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 entropy density functional $s(\gamma)$ and the local (Lagrangian) entropy flux $J_S(\gamma)$, it allows to write the local entropy balance equation in the usual form

\[
\frac{\partial s}{\partial t} + \nabla \cdot J_S = \Pi_S
\]

where $\nabla \cdot J_S$ 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 $\Pi_S$ (often denoted by $\sigma$ in non-equilibrium thermodynamics) is controlled by the dissipative vector field $\mathbf{Y}^S$ while the transport term $\nabla \cdot \mathbf{J}_p$ is controlled by the reversible vector field $\mathbf{X}^H$ (which of course controls also the local fluxes of other properties such as mass, momentum, angular momentum, energy). In order for GENERIC to be extended so as to include this class of descriptions, the degeneracy condition \[ [25] \] must be relaxed so as to properly account for mass, momentum, angular momentum, energy, and entropy fluxes across the boundaries of the system. Some progress in this direction has already been made in Refs. [38, 39].

This version of the GENERIC 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.

The geometric structure of the dissipative dynamics of metriplectic manifolds is similar to a sub-Riemannian structure. The difference lies in the nature of the distribution \[ [40] D^I(T^*M) \] : whereas, in the sub-Riemannian case, this would be a regular distribution (i.e., of constant dimension), in the case of GENERIC this may not happen (since the rank of $D^I$ may vary from point to point), and one has to deal with a generalized (or singular) distribution, whose dimension is not constant. Hereafter, we shall consider finite-dimensional manifolds, because the theorems we will mention are valid for this case.

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 [11, 32], 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 supposed to preserve the cometric structure. For this reason, the distribution $D^I(T^*M)$ is not integrable, and we do not even have the notion of distance, as we would have in the sub-Riemannian (constant rank) case (Carnot-Carathéodory distance; see, e.g., [43]).

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

\[ [\{A, B\}, C] = [\{B, C\}] + [\{A, C\}, B], \quad (36) \]

which is a generalization of Jacobi identity for non skew-symmetric brackets, we would obtain that dissipative flows preserve the cometric tensor, thus guaranteeing the integrability of the generalized distribution $D^I(T^*M)$ to metric leaves. Then, on metric leaves, we would gain a (non-degenerate) metric, we could calculate distances with it, and we could define gradients by Eq. [7]. 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 that time evolution is confined on a metric leaf in which the degenerate contravariant tensor $D$ is restricted into the non-degenerate one $D_L$. In this way, we can build the corresponding covariant metric tensor $g_L$, which acts on vectors as

\[ g_L(u, v) = D_L\left(D_L^*(u), D_L^*(v)\right). \quad (37) \]

In finite dimension, it has matrix $[g_L, ij] = [D_L^T]^{-1}$ (for a more rigorous treatment of this procedure for the case of symplectic leaves, see [31]). 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 of gradient of a smooth functional (given the non-degenerate bilinear form $g_L$) and the Cauchy-Schwarz inequality, we have

\[ |dS_p(v)|^2 = |g_L(\text{grad}_L S|_p, v_p)|^2 \leq g_L(\text{grad}_L S|_p, \text{grad}_L S|_p) \cdot g_L(v_p, v_p) = ||\text{grad}_L S|_p||^2_L, \quad (38) \]

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

\[ v_p = \frac{\text{grad}_L S|_p}{||\text{grad}_L S|_p||_L}. \quad (39) \]

The restriction of the total entropy `gradient' $D_L^* (dS_p)$ to the metric leaf is indeed $\text{grad}_L S|_p$, which is sometimes called horizontal gradient. Therefore, any nonequilibrium dynamics that can be written in GENERIC form and which satisfies the Leibniz identity (36) 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. (36) 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. [14, 40]) 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. [15]) or some “relevant information that must be included in the analysis” (in the information theory sense, see, e.g., Ref. [47][19]). For example, the recent Ref. [15] 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. [26] provides another example of maximal-entropy-generation model dynamics for a maximum-entropy discrete-probability-distribution landscape with time-dependent constraints.

C. Relaxation time

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. This choice represents the “modeling nob” 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 non-equilibrium dynamics: when in the same state they evolve differently. It is the metric field $q$ which characterizes the non-equilibrium behavior of the system. As argued in [13], 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 is the scalar

$$\|\dot{\gamma}(t)\| = \sqrt{g(\dot{\gamma}(t), \dot{\gamma}(t))},$$

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

In the previous 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. On the other hand, because of the novelty of the theory, there was no equation having to be reproduced by the model, as in the other meso- and macroscopic frameworks. Due to this fact, the relaxation time $\tau$ was allowed to be a functional of the state, in order to keep a “modeling nob” to control the rate of evolution along the trajectories of the dynamics.

But now that the metric is not chosen a priori, the SEA relaxation time may be merged in the metric tensor (indeed, the operator $\hat{L} \overset{\text{def}}{=} q^2/\tau$ introduced in [13] does so), since it simply scales the intensity of the dissipative vector field in the direction of the entropy gradient. That is why, in this work, we assume $\tau$ to be only a dimensionality constant.

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

$$\frac{\partial f(r,p;t)}{\partial t} = \left[ \frac{\partial \phi(r)}{\partial r} \cdot \frac{\partial}{\partial p} - \frac{p}{m} \cdot \frac{\partial}{\partial r} \right] f(r,p;t) + \int d^3p_2 \int d^3q_1 \int d^3q_2 w(q_1,q_2|p,p_2) \times \left[ f(r,q_1;t)f(r,q_2;t) - f(r,p;t)f(r,p_2;t) \right],$$

where $f(r,p)$ is the one-particle distribution function, $\phi(r)$ is the potential of external forces, $w(q_1,q_2|p_1,p_2)$ the transition probability given by

$$w(q_1,q_2|p_1,p_2) = \delta^{(3)}(q_1 + q_2 - p_1 - p_2) \times \delta^{(3)}(q_1^2 + q_2^2 - p_1^2 - p_2^2 - \frac{8}{m} \sigma(q_1,q_2|p_1,p_2),$$

and $\sigma$ the differential cross section calculated in the centre-of-mass frame. This is the formulation given by Grmela [60] and Ottinger in [51]. The state space is the infinite-dimensional Hilbert manifold $M$ of the distribution functions $f(r,p)$ that are well-defined, i.e., non-negative and with finite mean values of the meaningful moments.

At variance with Ref. [51], we choose as suggested in Ref. [13] to reformulate the state description not in terms of the distribution function but of its square-root

$$\gamma(r,p) \overset{\text{def}}{=} \sqrt{f(r,p)}.$$  

This is done in order to accomplish three different scopes:

- preserving the non-negativity of the distribution function;
- making the gradients of the relevant physical properties belong to a Hilbert space;
- avoiding the divergence of the entropy gradient outside of the support of $f(r,p)$, at the expense of an apparent singularity in the equation of motion.

The Boltzmann equation rewritten in terms of $\gamma(r,p;t)$ takes the form

$$\frac{\partial \gamma(r,p,t)}{\partial t} = \left[ \frac{\partial \phi(r)}{\partial r} \cdot \frac{\partial}{\partial p} - \frac{p}{m} \cdot \frac{\partial}{\partial r} \right] \gamma(r,p;t) + \frac{1}{2\gamma(r,p,t)} \int d^3q_1 \int d^3q_2 \int d^3p_2 w(q_1,q_2|p,p_2) \times [\gamma(r,q_1;t)^2\gamma(r,q_2;t)^2 - \gamma(r,p;t)^2\gamma(r,p_2;t)^2].$$

Eq. (44) does present a divergence problem outside of the support of $\gamma(r,p)$, 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 $\alpha^2/\beta$ 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 $\alpha : I \to M$ where

$$\alpha(t) = \gamma(r, p; t)$$

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

$$\dot{\alpha}(t) = X_{\alpha(t)}^H + Y_{\alpha(t)}^S,$$

where the explicit expressions of $X_{\alpha(t)}^H$ and $Y_{\alpha(t)}^S$ 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

$$\langle x, y \rangle = \int \! \! d^3r \int \! \! d^3p x(r, p) y(r, p).$$

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

$$A[\gamma(r, p)] = \int \! \! d^3r \int \! \! d^3p \gamma(r, p)^2 \hat{a}(r, p, \gamma(r, p))$$

$$= (\gamma, \gamma a) = A \quad \text{with} \quad |A| < \infty.$$

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

The functional derivative has the usual definition, analogous to Eq. (7).

$$\left\langle \frac{\delta A}{\delta \gamma}, y \right\rangle = dA_{\gamma o}(y) \quad (\gamma_0, y \in \mathcal{H}_{\text{GENERIC}}).$$

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

$$S[\gamma(r, p)] = -k_B \int \! \! d^3r \int \! \! d^3p \gamma(r, p)^2 \ln \frac{\gamma(r, p)^2}{\beta} = S,$$

where $b$ is a suitable constant with the same dimensions as $\gamma^2$, 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

$$C^0[\gamma(r, p)] = \int \! \! d^3r \int \! \! d^3p \gamma(r, p)^2 = N,$$

$$C^1[\gamma(r, p)] = \int \! \! d^3r \int \! \! d^3p p_x \gamma(r, p)^2 = P_x,$$

$$C^2[\gamma(r, p)] = \int \! \! d^3r \int \! \! d^3p p_y \gamma(r, p)^2 = P_y,$$

$$C^3[\gamma(r, p)] = \int \! \! d^3r \int \! \! d^3p p_z \gamma(r, p)^2 = P_z,$$

$$C^4[\gamma(r, p)] = \int \! \! d^3r \int \! \! d^3p \left[ \frac{p_x^2 + p_y^2 + p_z^2}{2m} + \phi(r) \right] \gamma(r, p)^2 = H.$$

These can be rewritten in compact notation as

$$C^j[\gamma(r, p)] = \int \! \! d^3r \int \! \! d^3p \psi^j(r, p) \gamma(r, p)^2 = C^j,$$

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

The expressions for the functional derivatives are

$$\frac{\delta S}{\delta \gamma}_{\gamma(r, p)} = -2k_B \gamma(r, p) \left[ \ln \frac{\gamma(r, p)^2}{\beta} + 1 \right],$$

$$\frac{\delta C^j}{\delta \gamma}_{\gamma(r, p)} = 2\gamma(r, p) \psi^j(r, p).$$

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

The functionals

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

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. [71], simply recast in terms of $\gamma(r, p)$ instead of $f(r, p)$.

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

$$\dot{\alpha}(t) = X_{\alpha(t)}^{H, \text{GENERIC}} + Y_{\alpha(t)}^{S, \text{GENERIC}}$$

where

$$X_{\alpha(t)}^{H, \text{GENERIC}} = P^i_{\gamma_{\alpha(t)}}(dH_{\alpha(t)}),$$

$$Y_{\alpha(t)}^{S, \text{GENERIC}} = D^i_{\gamma_{\alpha(t)}}(dS_{\alpha(t)}).$$

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

$$\frac{\partial \gamma(r, p; t)}{\partial t} = P^i_{\gamma(r, p; t)}(dH_{\gamma(r, p; t)})$$

$$+ D^i_{\gamma(r, p; t)}(dS_{\gamma(r, p; t)}).$$
We use the additional subscript $\gamma$ in $P_\gamma^2\big|_{\gamma=\omega(t)}$ and $D_\gamma^2\big|_{\gamma=\omega(t)}$ to distinguish these operators from the more standard ones that we give below in terms of $f = \gamma^2$, that we will denote by $P_f^2\big|_{f(r,p,t)}$ and $D_f^2\big|_{f(r,p,t)}$.

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

$$ P_\gamma^2\big|_{\gamma(r,p)}(dA_\gamma(r,p)) = \frac{1}{2\gamma(r,p)} \left[ \frac{\partial}{\partial p} \gamma(r,p)^2 \cdot \frac{\partial}{\partial r} \gamma(r,p)^2 \cdot \frac{\partial}{\partial p} \right] \left( \frac{1}{2\gamma(r,p)} \frac{\delta A}{\delta \gamma} \big|_{\gamma(r,p)} \right), \quad (58) $$

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

$$ \{A,B\}_{\gamma(r,p)} = P_\gamma\big|_{\gamma(r,p)}(dA_\gamma(r,p), dB_\gamma(r,p)) = P_\gamma^2\big|_{\gamma(r,p)}(dA_\gamma(r,p))(dB_\gamma(r,p)) = dB_\gamma(r,p)\left( P_\gamma^2\big|_{\gamma(r,p)}(dA_\gamma(r,p)) \right) = $$

$$ = \frac{1}{4} \int d^3r \int d^3p \frac{1}{\gamma(r,p)} \delta B \big|_{\gamma(r,p)} \left[ \frac{\partial}{\partial p} \gamma(r,p)^2 \cdot \frac{\partial}{\partial r} \gamma(r,p)^2 \cdot \frac{\partial}{\partial p} \right] \left( \frac{1}{2\gamma(r,p)} \frac{\delta A}{\delta \gamma} \big|_{\gamma(r,p)} \right) $$

$$ = \frac{1}{4} \int d^3r \int d^3p \int d^3p \frac{1}{\gamma(r,p)} \delta A \big|_{\gamma(r,p)} \frac{\delta B}{\delta \gamma} \big|_{\gamma(r,p)} \left[ \frac{\partial}{\partial p} \gamma(r,p)^2 \cdot \frac{\partial}{\partial r} \gamma(r,p)^2 \right] $$

$$ = \{A,B\}_{f(r,p)=\gamma(r,p)^2}. \quad (59) $$

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

$$ D_\gamma^2\big|_{\gamma(r,p)}(dA_\gamma(r,p)) = $$

$$ = \int d^3p_1 \hat{M}_\gamma[\gamma(r,p)](r,p,p_1) \frac{\delta A}{\delta \gamma}\big|_{\gamma(r,p_1)} $$

$$ = \hat{M}_{\text{generic}} \left( \frac{\delta A}{\delta \gamma}\big|_{\gamma(r,p)} \right), \quad (60) $$

where

$$ \hat{M}_\gamma[\gamma(r,p)](r,p,p_1) = $$

$$ = \frac{1}{4k_B \gamma(r,p)\gamma(r,p_1)} \int d^3q_1 \int d^3q_2 \int d^3p_2 w(q_1, q_2, p, p_2) \times $$

$$ \times \left[ \delta^{(3)}(p - p_1) + \delta^{(3)}(p_2 - p_1) - \delta^{(3)}(q_1 - p_1) - \delta^{(3)}(q_2 - p_1) \right] $$

$$ \times \frac{\gamma^2(r,q_1)\gamma^2(r,q_2) - \gamma^2(r,p)\gamma^2(r,p_2)}{\ln[\gamma^2(r,q_1)\gamma^2(r,q_2)] - \ln[\gamma^2(r,p)\gamma^2(r,p_2)]}, \quad (61) $$

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

$$ \{A,B\}_{\gamma(r,p)} = D_\gamma\big|_{\gamma(r,p)} \left( \frac{\delta A}{\delta \gamma}\big|_{\gamma(r,p)} \cdot \frac{\delta B}{\delta \gamma}\big|_{\gamma(r,p)} \right) $$

$$ = D_\gamma^2\big|_{\gamma(r,p)}(dA_\gamma(r,p))(dB_\gamma(r,p)) $$

$$ = dB_\gamma(r,p)\left( D_\gamma^2\big|_{\gamma(r,p)}(dA_\gamma(r,p)) \right) $$

$$ = \int d^3r \int d^3p \frac{\delta B}{\delta \gamma} \big|_{\gamma(r,p)} D_\gamma^2\big|_{\gamma(r,p)}(dA_\gamma(r,p)) $$

$$ = \int d^3r \int d^3p \frac{\delta B}{\delta \gamma} \big|_{\gamma(r,p)} \hat{M}_\gamma[\gamma(r,p)](r,p,p_1) \frac{\delta A}{\delta \gamma}\big|_{\gamma(r,p_1)} $$

$$ = \int d^3r \int d^3p \frac{\delta B}{\delta \gamma} \big|_{f(r,p)} \hat{M}_f[f(r,p)](r,p,p_1) \frac{\delta A}{\delta \gamma}\big|_{f(r,p_1)} $$

$$ = dB_f(r,p)\left( D_f^\gamma\big|_{f(r,p)}(dA_f(r,p)) \right) $$

$$ = \{A,B\}_{f(r,p)} \big|_{f(r,p)} $$

$$ = \hat{M}_f[f(r,p)](r,p,p_1) $$

$$ = \frac{1}{k_B} \int d^3q_1 \int d^3q_2 \int d^3p_2 w(q_1, q_2, p, p_2) \times $$

$$ \times \left[ \delta^{(3)}(p - p_1) + \delta^{(3)}(p_2 - p_1) - \delta^{(3)}(q_1 - p_1) - \delta^{(3)}(q_2 - p_1) \right] $$

$$ \times \frac{f(r,q_1)f(r,q_2) - f(r,p)f(r,p_2)}{\ln[f(r,q_1)f(r,q_2)] - \ln[f(r,p)f(r,p_2)]}, \quad (62) $$
and the corresponding friction operator is
\[ D^j_t \big|_{H \gamma} \left( \frac{\delta A}{\delta \gamma_j} \right) = \int d^3 p_2 \tilde{M}_j[f(r, p)](r, p, p_2) \frac{\delta A}{\delta \gamma_j} \bigg|_{f(r, p_2)}, \]

It is easy but important to verify that the degeneracy requirements
\[ D^j_t \big|_{\gamma(r, p, t)} \left( \frac{\delta C^j}{\delta \gamma} \right) = 0 \quad \forall j \]
are consequence of the symmetry property (invariance upon exchange of \(q_1, q_2\) with \(p_1, p_2\)) of both the transition probabilities \(w(q_1, q_2|p_1, p_2)\) and the positive semi-definite resistance ‘matrix’
\[ \Gamma(q_1, q_2|p_1, p_2) = \frac{\ln[f(r, q_1)f(r, q_2)] - \ln[f(r, p_1)f(r, p_2)]}{f(r, q_1)f(r, q_2) - f(r, p)f(r, p)} \]
whose form was suggested by the related work 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
\[ \Sigma = k_B \int d^3 q_1 \int d^3 q_2 \int d^3 p_1 \int d^3 p_2 w(q_1, q_2|p_1, p_2) \times \Gamma(q_1, q_2|p_1, p_2) \left[ f(r, q_1)f(r, q_2) - f(r, p_1)f(r, p_2) \right]^2. \]

In the case of GENERIC, the effort has been to put the Boltzmann Equation in GENERIC form, so that the Poisson operator and the friction operator \(M\) have arisen from this procedure. The friction operators \(M_s\) and \(M_f\) given above lead exactly to 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 given better approximations in the far non-equilibrium domain. Early attempts along these lines are discussed in [63].

**B. SEA**

For the SEA construction, the Hilbert space is \(\mathcal{H}_{SEA} = L^2(\mathbb{R}^3)\) with (local) inner product is
\[ \langle x | y \rangle (r) = \int d^3 p x(r, p) y(r, p), \]
the local densities of the physical properties are \(r\)-dependent functionals \(a(r)\gamma(r, p)\) with associated underlying field \(\tilde{a}(r, p, \gamma(r, p))\) such that, for each fixed \(r\), \(\gamma(r, p)\) \(\tilde{a}(r, p, \gamma(r, p))\) belongs to \(\mathcal{H}_{SEA}\). As a result, the local density functionals are
\[ a(r)\gamma(r, p) = \int d^3 p \gamma(r, p)^2 \tilde{a}(r, p, \gamma(r, p)) = (\gamma|\gamma) = a(r) \quad \text{with} \quad |\tilde{a}(r)| < \infty. \]

The functional derivative has again the usual definition analogous to Eq. (7), but on \(\mathcal{H}_{SEA}\),
\[ \left( \frac{\delta a}{\delta \gamma} \bigg|_{\gamma_0} \right)(y) = da_{\gamma_0}(y) \quad (\gamma_0, y \in \mathcal{H}_{SEA}). \]
Clearly,
\[ \langle A, B \rangle = \int d^3 r \left( a|b \right)(r). \]

For the SEA formulation the local properties which generate the dynamical equation are the local density and flux fields defined as follows
\[ s(r)\gamma(r, p) = -k_B \int d^3 p \gamma(r, p)^2 \ln \frac{\gamma(r, p)^2}{b} = s(r), \]
\[ c^i(r)\gamma(r, p) = \int d^3 p \psi^i(r, p) \gamma(r, p)^2 = c^i(r), \]
\[ J_{C^i}(r)\gamma(r, p) = \int d^3 p \psi^i(r, p) \gamma(r, p)^2 = J_{C^i}(r). \]

The expressions for the functional derivatives are
\[ \frac{\delta s}{\delta \gamma} \bigg|_{\gamma(r, p)} = -2k_B\gamma(r, p) \left[ \ln \frac{\gamma(r, p)^2}{b} + 1 \right] = (68) \]
\[ \frac{\delta c^i}{\delta \gamma} \bigg|_{\gamma(r, p)} = 2\gamma(r, p) \psi^i(r, p). \]

We note that the rhs of Eqs. (68) and (69) are identical, and the same for Eqs. (68) and (69).

Here, the functionals
\[ c^i c^j\gamma(r, p) = \frac{1}{4} \left( \frac{\delta c^i}{\delta \gamma} \bigg|_{\gamma(r, p)} \gamma(r, p) \right) \left( \frac{\delta c^j}{\delta \gamma} \bigg|_{\gamma(r, p)} \gamma(r, p) \right) = c^i c^j(r) \]
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
\[ \dot{\alpha}(t) = X^{H,SEA}_{\alpha(t)} + Y^{S,SEA}_{\alpha(t)} \]
where we recall that \(\alpha(t) = \gamma(r, p; t)\), the transport vector field
\[ X^{H,SEA}_{\alpha(t)} = - \frac{P}{m} \frac{\partial \gamma(r, p; t)}{\partial r} + \frac{\partial \phi(r)}{\partial r} \cdot \frac{\partial f(r, p; t)}{\partial p} \]
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,

\[ Y_{\alpha(t)}^{S,SEA} = g_\alpha^{\gamma} \left( \frac{\delta S}{\delta \gamma} |_{\alpha(t)} - \sum_j \beta_{\alpha(t)}^j \frac{\delta c_j}{\delta \gamma} |_{\alpha(t)} \right). \] (72)

The values of the (Lagrange multipliers) \( \beta^j \)'s are found by solving the following system of five algebraic equations,

\[ \sum_{j=0}^{4} g_{\alpha(t)} \left( g_{\alpha(t)}^{\gamma} \frac{\delta c^i}{\delta \gamma} |_{\alpha(t)} , g_{\alpha(t)}^{\gamma} \frac{\delta c^j}{\delta \gamma} |_{\alpha(t)} \right) \beta_{\alpha(t)}^j = g_{\alpha(t)} \left( g_{\alpha(t)}^{\gamma} \frac{\delta c^i}{\delta \gamma} |_{\alpha(t)} , g_{\alpha(t)}^{\gamma} \frac{\delta s}{\delta \gamma} |_{\alpha(t)} \right) \] \( i \in [0, 4] \) . (73)

which can be written in the equivalent form of Eq. (16),

\[ \sum_{j=0}^{4} g_{\alpha(t)} \left( \text{grad } c^i |_{\alpha(t)} , \text{grad } c^j |_{\alpha(t)} \right) \beta_{\alpha(t)}^j = g_{\alpha(t)} \left( \text{grad } c^i |_{\alpha(t)} , \text{grad } s |_{\alpha(t)} \right) \] \( i \in [0, 4] \) . (74)

In contrast to the GENERIC, which imposes restricting conditions on the friction operator \( D^2 \), the SEA method is that it does not assume \textit{a priori} any form for the metric tensor \( g \). So, without a particular choice of \( g \) the gradients remain unspecified. The subsequent effort in the SEA philosophy, is to find a metric tensor that models correctly and efficiently the collision integral of the Boltzmann Equation in the best way, so as to extend the validity of the traditional Kinetic Models, such as BGK, ES-BGK, etc. from the near-equilibrium to the far non-equilibrium domain. The problem of identifying criteria to that choice is still open. Recent numerical results \(^{[30]}\) 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 non-equilibrium 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 provides hints to find a suitable metric for this purpose.

On the other hand, the metric tensor \( g \) 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 \( \dot{M}^{\text{GENERIC}} \) defined by Eqs. \( [60] \) and \( [64] \), which corresponds to the full Boltzmann collision integral. In fact, in the next section we prove that given a GENERIC friction operator \( \dot{M} \), the metric tensor \( g \) identified by Eq. \( [106] \) yields the equivalent SEA formulation. In particular, such \( g \) is given by the uniform metric inside the kernel \( \text{ker}(\dot{M}) \) of the GENERIC friction operator, while inside the orthogonal component \( \text{ker}(\dot{M})^\perp \) it is proportional through a scaling time constant \( \tau \) to the inverse of \( \dot{M} \) (more precisely, of its restriction to \( \text{ker}(\dot{M})^\perp \)). The challenge of deriving the explicit expression of such metric tensor \( g \) is left for future work.

\section{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 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. \([13]\). To show such broader validity, below we state the result with explicit reference to the Kinetic Theory framework but by using a more compact notation which points directly to the notation introduced in \([13]\) in order to unify several different non-equilibrium 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 \( \gamma(r,p) \) to denote the states in GENERIC and SEA, even though in SEA the position \( r \) is a fixed parameter also for the local functionals. What is important, though, is that proper functional derivatives in the two frameworks end up being identical functions of \( r \) and \( p \). Therefore, we denote them by the same symbol. We write the functional derivative of entropy as

\[ \delta S \big|_{\gamma(r,p)} = \delta S \bigg|_{\gamma(r,p)} , \] (75)

collect the conserved quantities in the vectors

\[ \mathbf{c} = \{ c^3 \} , \quad \mathbf{C} = \{ C^3 \} , \] (76)

and write their functional derivatives as

\[ \Psi = \frac{\delta c}{\delta \gamma} \bigg|_{\gamma(r,p)} = \frac{\delta C}{\delta \gamma} \bigg|_{\gamma(r,p)} . \] (77)

We use the GENERIC friction operator \( \dot{M} \) (dropping the apex ‘GENERIC’), which acts on a vector \( b \) according to Eq. \( [60] \):

\[ \dot{M} : \dot{M}(b) = D^2_b(b^*) \] (78)

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
\[ \hat{G} : \hat{G}|b\rangle = g_h^b|b\rangle, \quad (79) \]
\[ \hat{L} : \hat{L}|b\rangle = \frac{1}{\tau^{\gamma}} \hat{G}^{-1}|b\rangle = \frac{1}{\tau^{\gamma}} g_h^b(b^*), \quad (80) \]
\[ (a|\hat{G}|b\rangle = (a, g_h^b(b)), \quad (81) \]
\[ (a|\hat{L}|b\rangle = g_a(a, b), \quad (82) \]

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:
\[ |\Pi_\gamma\rangle = Y_\alpha^{S(t)}, \quad (83) \]
\[ \beta = \{ \beta^j_{\alpha(t)} \}, \quad (84) \]
\[ |\beta \cdot \Psi\rangle = \sum_j \beta^j_{\alpha(t)} \delta_c |\delta^{(r,p)}\rangle, \quad (85) \]

Within the GENERIC framework, \(|\Pi_\gamma\rangle\) takes the form
\[ |\Pi_\gamma\rangle = \hat{M}|\Phi\rangle, \quad (86) \]
subject to the conditions
\[ \hat{M}(|\Psi\rangle) = 0, \quad \hat{M} \geq 0 \quad \text{and} \quad \hat{M} \text{ symmetric}, \quad (87) \]
whereas within the SEA framework it takes the form
\[ |\Pi_\gamma\rangle = \hat{L}|\Phi - \beta \cdot \Psi\rangle, \quad (88) \]
subject to the conditions
\[ \hat{L} > 0 \quad \text{and symmetric}, \quad (89) \]
and \(\beta\) given by the solution of the system of equations
\[ (\Psi|\hat{L}|\Psi\rangle \cdot \beta = (\Psi|\hat{L}|\Phi\rangle), \quad (90) \]
that is,
\[ \beta = (\Psi|\hat{L}|\Psi\rangle^{-1} \cdot (\Psi|\hat{L}|\Phi\rangle, \quad (91) \]
where, of course, \((\Psi|\hat{L}|\Psi\rangle^{-1}\) denotes the inverse of matrix \((\Psi|\hat{L}|\Psi\rangle\), and \((\Psi|\hat{L}|\Psi)\) is a shorthand to indicate the matrix \([(|\Psi|\hat{L}|\Psi\rangle)]\), i.e., we have the identity
\[ (\Psi|\hat{L}|\Psi\rangle^{-1} \cdot (\Psi|\hat{L}|\Psi) = I, \quad (92) \]
which, again, is a shorthand for \(\sum_{kl} (|\Psi|\hat{L}|\Psi\rangle^{-1})_{kl} (\Psi^k|\hat{L}|\Psi^l) = \delta_{ij}\).

Now, to prove that every SEA model admits a GENERIC form, we note that we can rewrite Eq. (86) as
\[ |\Pi_\gamma\rangle = \hat{L}|\Phi\rangle - \hat{L}|\Psi\rangle \cdot (\Psi|\hat{L}|\Psi\rangle^{-1} \cdot (\Psi|\hat{L}|\Phi\rangle, \quad (93) \]
which takes the form of Eq. (83) if we define the operator
\[ \hat{M} = \hat{L} - \hat{L}|\Psi\rangle \cdot (\Psi|\hat{L}|\Psi\rangle^{-1} \cdot (\Psi|\hat{L}. \quad (94) \]

Before we conclude that the matrix \(\hat{M}\) defined by Eq. (92) provides the GENERIC form (84) of the SEA dynamical equation (86), we must show that \(\hat{M}\) satisfies the requirements stated in Eq. (85). In fact, the first condition is a readily verified consequence of Eq. (90),
\[ \hat{M}(|\Psi\rangle) = \hat{L}(|\Psi\rangle) - \hat{L}(|\Psi\rangle) \cdot (\Psi|\hat{L}|\Psi\rangle^{-1} \cdot (\Psi|\hat{L}|\Psi\rangle = \hat{L}(|\Psi\rangle) - \hat{L}(|\Psi\rangle) = 0, \quad (95) \]
the third condition is a direct consequence of the symmetry of \(\hat{L}\), while the second condition requires that we prove that \(\hat{M}\) is positive semi-definite. This follows from the fact that \(\hat{L}\) is positive definite, together with the following two observations:

- Consider the two operators
  \[ \hat{P}_1 = \hat{L}^{-1} \hat{M} \quad (96) \]
  and
  \[ \hat{P}_2 = |\Psi\rangle \cdot (\Psi|\hat{L}|\Psi\rangle^{-1} \cdot (\Psi|\hat{L}. \quad (97) \]
  It may be easily verified that Eq. (90) implies that \(\hat{P}_2\) is idempotent, that is, \(\hat{P}_2^2 = \hat{P}_2\). By applying on the left of Eq. (92) the operator \(\hat{L}^{-1}\) we obtain \(\hat{P}_1 = \hat{I} - \hat{P}_2\) and from this follows that also \(\hat{P}_1\) is idempotent and that \(\hat{P}_1 \hat{P}_2 = 0\). Hence, the two projection operators provide the following orthogonal resolution of the identity operator
  \[ \hat{I} = \hat{P}_1 + \hat{P}_2 \quad (98) \]
  meaning that for any vector \(|b\rangle\) in the domains of \(\hat{M}\), \(\hat{L}\), and \(\hat{L}^{-1}\) we can write the decomposition
  \[ |b\rangle = |b_1\rangle + |b_2\rangle \quad \text{where} \quad |b_1\rangle = \hat{P}_1|b\rangle, \quad |b_2\rangle = \hat{P}_2|b\rangle, \quad (99) \]
  and we note in passing that the decomposition is orthogonal in the sense that relation \(\hat{P}_1 \hat{P}_2 = 0\) implies that \(|b_1|b_2\rangle = 0\).

- Applying operator \(\hat{L}\) on the left of the identity \(\hat{P}_2^2 = \hat{P}_2\) and using the definition (94) of \(\hat{P}_1\) we obtain the relation
  \[ \hat{M} = \hat{M} \hat{L}^{-1} \hat{M} = \hat{M} \hat{P}_1 \quad (100) \]
  therefore, Eq. (96) implies that
  \[ \hat{M} \hat{P}_2 = \hat{M} (\hat{I} - \hat{P}_1) = \hat{M} - \hat{M} \hat{P}_1 = 0. \quad (101) \]
Moreover, applying operator \(\hat{L}\) on the left of Eq. (94) we obtain
\[ \hat{M} = \hat{L} \hat{P}_1. \quad (102) \]
As a result of Eq. (102) we see that operator \(\hat{P}_2\) projects any vector \(|b\rangle\) onto the kernel of \(\hat{M}\), i.e., component \(|b_2\rangle\)
of the decomposition \( \hat{M} \) is in \( \ker(\hat{M}) \). Comparing Eqs. (98) and (100) we see that operator \( \hat{P}_i \) projects any vector \( |b\rangle \) onto a subspace (orthogonal to the kernel of \( \hat{M} \)) in which for any vector \( |b_1\rangle \) we have the identity

\[
\hat{M}|b_1\rangle = \hat{M}\hat{P}_i|b\rangle = \hat{L}|b_1\rangle . \tag{101}
\]

This proves that when restricted to this subspace operators \( \hat{M} \) and \( \hat{L} \) coincide and, since \( \hat{L} \) is positive definite, also this restriction of \( \hat{M} \) is positive definite, i.e., \( (b_1|\hat{M}|b_1) > 0 \) except for \( |b_1\rangle = 0 \).

These two observations finally put us in a position to prove that \( \hat{M} \) is positive semi-definite. In fact, for any vector \( |b\rangle \), using the decomposition (97) and Eq. (99), which implies that \( \hat{M}|b_2\rangle = 0 \), we have \( (b|\hat{M}|b) = (b_1 + b_2|\hat{M}|b_1 + b_2) = (b_1|\hat{M}|b_1) \geq 0 \) with the equal sign holding when \( |b_1\rangle = 0 \), i.e., when \( |b\rangle \) lies in the kernel of \( \hat{M} \).

This concludes the proof that any SEA formulation can always be put into GENERIC form. Therefore, all the frameworks discussed in [13], once put into SEA form by choosing the suitable metric \( G \) and the dissipative time \( \tau \), can also be put into GENERIC form by using \( \hat{M} \) given by Eq. (92) with \( \hat{L} = G^{-1}/\tau \). In other words, for any operator \( \hat{L} \), the operator \( \hat{M} \) given in Eq. (92) makes the rhs of Eq. (84) becomes identical to the rhs of Eq. (86), i.e.,

\[
\hat{M}|\Psi\rangle = \hat{L}|\Psi\rangle - \hat{L}|\Psi\rangle \cdot (\langle \Psi|\hat{L}|\Psi\rangle)^{-1} \cdot (\langle \Psi|\hat{L}|\Psi\rangle) = \hat{L}|\Psi\rangle - \hat{L}|\Psi\rangle \cdot \beta . \tag{102}
\]

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

\[
\ker(\hat{M}) = \text{span}(\Psi), \tag{103}
\]

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

\[
\hat{P}_{\ker(\hat{M})} = \hat{P}_{\text{span}(\Psi)} , \tag{104}
\]

where \( \hat{P}_{\ker(\hat{M})} \) denotes the projection operator onto the kernel of operator \( \hat{M} \) and \( \hat{P}_{\text{span}(\Psi)} \) denotes the projection operator onto the linear span of the set of vectors \( \langle \Psi| \).

The projection operator \( \hat{P}_{\text{span}(\Psi)} \) is given by

\[
\hat{P}_{\text{span}(\Psi)} = |\Psi\rangle \cdot (\langle \Psi|\Psi\rangle)^{-1} \cdot (\langle \Psi| , \tag{105}
\]

where \((\langle \Psi|\Psi\rangle)^{-1}\) denotes the inverse of matrix \((\langle \Psi|\Psi\rangle)\), and \((\langle \Psi|\Psi\rangle)^{-1}\) is a shorthand to indicate the matrix \([\langle \Psi|\Psi\rangle][, i.e., Eq. (105) is a shorthand for \( \hat{P}_{\text{span}(\Psi)} = \sum_i \sum_j \langle \Psi_i|[(\langle \Psi|\Psi\rangle)^{-1}]_{ij}|\Psi_j\rangle \].

In the framework of the Boltzmann equation, it is well known [54, 55] that the kernel of the collision integral coincides with the linear span of the five collision invariants \( \psi_0 = 1, \psi_1 = p_x, \psi_2 = p_y, \psi_3 = p_z, \psi_4 = p \cdot p / 2m + \phi(r) \), i.e., there exist no other linearly independent collision invariants. Since the friction operator given by Eq. (60) and Eq. (61) has been proven to be exactly equivalent to the full Boltzmann collision integral, by applying it to the functional derivatives in Eq. (53), it is easy to verify that the well known result implies that Eq. (104) holds for \( \hat{M} \).

In other frameworks, condition (104) appears as a reasonable additional condition in every GENERIC construction, for otherwise the structure would admit more distinguished functionals of the dissipative structure than the actual conserved properties, i.e., in other words there would be some sort of hidden additional constants of the motion.

To proceed with the proof, we look for a solution of Eq. (92) for the unknown \( \hat{L} \) given any \( \hat{M} \) satisfying the conditions in Eq. (85).

To this end, let us consider the operator

\[
\hat{L} = \hat{P}_{\ker(\hat{M})} + \hat{M} . \tag{106}
\]

This operator may be shown to be a solution of Eq. (92) by using Eq. (104) and Eq. (105). The operator in Eq. (106) corresponds to a uniform (Fisher-Rao) metric in the kernel \( \hat{M} \) and the metric given by \( \hat{M} \) in \( \ker(\hat{M})^\perp \).

In order to identify the metric which makes the Boltzmann Equation fit exactly into the SEA form, we would need to identify \( \ker(\hat{M}_G^{\text{GENERIC}}) \) with \( \hat{M}_G^{\text{GENERIC}} \) given by Eq. (61).

Even without knowing the explicit expression of \( \hat{P}_{\ker(\hat{M}_G^{\text{GENERIC}})} \), we can easily verify that for any operator \( \hat{M} \) satisfying the conditions (85), the operator \( \hat{L} \) given in Eq. (106) makes the rhs of Eq. (86) becomes identical to the rhs of Eq. (84), which is the thesis we would like to prove. In fact, it suffices to observe the following:

- The degeneracy requirements \( \hat{M}(\Psi) = 0 \) (e.g., Eqs. (64) satisfied by operator \( \hat{M} \) in the kinetic theory framework), implies that every component of vector \( |\Psi\rangle \) is in the kernel of \( \hat{M} \), therefore,

\[
\hat{P}_{\ker(\hat{M})}|\Psi\rangle = |\Psi\rangle . \tag{107}
\]

- The geometrical formalism of the SEA construction can be used to define explicitly the projection of vector \( |\Psi\rangle \) onto the linear span of vectors \( |\Psi\rangle \). Using the definition in Eq. (105), we have that

\[
\hat{P}_{\text{span}(\Psi)}|\Phi\rangle = |\Psi\rangle \cdot (\langle \Psi|\Psi\rangle)^{-1} \cdot (\langle \Psi|\Phi\rangle = |\Psi\rangle \cdot \beta' , \tag{108}
\]
where the last equality holds for the multipliers $\beta'$ given by the solution of the system of equations
\[
(\Psi | \Psi) \cdot \beta' = (\Phi | \Psi).
\]  
(109)

As a result, starting from (108), by virtue of condition (104), we can write
\[
\hat{P}_{\ker(M)} | \Phi \rangle = | \Psi \rangle \cdot \beta'
\]  
(110)
\[
\hat{P}_{\ker(M)} | \Phi - \beta \cdot \Psi \rangle = | \Psi \rangle \cdot (\beta' - \beta)
\]  
(111)
\[
\hat{M} | \Phi - \beta \cdot \Psi \rangle = \hat{M} | \Phi \rangle.
\]  
(112)

For $\hat{L}$ given by Eq. (106), we have the following relations
\[
(\Psi | \hat{L} | \Psi) = (\Psi | \hat{P}_{\ker(M)} + \hat{M} | \Psi)
\]  
(113)
\[
(\Phi | \hat{L} | \Psi) = (\Phi | \hat{P}_{\ker(M)} + \hat{M} | \Psi)
\]  
(114)
so that Eqs. (109) and (88) become identical and so do the Lagrange multipliers, i.e., $\beta' = \beta$. As a result Eq. (111) yields
\[
\hat{P}_{\ker(M)} | \Phi - \beta \cdot \Psi \rangle = 0
\]  
(115)

so that we finally have
\[
\hat{L} | \Phi - \beta \cdot \Psi \rangle = \left[ \hat{P}_{\ker(M)} + \hat{M} \right] | \Phi - \beta \cdot \Psi \rangle = \hat{M} | \Phi \rangle.
\]  
(116)
This concludes the proof that we can construct the SEA form of any given GENERIC model provided it admits an inner product.

VI. CONCLUSIONS

The main objective of the present paper is the comparison between the Steepest Entropy Ascent (SEA) dynamical model, initially proposed by Beretta in a quantum thermodynamics framework and recently adapted to meso- and macroscopic systems, and the GENERIC (General Equation for Non-Equilibrium Reversible-Irreversible Coupling) formalism, developed by Gümüsa 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.

We show that the two non-equilibrium 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 irreversible component of the time evolution of the state of a thermodynamic system is determined by the entropy gradient. In the SEA model it is in the direction of the projection of the entropy gradient onto the submanifold orthogonal to the gradients of the conserved properties. 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 section IIB).

Both structures have been motivated by the search for Non-Equilibrium Thermodynamics formulations that are fully compatible with the Second Law of Thermodynamics. However, specific differences must be pointed out:

- GENERIC tackles with equal emphasis both the reversible and the irreversible components of the dynamics, while SEA focuses only on the irreversible component;
- the SEA construction assumes the existence of a non-degenerate Riemannian metric tensor that regulates the dissipative component of the evolution equation, while the GENERIC construction sets a more structured geometrical environment, by assuming a Poisson structure to describe the reversible part of the dynamics and a degenerate co-Riemannian structure to describe the irreversible part;
- as SEA dynamics is set in a less-structured manifold, the constraints related to the conservation laws are imposed by forcing the term in the evolution equation that is responsible for the production terms in the balance equations to be locally orthogonal to the gradients of the conserved properties, while in the GENERIC formalism, the conservation laws are already embedded in the degeneracy of the two assumed geometric structures;
- related to the last point is the fact that GENERIC imposes restricting conditions on the friction operator $D^2$, while the SEA method requires no a priori assumption about the form of the metric tensor $g$;
- in GENERIC, the conserved quantities of the process are set once the reversible and irreversible structures have been given, while in SEA the conserved quantities must be known in order to build the dynamics;
- in SEA dynamics, the choice of a non-degenerate metric allows 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;
- 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 aims at finding an easier metric to model the collision integral in order to create efficient Kinetic Models capable of extending to the highly non-equilibrium 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:

- the reversible-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;
- the idea of imposing that the dissipative bracket in GENERIC satisfies the Leibniz identity in order to have a non-degenerate metric on the metric leaves, could be tested in practical instances by a symbolic algorithm as done for the Jacobi identity in [56];
- as far as open systems are concerned, a parallel could be undertaken between the approach used in [13] and the mathematical framework of Dirac structures, which the authors of GENERIC claim to play a role in this kind of modeling [16].

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We do not enter here into the details of the nonetheless important question of what is the operative definition of thermodynamics entropy and what specific functional represents it in a given level of description. [25–30]

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Generalizations of this point have been proposed especially in the context of contact manifolds [4, 36].

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More precisely, symplectic leaves are the equivalence classes of points that can be matched by a piecewise smooth curve, each element of which is a trajectory of a locally defined Hamiltonian vector field [5].

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