Modeling reparametrizations in thermodynamic phase space

V. Pineda-Reyes,1 L. F. Escamilla-Herrera,1,∗ C. Gruber,2,3,† Francisco Nettel,4,‡ and H. Quevedo1,5,6,¶

1Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, Mexico City 04510, México.
2Hanse-Wissenschaftskolleg Delmenhorst, Germany
3Institut für Physik, Universität Oldenburg, D-26111 Oldenburg, Germany
4Departamento de Física, Fac. de Ciencias
Universidad Nacional Autónoma de México,
A. P. 50-542, México D.F. 04510, México
5Dipartimento di Fisica and ICRA,
Università di Roma “La Sapienza”, I-00185 Roma, Italy
6Institute of Experimental and Theoretical Physics,
Al-Farabi Kazakh National University, Almaty, Kazakhstan

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Abstract

We investigate the consequences of reparametrizations in the geometric description of thermodynamics analyzing the effects on the thermodynamic phase space. It is known that the contact and Riemannian structures of the thermodynamic phase space are related to thermodynamic equilibrium and statistical fluctuations in the Boltzmann-Gibbs statistical mechanics. The physical motivation for this analysis rests upon the possibility of having, instead of a direct control of the intensive parameters determining the state of the corresponding physical reservoirs, the control of a set of differentiable functions of the original variables. Likewise, we consider a set of differentiable functions of the extensive variables accounting for the possibility of not having direct access to the original variables. We find that different geometric structures in the thermodynamic phase space can be used to describe its contact and Riemannian structures, while preserving the metric structure on the thermodynamic space of equilibrium states, if we restrict ourselves to a particular set of reparametrizations. We also single out a rank-two tensor that geometrically comprises the information about such reparametrizations in the thermodynamic phase space.

∗viridiana.pineda@correo.nucleares.unam.mx
†lenin.escamilla@correo.nucleares.unam.mx
‡christine.gruber@uni-oldenburg.de
¶fnettel@ciencias.unam.mx
§fnettel@ciencias.unam.mx
¶quevedo@nucleares.unam.mx
I. INTRODUCTION

The use of a geometric language in thermodynamics started with the works of Gibbs [1] and Caratheodory [2], introducing the notion of the thermodynamic space of equilibrium states, or thermodynamic equilibrium space (TES), as a (hyper-)surface determined by a fundamental relation and the first law as a Pfaffian differential equation whose solutions form the TES. It was Hermann who first introduced the concept of a thermodynamic phase space (TPS) as a \((2n + 1)\)-dimensional manifold equipped with a contact structure, whose maximally integrable submanifolds constitute the TES [3]. A different approach to thermodynamic geometry using Riemannian geometry was later proposed by Weinhold [4] and Ruppeiner [5, 6]. In these two approaches a metric is defined on TES. In the Weinhold geometry, the components of the metric are given by the Hessian of the internal energy, while in Ruppeiner’s case by the negative Hessian of the entropy; later, in Ref. [7] it was shown that these two metrics are related by a conformal factor and in [8] the same result is established in terms of a conformal gauge transformation in the TPS. In the two decades following the proposal of these two formalisms there was a significant number of works devoted to the physical implications of these Riemannian structures in thermodynamics, where the physical significance of the thermodynamic length associated to these two metrics was studied, as well as the relation to thermodynamic fluctuations and the link between the thermodynamic curvature, stability and phase transitions, among other related topics [5, 7, 9–13]. Ref. [6] contains an extensive account of the different results concerning thermodynamic geometry, as well as a comprehensive collection of bibliographic references up to the date of its publication. More recently, there has also been established a parallelism between statistical inference theory, statistical mechanics and their geometric descriptions [14–17].

In [18] a statistical approach to thermodynamic geometry was explored by the construction of a contact Riemannian manifold associated to a family of exponential probability distributions. Inspired by Jaynes’ perspective on the interpretation of statistical mechanics as a theory of maximum entropy inference, that work establishes that the contact structure determines the thermodynamic equilibrium and that the metric structure is related to statistical fluctuations. Further explorations on the contact geometry of thermodynamics have followed [8, 19–26].

In the TPS, Legendre transformations are described as a set of strict contactomorphisms, that is, transformations which leave the Gibbs fundamental (contact) one-form invariant, thus expressing in geometrical language the invariant description of thermodynamics under this set of transformations. This idea served as a motivation for the formulation of Geometrothermodynamics (GTD), whose basic premise is that the geometric description of thermodynamics must also be invariant under Legendre transformations. Consequently, the metric in the TES should be invariant under this set of transformations. Legendre transformations are naturally defined on the TPS, therefore in the GTD formalism the metric on the TPS must be invariant, in this way guaranteeing an invariant metric on the TES, as these latter metrics inherit the Legendre invariant property of the metric in the TPS [27–30].

A geometric theory of thermodynamics in the TES in terms of a Riemannian structure naturally entails the idea of an invariant description under reparametrizations of the intensive and/or extensive variables used to describe the system. In this work, we are interested in analyzing the effects that such reparametrizations have on the TPS from a geometric point of view. To this end, we consider here reparametrizations as determined by mappings that are at least \(C^2\) functions of their corresponding parameters. The physical motivation for
considering this kind of situation arises from the possibility of sometimes not being able to control the intensive variables of a thermodynamic system in contact to some reservoirs, or not having a direct access to the extensive variables by means of measurements, but only through some general functions of the original variables instead.

As a result of these investigations we find that different contact and Riemannian structures of the TPS can be considered to account for the reparametrization, while the Riemannian structure of the TES remains unaltered. That is, for each different parametrization, the TES, as a Riemannian manifold, can be embedded in a TPS with a different contact structure and metric. However, under the corresponding pullbacks these different geometric structures on the TPS are mapped to the same Riemannian submanifold of equilibrium states. In this sense, we have different TPS’s for the same TES, depending on the parametrization chosen for the thermodynamic variables.

The structure of the paper is as follows. In Section II, we review how the Boltzmann-Gibbs distribution is obtained using the optimized Lagrange multipliers method for maximizing the Boltzmann entropy and explore how some quantities transform under reparametrizations of the intensive variables. In Section III, we present the link between statistical fluctuations and the geometry of the TES. In Section IV, we analyze the consequences that the reparametrizations have on the contact and Riemannian structures of the TPS and show that despite having different TPS’s the Riemannian structure of the TES remains unchanged. Finally, in Section V a discussion of the results found in this work is presented.

II. STATISTICAL REPARAMETRIZATION

In this section, we analyze how the proposed reparametrization can be cast in terms of the maximum entropy principle using the optimized Lagrange multipliers (OLM) method, and how, from this starting point, the TPS and the TES are constructed. This procedure was used in the work of Mrugala et al. in [18], where a link between statistical mechanics and a geometric description of thermodynamics was established in terms of a Riemannian contact manifold. The underlying idea is the interpretation proposed by Jaynes of viewing statistical mechanics as a theory of maximum entropy inference [31], which from a mathematical point of view renders statistical inference almost indistinguishable from (subjective) statistical mechanics, allowing one to trade physical assumptions for statistical inference based on the least biased information input. This approach was retaken in [18] to establish a link between statistics and the geometric structures of thermodynamics.

Thus following [18], let us consider a (mechanical) phase space $\Gamma$ along with a set of $n$ functions $H^a : \Gamma \to \mathbb{R}$ where $a = 1, \ldots, n$. Given the set of statistical averages $\{\langle H^a \rangle\}$, the task is to find the probability distribution $\tilde{\rho} : \Gamma \to \mathbb{R}^+$ maximizing the Boltzmann entropy

$$S[\tilde{\rho}] = -\int \tilde{\rho} \ln \tilde{\rho} \, d\Gamma,$$

subject to the following set of $n + 1$ generalized constraints:

$$1 = \int \tilde{\rho} \, d\Gamma,$$

$$\tilde{E}^a(E^a) = \langle H^a \rangle = \frac{\int H^a \tilde{\rho} \, d\Gamma}{\int \tilde{\rho} \, d\Gamma}. \tag{2}$$
Here, we first consider a reparametrization of what will later be identified as the set of extensive variables $E^a$ through a set of $n$ arbitrary functions $E^a(\bar{E}^a)$. Each $E^a$ is associated to the statistical average of the corresponding functions $H^a(x) \in \Gamma$, instead of just considering the macroscopic physical quantity $E^a = \langle H^a \rangle$. For instance, in the context of statistical mechanics, rather than identifying the average of the Hamiltonian with the internal energy $U$, we consider for the average value a general function of the energy $f(U)$.

The second reparametrization is introduced via the OLM method when maximizing the entropy functional (1) subject to the set (2) of $n + 1$ constraints,

$$S[\tilde{\rho}] = - \int \tilde{\rho} \ln \tilde{\rho} \, d\Gamma - \tilde{\phi} \left[ \int \tilde{\rho} \, d\Gamma - 1 \right] + \bar{I}_a(I_a) \left[ \int H^a \tilde{\rho} \, d\Gamma - \bar{E}^a(\bar{E}^a) \right],$$

where $\tilde{\phi}$ is the Lagrange multiplier associated to the normalization condition which later we will identify as the total Massieu potential, and $\{\bar{I}_a(I_a)\} = \{\bar{I}_1(I_1), \ldots, \bar{I}_n(I_n)\}$ is a set of $n$ functions on the set of what we will identify as the intensive variables $\{I_a\}$. Given the particular reparametrization proposed, imposing the constraints varying $S[\tilde{\rho}]$ with respect to $\bar{I}_a$ or $I_a$ yields exactly the same result.

The result of the extremization process of the entropy functional presented in Eq. (3) is the reparametrized distribution given by

$$\tilde{\rho} \left( \Gamma; \tilde{\phi}, \bar{I}_1(I_1), \ldots, \bar{I}_n(I_n) \right) = \exp \left( -\tilde{\phi} + \bar{I}_a(I_a)H^a \right),$$

where a summation over $a$ in $\bar{I}_a(I_a)H^a$ is implicit. Throughout this work, we will adopt the convention that any set of repeated indices indicates a sum over all its values, unless stated otherwise. If $\bar{I}_a(I_a) = I_a$ and $\bar{E}^a(\bar{E}^a) = E^a$, the reparametrized distribution (4) reduces to the Boltzmann-Gibbs distribution in terms of the canonical intensive variables and the total Massieu potential $\tilde{\phi} = \phi$ as presented in [18, 31],

$$\rho = \exp(-\phi + I_aH^a).$$

Eq. (5) will be labeled as the canonical case. If the reparametrizations $E^a \xrightarrow{\psi_a} \bar{E}^a$ and $I_a \xrightarrow{\psi_a} \bar{I}_a$ constitute a diffeomorphism, then (4) and (5) are the same distribution (i.e. diffeomorphically equivalent), namely, the Boltzmann-Gibbs distribution $\tilde{\rho}(\Gamma; \phi, \bar{I}_a(I_a)) = \rho(\Gamma; \phi, I_a)$, where $I_a = \psi_a^{-1}(\bar{I}_a)$. Therefore, in order to have physically equivalent statistical descriptions, $\psi_a$ must be a diffeomorphism, since in any other case we will not be able to describe the complete TES through the proposed reparametrization. From now on, we will assume that the reparametrization is a diffeomorphism, and thus the distribution behaves as a scalar function $\tilde{\rho} = \rho(\bar{I})$. Similarly, $\phi(I)$ also behaves as a scalar function under the diffeomorphism and we will use the notation $\phi$ for the total Massieu potential instead of $\tilde{\phi}$ from here on.

The parameter $\phi$ can be obtained as a function of the parameters $\{\bar{I}_a\}$ by imposing the first condition in Eq. (2),

$$\phi(\bar{I}) = \ln \int \exp(\bar{I}_aH^a) \, d\Gamma \equiv \ln Z(\bar{I}),$$

where

$$Z = \int \exp(\bar{I}_aH^a) \, d\Gamma,$$
i.e., the partition function is a scalar function of the intensive parameters. For the canonical
distribution (5), the expression (6) reduces to
\[
\phi(I) = \ln \int \exp(I_a H^a) \, d\Gamma.
\]
(8)

In this case \( \bar{E}^a \) can be expressed (for each fixed value of \( a \)) as
\[
\bar{E}^a = \langle H^a \rangle_I = \frac{dI_a}{dI_a} \partial I_a \ln Z,
\]
(9)
where no sum is intended and the subindex \( \tilde{I} \) in the average indicates that it is an explicit
function of the parameters \( \{ \tilde{I}_a \} \). This last relation can be also written as
\[
\frac{\partial \phi}{\partial I_a} = \frac{dI_a}{dI_a} \langle H^a \rangle_{\tilde{I}} = \frac{dI_a}{dI_a} \bar{E}^a,
\]
(10)
establishing a relation between the conjugate variables \( E^a \) and \( I_a \). Taking a second derivative
of the above equation leads to the following matrix,
\[
\ell_{ab}(I) = \frac{\partial^2 \phi}{\partial I_a \partial I_b} = \tilde{I}_a \tilde{I}_b \left\langle (H^a - \langle H^a \rangle_{\tilde{I}})(H^b - \langle H^b \rangle_{\tilde{I}}) \right\rangle_{\tilde{I}} + \tilde{I}_a \tilde{I}_b \delta_{ab}(H^a)_{\tilde{I}}
\]
\[
= \tilde{I}_a \tilde{I}_b \left\langle \frac{\partial^2 \phi}{\partial I_a \partial I_b} \right\rangle_{\tilde{I}} + \tilde{I}_a \partial I_a \frac{\partial \phi}{\partial I_b},
\]
(11)
where \( \tilde{I}_a' \equiv d\tilde{I}_a/dI_a \). It is also possible to use the definition of the Fisher matrix [32] for \( \rho \),
\[
g_{ab}(I) = \left\langle \frac{\partial \ln \rho}{\partial I_a} \frac{\partial \ln \rho}{\partial I_b} \right\rangle_{\tilde{I}} = \text{Cov}_{\tilde{I}}(H^a, H^b)
\]
\[
= \tilde{I}_a \tilde{I}_b' \left\langle \frac{\partial \ln \rho}{\partial I_a} \frac{\partial \ln \rho}{\partial I_b} \right\rangle_{\tilde{I}} = \tilde{I}_a \tilde{I}_b' \text{Cov}_{\tilde{I}}(H^a, H^b),
\]
(12)
where the subindex in the covariance is to indicate that its elements are explicit functions
of \( \{ \tilde{I}_a \} \). Note that the matrices (11) and (12) are related as
\[
\ell_{ab} = g_{ab} + \tilde{I}_a'' \delta_{ab}(H^a)_{\tilde{I}}. 
\]
(13)
If the reparametrization is a linear function, and in particular for the canonical case \( \tilde{I}_a = I_a \),
these two matrices coincide (c.f. equations (4) and (6) in Ref. [17] where the covariance
matrix for \( \rho \) is identical to the Fisher information matrix). This last equation resembles Eq.
(11) in [33] which relates the Fisher information to the negative second derivative of the free
entropy when the energy is not a linear function of the control parameter.

III. THE GEOMETRY OF FLUCTUATIONS

In the preceding section, a maximum entropy principle was considered to find a probabilistic
distribution; in that case, the relevant quantity from a physical and statistical mechanical
point of view was the Boltzmann entropy given by Eq. (1). The functional $S$ can be understood as the average with respect to the corresponding distribution of the microscopic entropy,

$$s = -\ln \rho,$$

which implies

$$S = \langle s \rangle = -\int \rho \ln \rho \, d\Gamma.$$  

If the normalization constraint is not imposed on the distribution, the microscopic entropy is a function on the set of $n + 1$ parameters $\{\phi, I_a\}$, i.e., $s = s(\Gamma; \phi, I_a)$. In the canonical case,

$$s = \phi - I_a H^a(\Gamma).$$

Considering the reparametrization, we will denote the generalized microscopic entropy as $\tilde{s}$,

$$\tilde{s} = \phi - \tilde{I}_a H^a(\Gamma).$$

If we consider $\tilde{s}$ as a function on the $(n + 1)$-dimensional space, its differential is given by

$$d\tilde{s} = d\phi - H^a \tilde{I}_a' \, dI_a.$$  

We are interested in the average and the variance of the differential $d\tilde{s}$. The average value of the differential of the generalized micro-entropy is

$$\langle d\tilde{s} \rangle_I = d\phi - \langle H^a \rangle_I \tilde{I}_a' \, dI_a,$$

while its variance $\langle (d\tilde{s} - \langle d\tilde{s} \rangle_I)^2 \rangle_I$ can be used to define a metric $g$,

$$\langle (d\tilde{s} - \langle d\tilde{s} \rangle_I)^2 \rangle_I = \tilde{I}_a' \tilde{I}_b' \langle (H^a - \langle H^a \rangle_I)(H^b - \langle H^b \rangle_I) \rangle_I \, dI_a dI_b,$$

$$g = \tilde{I}_a' \tilde{I}_b' \text{Cov}_I(H^a, H^b) \, dI_a dI_b.$$  

In the canonical setting, for the micro-entropy $s$ the results presented in [18] are recovered,

$$\langle ds \rangle = d\phi - \langle H^a \rangle_I dI_a,$$

with the variance and the metric as

$$\langle (ds - \langle ds \rangle_I)^2 \rangle_I = \langle (H^a - \langle H^a \rangle_I)(H^b - \langle H^b \rangle_I) \rangle_I \, dI_a dI_b,$$

$$g = \text{Cov}_I(H^a, H^b) \, dI_a dI_b.$$  

We recognize Eq. (22) as the variance-covariance metric for $\{H^a\}$, and from (20) we note that under the reparametrization the metric transforms accordingly. Therefore, this metric contains the information about statistical fluctuations for the Boltzmann-Gibbs distribution. This metric can be utilized to define a Riemannian manifold $(\mathcal{E}, g)$ where $\mathcal{E}$ is the TES. Additionally, it can be shown that in this coordinate system $\{I_a\}$ the components of the metric $g$ can be expressed in terms of the Hessian of the potential $\phi$,

$$g_{ab}(I) = \frac{\partial^2 \phi}{\partial I_a \partial I_b}.$$  

However, as is clear from Eq. (13), the above equation is not a covariant expression for the components of the metric, since it is written in terms of partial derivatives of a scalar function.
IV. RIEMANNIAN STRUCTURE ON THE THERMODYNAMIC PHASE SPACE

In this section we analyze the consequences of reparametrizations on the TPS, and we find a tensor field on this space which contains the information about these impacts, i.e., a scaling of thermodynamic variables.

From the set of constraints given by Eq. (2) we notice that $\langle H^a \rangle_I$ is a function of the intensive parameters $\{I_a\}$ through $\tilde{I}_a(I_a)$ and, therefore, differentiating leads to

$$\frac{\partial \langle H^a \rangle_I}{\partial I_b} = \tilde{I}_b' \text{Cov}_I(H^a, H^b),$$

with no sum over the indices. This relation allows us to write the differential of $\langle H^a \rangle_I$ as

$$d\langle H^a \rangle_I = d\tilde{E}^a = \tilde{I}_b' \langle (H^a - \langle H^a \rangle_I)(H^b - \langle H^b \rangle_I) \rangle_I dI_b.$$  \hspace{1cm} (25)

Using the above relation we can rewrite (20) as

$$\langle (d\tilde{s} - (d\tilde{s})_I) \rangle_I = \tilde{I}_a' \tilde{d} \tilde{E}^a dI_a = d\tilde{E}^a d\tilde{I}_a,$$  \hspace{1cm} (26)

while for the canonical case, where $\tilde{E}^a(E^a) = E^a$ and $\tilde{I}_a(I_a) = I_a$, we have the analogous relations

$$dE^a = \langle (H^a - \langle H^a \rangle_I)(H^b - \langle H^b \rangle_I) \rangle_I dI_b,$$  \hspace{1cm} (27)

and

$$\langle (ds - (ds)_I) \rangle_I = dE^a dI_a,$$  \hspace{1cm} (28)

which suggest that $\{\phi, E^a, I_a\}$ (or $\{\phi, \tilde{E}^a, \tilde{I}_a\}$, respectively) can be considered as a set of independent coordinates for a higher dimensional space, and the $n$-dimensional space of parameters $\{I_a\}$ (or $\{\tilde{I}_a\}$ respectively) can be understood as an embedded submanifold. Therefore, in the following we will construct a $(2n+1)$-dimensional manifold with a contact structure using $\{\phi, E^a, I_a\}$ as a set of (local) coordinates.

Before we continue, let us first briefly recall what a contact manifold is. Consider a $(2n+1)$-dimensional manifold $\mathcal{T}$. A contact structure is a maximally non-integrable distribution $D \subset T\mathcal{T}$ of $2n$-dimensional hyperplanes. Such a structure is characterized by means of the equivalence class of 1-forms $[\eta]$ such that for any representative $\eta$ the relation

$$D = \text{ker}(\eta)$$

is satisfied, and the condition of non-integrability

$$\eta \wedge (d\eta)^n \neq 0$$

is fulfilled. The equivalence class $[\eta]$ is defined by a conformal relation, that is, $\eta$ and $\eta'$ are equivalent if $\eta = \Omega \eta'$, where $\Omega$ is a non-vanishing real function. The condition means that a well-defined volume form exists on $\mathcal{T}$. Introducing a set of local coordinates $\{\phi, x^a, y_a\}$ it is possible to express $\eta$ in its canonical (Darboux) form,

$$\eta = d\phi - x^a dy_a.$$  \hspace{1cm} (31)
A transformation \( f : \mathcal{T} \to \mathcal{T} \) preserving the contact structure, \( f^*(\eta) = \Omega \eta \), is called a contact transformation. A (discrete) Legendre transformation leaves invariant the contact form, \( f^*(\eta) = \eta \), i.e., it represents a symmetry of the contact form and is defined as follows. Let \( I \cup J \) be any partition of a set of \( n \) indices into two disjoint sets \( I \) and \( J \), then a Legendre transformation on \( \mathcal{T} \) is given by the following \( 2n + 1 \) equations between the sets of coordinates \( \{ \phi, x^a, p_a \} \) and \( \{ \bar{\phi}, \bar{x}^a, \bar{y}_a \} \),

\[
\bar{\phi} = \phi - y_i x^i, \quad \bar{y}_i = -x^i, \quad \bar{y}_j = y_j, \quad \bar{x}^i = y_i, \quad \bar{x}^j = x_j , \tag{32}
\]

with \( i \in I \) and \( j \in J \). A direct calculation shows that

\[
\eta = d\phi - x^a dy_a = d\bar{\phi} - \bar{x}^a d\bar{y}_a . \tag{33}
\]

For \( J = \emptyset \), we say that \( f \) is a total Legendre transformation, otherwise we have a partial Legendre transformation.

A Legendre submanifold is a maximally integral embedded submanifold \( \mathcal{E} \subset \mathcal{T} \) whose tangent bundle is completely contained in the distribution \( D \), \( T\mathcal{E} \subset D \). A characterization in terms of local coordinates is given by the following theorem [34]. Let \( I \cup J \) be the same partition as before and consider any function \( \Phi = \Phi(x^i, y_j) \) where \( i \in I \) and \( j \in J \). The following set of \( n + 1 \) equations defines a Legendre submanifold \( \mathcal{E} \) of \( \mathcal{T} \),

\[
x^j = \frac{\partial \Phi}{\partial y_j}, \quad y_i = -\frac{\partial \Phi}{\partial x_i}, \quad \phi = \Phi + x^i \frac{\partial \Phi}{\partial x^i} . \tag{34}
\]

Conversely, any Legendre submanifold is defined locally by these equations for at least one of the \( 2^n \) partitions of the set \( I \cup J \). Such a maximally integrable submanifold is of dimension \( n \) and is determined by the condition \( \varphi^*(\eta) = 0 \), where \( \varphi : \mathcal{E} \to \mathcal{T} \) is the embedding mapping.

Finally, we can furnish the contact manifold with a Riemannian structure, defining a metric \( G \) on \( \mathcal{T} \). If \( \varphi(\mathcal{E}) \) represents the embedded Legendre submanifold in \( \mathcal{T} \), then a metric \( g = \varphi^*(G) \) is induced on the submanifold.

We can now proceed to define the TPS as a \((2n+1)\)-dimensional contact manifold \((\mathcal{T}, \tilde{\eta}, \tilde{G})\) with a contact one-form \( \tilde{\eta} \) and a Riemannian structure from which the metric \( (20) \) can be obtained as the pullback induced by the embedding map \( \tilde{\varphi} : \mathcal{E} \to \mathcal{T} \), where \( \mathcal{E} \) is the TES. Therefore, we choose to endow \( \mathcal{T} \) with the contact structure defined by Eq. (19),

\[
\tilde{\eta} = \langle d\tilde{s} \rangle_I = d\phi - \tilde{E}^a(E^a)\tilde{I}_a' dI_a . \tag{35}
\]

As we have shown above, the Legendre submanifold \( \mathcal{E} \) is determined by the condition \( \tilde{\varphi}^*(\tilde{\eta}) = 0 \), where \( \tilde{\varphi} : \mathcal{E} \to \mathcal{T} \). In terms of the coordinates \( \{ \phi, E^a, I_a \} \) this embedding is determined by the equations

\[
d\phi = \tilde{E}^a(E^a)\tilde{I}_a' dI_a , \tag{36}
\]

and

\[
\tilde{E}^a(E^a) = \frac{1}{\tilde{I}_a'} \frac{\partial \phi}{\partial I_a} . \tag{37}
\]

Regarding the definition of a metric for the contact manifold \((\mathcal{T}, \tilde{\eta})\), we note that Eq. (26) can be used to define a bilinear symmetric tensor field \( \tilde{t} \) on \( \mathcal{T} \),

\[
\tilde{t} = \tilde{I}_a' d\tilde{E}^a \otimes dI_a = \tilde{I}_a' \tilde{E}^a' dE^a \otimes dI_a . \tag{38}
\]
As such, Eq. (38) cannot be considered as a metric for \( T \) since it is a degenerate symmetric tensor field on the \((2n + 1)\)-dimensional space. However, it is possible, as done in \([18]\), to remedy this flaw by adding the tensor product of \( \tilde{\eta} \) to obtain
\[
\tilde{G} = \tilde{\eta} \otimes \tilde{\eta} + \tilde{t}.
\] (39)

This metric can also be written in terms of the local coordinates \( \{\phi, E^a, I_a\} \) as
\[
\tilde{G} = (d\phi - \tilde{E}^a \tilde{I}_a' dI_a) \otimes (d\phi - \tilde{E}^b \tilde{I}_b' dI_b) + \tilde{I}_a' \tilde{E}^a \tilde{I}_a' dI_a \\
= (d\phi - \tilde{E}^a \tilde{I}_a' dI_a) \otimes (d\phi - \tilde{E}^b \tilde{I}_b' dI_b) + \tilde{I}_a' \tilde{E}^a \tilde{I}_a' dE^a \otimes dI_a,
\] (40)

where \( \tilde{E}^a = \tilde{E}^a(E^a) \), \( \tilde{E}^a' \equiv d\tilde{E}^a/dE^a \) and \( dE^a \otimes dI_a \equiv \frac{1}{2} (dE^a \otimes dI_a + dI_a \otimes dE^a) \) denotes the symmetric tensor product.

If we set \( \tilde{E}^a(E^a) = E^a \) and \( \tilde{I}_a(I_a) = I_a \), the canonical case is recovered and the contact one-form becomes
\[
\eta = d\phi - E^a dI_a,
\] (41)

and the metric on \( T \) is
\[
G = \eta \otimes \eta + t.
\] (42)

In terms of a coordinate basis \( t \) is expressed as
\[
t = dE^a \otimes dI_a,
\] (43)

and the metric takes the form
\[
G = (d\phi - E^a dI_a) \otimes (d\phi - E^b dI_b) + dE^a \otimes dI_a.
\] (44)

The TES is determined by the embedding \( \varphi : \mathcal{E} \rightarrow \mathcal{T} \) and the condition \( \varphi^*(\eta) = 0 \), which describes geometrically the first law of thermodynamics and the equations of state expressed in terms of the total Massieu potential \( \phi \),
\[
d\phi = E^a dI_a \quad \text{and} \quad E^a = \frac{\partial \phi}{\partial I_a}.
\] (45)

The pullback \( g = \varphi^*(G) \) induced by \( \varphi \) yields the metric \((22)\) on \( \mathcal{E} \), cf. Eq. (16) in Ref. \([18]\) and Eq. (25) in Ref. \([25]\) (note that our convention differs from that of \([25]\) by a sign). From the pullback of the metric \((39)\) induced by the mapping \( \tilde{\varphi} : \mathcal{E} \rightarrow \mathcal{T} \) we obtain Eq. (20), that is, the same metric \( g \) on \( \mathcal{E} \), just written in the reparametrized variables. Indeed, using \((36)\) we obtain
\[
g = \tilde{\varphi}^*(\tilde{G}) = \left( \ell_{ab} - \tilde{I}_a' \delta_{ab}(H^a)(I) \right) dI_a \otimes dI_b \\
= \tilde{I}_a' \tilde{I}_b' \text{Cov}_{I_a}(H^a, H^b) dI_a \otimes dI_b,
\] (46)

where relation \((13)\) was considered in order to arrive at the last result.
V. CONCLUSIONS

Let us summarize the different geometric structures we have found so far in the previous section and single out some of their properties, starting with the Riemannian manifold \((\mathcal{E}, g)\) with the metric \(g\) given by (22). This is an embedded manifold in a higher-dimensional manifold possessing a contact structure and a metric \((\mathcal{T}, \eta, \mathcal{G})\). In physical terms, these correspond to the TES and the TPS, respectively. In [18] it is shown that under a total Legendre transformation the metric (44) gives rise, after the pullback, to Ruppeiner’s metric [5] on the space of equilibrium states \(\mathcal{E}\), which takes the form of the negative Hessian of the entropy with respect to the extensive variables.

We have seen that under a reparametrization \(\tilde{I}_a = \tilde{I}_a(I_a)\) we can describe the manifold \((\mathcal{E}, g)\) in terms of a different TPS \((\mathcal{T}, \tilde{\eta}, \tilde{\mathcal{G}})\). We identify this as a different TPS because the contact one-form (35) is not related to (41) via a contact transformation. Nevertheless, the thermodynamic description on \(\mathcal{E}\) is the same, since the first law (45) is recovered from the condition \(\tilde{\varphi}^*(\tilde{\eta}) = 0\), as can be verified from the embedding conditions (36) and (37). Moreover, the metric on the TES, which is related to the statistical (thermodynamic) fluctuations, is obtained as \(g = \tilde{\varphi}^*(\tilde{G})\).

Finally, it was found that the pullbacks of the two different metrics in the TPS can be expressed only in terms of the tensors (38) and (13), that is, \(g = \tilde{\varphi}^*(\tilde{t})\) and \(g = \varphi^*(t)\), respectively. In [18] it is argued that the contact structure describes the thermodynamic equilibrium, whilst the metric structure describes the thermodynamic fluctuations. As we have seen, both contact one-forms, \(\eta\) and \(\tilde{\eta}\), lead to the first law of thermodynamics on \(\mathcal{E}\) and the two tensors \(t\) and \(\tilde{t}\) give the same geometric description of the thermodynamic fluctuations on \(\mathcal{E}\) through the metric \(g\). Therefore, despite having different TPS’s via these particular reparametrizations of the intensive and extensive thermodynamic variables, the geometric structures in the thermodynamic state space remain invariant. This suggests that it is only in the TPS that there are consequences of having this particular reparametrization of the thermodynamic variables on the geometric structures. Thus, we can conclude that the tensor field \(\tilde{t}\) geometrically comprises the information in the TPS that these particular reparametrizations of the thermodynamic state variables have in the description of statistical fluctuations. It could be attempted to construct a TPS with the contact structure \(\eta\) and a metric resulting from combining the canonical one-form with the tensor field \(\tilde{t}\), and analyze the geometric information about reparametrizations inherited on the TES to single out the effects that these reparametrizations have on the description of fluctuations. These investigations will be left for future work.

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