In this work we analyze several aspects of the application of contact geometry to thermodynamics. We first investigate the role of gauge transformations and Legendre symmetries in thermodynamics, with respect to both the contact and the metric structures. Then we present a novel mathematical characterization of first order phase transitions as equilibrium processes on the thermodynamic phase space for which the Legendre symmetry is broken. Moreover, using contact Hamiltonian dynamics, we propose a formalism for thermodynamics that resembles the classical Hamiltonian formulation of conservative mechanics. We find out the general functional form for the relevant contact Hamiltonian in thermodynamics and show that it is a measure of the entropy production along thermodynamic processes. Therefore, we use such property to give a precise definition of thermodynamically admissible processes according to the Second Law of thermodynamics. Finally, we also show that we can give an equivalent formulation in terms of the Fisher-Rao metric, in analogy with the Theory of Relativity, where the metric structure defines admissible paths.
I. INTRODUCTION

Several programmes for the geometrization of equilibrium thermodynamics have been proposed so far and the literature on the subject is vast (see e.g. [1, 21]). In particular, it has been argued that there are two relevant manifolds: the thermodynamic phase space (TPS), which is endowed with a contact structure, and the manifold of equilibrium states, which is an integral (Legendre) sub-manifold of the TPS. We refer to [4, 5] and [13] for the definitions of these two manifolds and the description of the embedding between the two. Moreover, considering also thermodynamic fluctuations out of the equilibrium values, one can equip the TPS with a (pseudo-)Riemannian structure and the equilibrium manifold with the induced metric. Although most of the work so far has been focused on the investigation of the properties of the equilibrium manifold as a Riemannian sub-manifold of the TPS [6–17], it has been shown in [21] and [22] that both the contact and the metric structures on the TPS can be derived from statistical mechanics and information theory. In particular, the contact 1-form represents the first variation of the relative entropy near the Gibbs equilibrium distribution, providing us with an expression of the First Law, while the Riemannian metric, obtained from the second variation, represents thermodynamic fluctuations [22]. Furthermore, such Riemannian structure coincides with the well-known Fisher-Rao Information Metric [14, 15]. Finally, by exploring further the geometric properties of the TPS, it has been shown in [22] that it is a Sasakian and $\eta$-Einstein manifold [23, 24]. All this construction is appealing, because at this point several connections with other branches of theoretical physics become apparent. In particular, Sasakian manifolds are ubiquitous in the context of the AdS/CFT correspondence [25] and their symmetries give important informations about the dual field theory [26]. Therefore, from this point of view, it is interesting to study the mathematical symmetries of the TPS and eventually also give them a physical significance.

This work is meant to be a comprehensive presentation of several topics in the contact Riemannian description of thermodynamics. Therefore it can be divided into two parts. In the first part, Secs. III and IV we give new results on the application of contact transformations to the Sasakian structure of the TPS. In the second part, Sec. V we present the main result, that is a contact Hamiltonian formulation for ‘thermo-dynamics’. Readers interested only in the latter result in principle can skip Secs. III and IV.

In particular, in the first part we consider two types of well-known transformations of the contact metric structure of the TPS: the re-scalings of the contact 1-form by a conformal factor (or gauge transformations) and those transformations leaving the contact 1-form unchanged (or
contact symmetries). In particular, a gauge transformation is a re-scaling of the contact 1-form, but it does not preserve the corresponding Reeb vector field nor the contact splitting of the TPS. For this reason, we say that it does not induce a symmetry of the TPS. Therefore, our focus in this work is on the second type of transformations, i.e. contact symmetries, leaving the discussion about the physical interpretation of gauge transformations to future work. Here we just limit to mention that a change in the thermodynamic representation is a particular example of these transformations and we show that this particular change of the gauge induces the well-known conformal scaling between the Weinhold and the Ruppeiner metrics on the equilibrium manifolds \[27\].

By investigating contact symmetries, we present the Legendre transformations as an example of this class. We then show that the Legendre symmetry is a necessary and sufficient condition in order to reduce the thermodynamic degrees of freedom from the \(2n+1\) variables of the TPS to the \(n\) degrees of freedom of the sub-manifold of equilibrium states. However, when passing from the TPS to the equilibrium manifold representing a particular thermodynamic system, the Legendre symmetry can break. In fact, as we will show, there is not just one sub-manifold of equilibrium, but there are in principle as many as the different statistical ensembles (this was already observed in \[19, 20\]). When the Legendre symmetry is valid, the different ensembles are equivalent and the change from one ensemble to the other is interpreted geometrically simply as a diffeomorphism between the equilibrium manifolds. However, when the Legendre symmetry breaks, the ensembles are inequivalent and geometrically the map from one equilibrium sub-manifold to the other is not a diffeomorphism. In this case the full description of the system cannot be achieved by means of a single ensemble. Therefore, we need to consider the full TPS instead of just one of its equilibrium sub-manifolds. In ordinary thermodynamics this happens only at first order phase transitions. Thus we give a geometric characterization of first order phase transitions as equilibrium processes on the full thermodynamic phase space for which the Legendre symmetry is broken. This is the first result of the present work.

Notice that if one considers also fluctuations, these are different in the different ensembles. Therefore in general the Legendre symmetry need not be also an isometry between the different metric structures induced on the equilibrium sub-manifolds. However, we will show that a total Legendre transformation always induces an isometry. This is the second result of this work.

Finally, in the second part of the work we consider a contact Hamiltonian formulation for thermodynamics, generalizing the work in \[35\]. In particular, we define a precise contact Hamiltonian system on the TPS and show that it is completely integrable. It turns out that the integral curves of this system define thermodynamic processes at equilibrium or near equilibrium. Moreover, we
identify the Hamiltonian of the system with the entropy production potential along a process. With this definition and based on the Second Law of thermodynamics we give a simple characterization of thermodynamically admissible paths on the TPS and show that this equips the TPS with a cone-like structure as it is for spacetime in Relativity. Finally, we show that this construction can also be built up in a completely equivalent way starting from the Fisher-Rao metric structure on the TPS. We will conclude highlighting that in some sense this contact Hamiltonian formulation of thermodynamic processes naturally entails the Laws of thermodynamics. This is the third and main result presented in this work.

The outline of the paper is as follows. In Sec. II we will review briefly the construction of the contact metric structure in the TPS. In Sec. III we will discuss the role of gauge and Legendre transformations in the geometry of thermodynamics. In particular, we will argue that the first kind of transformations is not a symmetry of the contact bundle, while the second type is. In Sec. IV we will study in more detail the physical consequences of the Legendre symmetry of the thermodynamic phase space and show that the breaking of such symmetry for particular systems implies that there can be intersections between the equilibrium sub-manifolds and inequivalence of the ensembles. As a special case from ordinary thermodynamics, we will present the example of first order phase transitions. In Sec. V we will derive a contact Hamiltonian formulation of thermodynamics. We show that such system is a completely integrable contact Hamiltonian system and that the Hamiltonian is related with the entropy production. Moreover, we will define thermodynamically admissible processes and show that this is completely consistent with the same definitions given in terms of the metric structure. We conclude in Sec. VI with a review of our results and a discussion about possible future investigations.

II. CONTACT AND METRIC STRUCTURES IN THERMODYNAMICS

Let us consider the contact description of the thermodynamic phase space as given e.g. in [4, 5, 18]. Given a thermodynamic system with \( n \) degrees of freedom, the thermodynamic phase space (TPS) is the \((2n + 1)\)-dimensional manifold \( \mathcal{T} \), endowed with a contact structure, that is, a maximally non-integrable distribution \( \mathcal{D} \subset T\mathcal{T} \) of co-dimension one hyperplanes. We can characterize such a distribution with the aid of a 1-form \( \eta \) such that

\[
\mathcal{D} = \ker(\eta),
\]
and the non-integrability condition

\[ \eta \wedge (d\eta)^n \neq 0 \]  \hspace{1cm} (2)

is fulfilled. Equation (2) can be understood as the condition for a well defined volume form on the TPS. Additionally, it is always possible to find a set of local (Darboux) coordinates for \( \mathcal{T} \) such that the 1-form \( \eta \) can be written in the form

\[ \eta = dw - p_a dq^a, \]  \hspace{1cm} (3)

where we have used Einstein’s convention for repeated indices and \( a \) takes values from 1 to \( n \) – the number of degrees of freedom. Note that at this level \( w, q^a \) and \( p_a \) are coordinates for \( \mathcal{T} \) whose thermodynamic significance is linked to the underlying statistical mechanics \[22\].

In the present work, we focus on the contact structure of \( \mathcal{T} \). First, note that the contact 1-form \( \eta \) is not unique. Indeed, any other 1-form defining the same family of hyperplanes, equation (1), is necessarily conformally equivalent to \( \eta \), i.e. for any two 1-forms \( \eta_1 \) and \( \eta_2 \) in the same equivalence class \([\eta]\), one has \( \eta_2 = \Omega \eta_1 \) for some non-vanishing real function \( \Omega \).

In the coming Sections, we will consider the particular transformations that leave invariant the contact structure \( \mathcal{D} \). In particular, we will consider homotheties – also known as ‘gauge transformations’ – of the contact 1-form \( \eta \). We will see that a change of representation in thermodynamics corresponds to a specific choice for the conformal factor \( \Omega \). We will also consider infinitesimal symmetries of \( \eta \) and show that Legendre transformations form a particular class of such transformations.

Let us consider a contact 1-form \( \eta \) defining the contact distribution \( \mathcal{D} \). Associated to \( \eta \) there is always a global vector field \( \xi \) – the Reeb vector field – defined uniquely by the two conditions

\[ \eta(\xi) = 1 \quad \text{and} \quad d\eta(\xi) = 0. \]  \hspace{1cm} (4)

The Reeb vector field generates a natural splitting of the tangent bundle, that is

\[ T\mathcal{T} = L_\xi \oplus \mathcal{D}, \]  \hspace{1cm} (5)

where \( L_\xi \) is the vertical sub-space generated by \( \xi \). It will be convenient to work in a basis adapted to the splitting (5). Since we have already seen that the Reeb vector field generates the vertical part, it only remains to find a basis for the contact distribution. It is an easy exercise showing that the set of vectors

\[ \left\{ \frac{\partial}{\partial p_i} + p_i \frac{\partial}{\partial w} + \frac{\partial}{\partial q^i} \right\} \subset \ker (\eta) \]  \hspace{1cm} (6)
is linearly independent and generates $\mathcal{D}$. Therefore, the non-coordinate basis

$$\hat{e}_{(\alpha)} = \left\{ \xi, \hat{P}_i, \hat{Q}^i \right\} = \left\{ \xi, \frac{\partial}{\partial p_i}, p_i \frac{\partial}{\partial w} + \frac{\partial}{\partial q_i} \right\}, \quad \alpha = 1, \ldots, 2n + 1. \quad (7)$$

is naturally adapted to the splitting (5) induced by the gauge choice $\eta \in [\eta]$. Notably, the generators of such basis satisfy the commutation relations

$$[\hat{Q}^i, \hat{P}_j] = -\delta^i_j \xi, \quad [\xi, \hat{Q}^i] = 0 \quad \text{and} \quad [\xi, \hat{P}_i] = 0, \quad (8)$$

defining the Lie-algebra of the $n$th Heisenberg group, $\mathcal{H}_n$. For this reason, we call the set (7) an $\eta$-canonical basis of $\mathcal{T}\mathcal{T}$.

Analogously to the almost complex structures of symplectic manifolds, associated to each $\eta$ in the class generating the contact structure there is a $(1, 1)$ tensor field $\phi$ such that

$$L_\xi = \ker(\phi), \quad \mathcal{D} = \text{Im}(\phi) \quad \text{and} \quad \phi^2 = -\text{id}_\mathcal{T} + \eta \otimes \xi. \quad (9)$$

Thus, since $\phi(\xi) = 0$, we observe that the negative of $\phi^2$ plays the role of the projection into the horizontal space $\mathcal{D}$ and that the splitting (5) becomes

$$\mathcal{T}\mathcal{T} = \ker(\phi) \oplus \text{Im}(\phi). \quad (10)$$

The quadruple $(\mathcal{T}, \eta, \xi, \phi)$ is called an almost contact structure. In general the tensor field $\phi$ is not unique. However, if $\mathcal{T}$ is equipped with a metric tensor and there exists an almost contact structure such that

$$G(\phi X, \phi Y) = G(X, Y) - \eta(X) \eta(Y), \quad (11)$$

for any pair of vector fields $X, Y \in \mathcal{T}\mathcal{T}$ then we say that the metric $G$ is an associated metric of the almost contact structure $\phi$. Associated metrics are particularly important because they make the splitting (10) orthogonal. The structure $(\mathcal{T}, \eta, \xi, \phi, G)$ is called a contact metric manifold $\cite{24}$.

Now, considering thermodynamic fluctuation theory, the TPS is not just a contact manifold, but it also carries an almost contact structure and an associated metric. The derivation follows from information theory in the following way (c.f. $\cite{22}$ for details). Define the microscopic entropy of a distribution $\rho$ over the microscopic phase space as $s = -\ln \rho$. Let us denote by $\rho_{\text{Gibbs}}$ the Gibbs equilibrium distribution, obtained from maximizing the Shannon entropy functional subject to the $n$ independent constraints $p_a$. This allows us to construct an $(n + 1)$–dimensional control manifold embedded in $\mathcal{T}$ such that

$$\Phi^\star(\eta) = \langle ds \rangle_{\text{Gibbs}} = dw - p_i dq^i \quad (12)$$
and
\[ \Phi^*(G_{FR}) = \langle (ds)^2 \rangle_{Gibbs} = \langle ds \rangle_{Gibbs} \otimes \langle ds \rangle_{Gibbs} + dq^i \otimes dp_i, \tag{13} \]
where \( \Phi \) is the embedding of the control manifold into the TPS, \( \langle \cdot \rangle_{Gibbs} \) represents the ensemble average with respect to the equilibrium distribution \( \rho_{Gibbs} \) and \( G_{FR} \) is the metric on the TPS which reduces to the Fisher-Rao metric [3] over the control manifold. Here we have used the symbol \( \otimes \) to denote the symmetric tensor product
\[ dq^i \otimes dp_i \equiv \frac{1}{2} (dq^i \otimes dp_i + dp_i \otimes dq^i). \tag{14} \]
Thus, in the coordinate basis of \( TT \), the metric \( G_{FR} \) reads explicitly as
\[ G_{FR} = (dw - p_i dq^i) \otimes (dw - p_j dq^j) + dq^i \otimes dp_i. \tag{15} \]
The signature of \( G_{FR} \) is \((n + 1, n)\) and one can directly verify that the basis vectors \( \tilde{P}_a, \tilde{Q}_a \) for the horizontal space \( \mathcal{D} \) are all null, i.e.
\[ G_{FR}(\tilde{P}_a, \tilde{P}_a) = 0 \quad \text{and} \quad G_{FR}(\tilde{Q}^a, \tilde{Q}^a) = 0. \tag{16} \]
Thus, with respect to the dual \( \eta \)–canonical basis,
\[ \hat{\theta}^{(\alpha)} = \{ \eta, \tilde{\Pi}_i, \tilde{\Theta}^i \} = \{ dw - p_j dq^j, dp_i, dq^i \}, \quad \alpha = 1, \ldots, 2n + 1. \tag{17} \]
the metric takes the form
\[ G_{FR} = \eta \otimes \eta + \tilde{\Theta}^i \otimes \tilde{\Pi}_i, \tag{18} \]
whose matrix representation is
\[ [G_{FR}]_{ab} = \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & \delta_n \\ 0 & \delta_n & 0 \end{pmatrix}, \tag{19} \]
where \( \delta_n \) represents the \( n \)-dimensional Kronecker delta.

Note that \( \eta \) is naturally connected with the first moment of \( ds \) and hence with the First Law by means of [12], while \( G_{FR} \) is connected with the second moment of \( ds \) and hence with thermodynamic fluctuations. In fact, it turns out that the metric induced by \( G_{FR} \) into the equilibrium sub-manifolds is the Hessian of the corresponding thermodynamic potential. Therefore it coincides with the Weinhold or the Ruppeiner thermodynamic metrics or their Legendre transformed versions, depending on the representation and on the constraints that are considered [22].
The isometry group of $G_{FR}$ – $\text{Iso}(G_{FR})$ – is isomorphic to the the $(n + 1)^2$–dimensional group $GL(n, \mathbb{R}) \times \mathcal{H}_n$ generated by the $n^2$ ‘boosts’

$$\left\{ p_i q^j \xi + p_i \hat{P}_j - q^j \hat{Q}^i \right\}$$

(20)

and the $2n + 1$ ‘translations’

$$\left\{ \xi, -p_i \xi + \hat{Q}^i, q_i \xi + \hat{P}_i \right\}.$$  

(21)

We observe that the set (21) satisfies the Heisenberg algebra commutation relations whose center is the Reeb vector field, while the boosts are generators of $gl(n, \mathbb{R})$. In Figures 1 and 2 we show the orbits of the boosts and translations, respectively.

In the case when $n$ is an even number, the almost contact structure associated with $G_{FR}$ can be written as

$$\phi = \sum_{i=1}^{n} \left[ \hat{\theta}^{(2i)} \otimes \hat{e}_{(2i+1)} - \hat{\theta}^{(2i+1)} \otimes \hat{e}_{(2i)} \right].$$

(22)

For illustration purposes let us write it explicitly for the $n = 2$ case in the $\eta$–canonical basis, that is,

$$\phi = -\hat{\Theta} \otimes \hat{Q}^1 + \hat{\Theta}^1 \otimes \hat{Q}^2 - \hat{\Pi}_2 \otimes \hat{P}_1 + \hat{\Pi}_1 \otimes \hat{P}_2$$

(23)

whose matrix expression is

$$[\phi]_a^b = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & -1 & 0
\end{pmatrix}.$$  

(24)

### A. Legendre sub-manifolds

The set of coordinates $\{w, q^a, p_a\}$ has a natural thermodynamic interpretation on the integral sub-manifolds of the TPS. Of special interest are the maximal integral sub-manifolds, $\mathcal{E} \subset \mathcal{T}$, i.e. those of maximal dimension which can be embedded in $\mathcal{T}$ such that their tangent bundle is completely contained in the distribution $\mathcal{D}$. These are called Legendre sub-manifolds. One can show that these correspond to $n$-dimensional sub-manifolds defined through the embedding

$$\varphi : \mathcal{E} \longrightarrow \mathcal{T},$$

(25)
FIG. 1. Orbits of the ‘boosts’ generator \((20)\) of infinitesimal isometries mixing the \(q^i\) and \(p_i\) coordinates. The curves lie entirely on the hyper-surfaces \(w = \text{constant}\).

FIG. 2. Orbits of the ‘translations’ generators \((21)\) of infinitesimal isometries. We show the projections of the orbits on the \(w - p_i\) and \(w - q^i\) planes corresponding to the left and right panels, respectively.
\[ q^a \mapsto [w(q^a), p_b(q^a), q^a] \]  

satisfying the isotropy condition

\[ \varphi^*(\eta) = \left[ \frac{\partial}{\partial q^a} w(q^b) - p_a \right] dq^a = 0, \]  

equivalent to the First-Law of thermodynamics

\[ dw(q^b) = p_a dq^a, \quad \text{where} \quad p_a = \frac{\partial}{\partial q^a} w(q^b). \]  

Therefore, let us call \([3]\) the Gibbs 1-form and \(E\) the equilibrium manifold. On the equilibrium manifold the coordinate \(w\) can be interpreted as a thermodynamic potential depending on the variables \(q^a\), and the definition of their respective conjugate variables \(p_a\) – equation \([28]\) – corresponds to the set of equations of state.

Finally, the metric \(G_{FR}\) can be pulled back by means of \([26]\) to the Legendre sub-manifolds obtaining

\[ g = \varphi^*(G_{FR}) = \frac{\partial^2 w}{\partial q^a \partial q^b} dq^a \otimes dq^b. \]  

We observe that different choices of the embedding \([26]\) give in principle different Legendre sub-manifolds, each one equipped with its induced metric, given by the Hessian of the corresponding potential. We will analyze this aspect in more detail in \([III.B]\).

**III. CONTACT SYMMETRIES**

Transformations leaving the contact distribution unchanged determine diffeomorphisms between the sub-manifolds. Therefore, from the thermodynamic point of view, there is a large group of transformations in \(T\) that leave the equilibrium sub-manifold \(E\) unchanged, at least as long as we do not consider the induced Riemannian structure on \(E\). In this Section we study two particular examples of transformations that preserve the contact distribution, that is gauge transformations and Legendre symmetries.

**A. Gauge Transformations**

We have said that the contact distribution over a contact manifold is given by \(D = \ker(\eta)\) for some \(\eta\) in an equivalence class with respect to multiplication by a conformal factor. Therefore \(D\) is invariant with respect to a different choice of the Gibbs 1-form in the same equivalence class.
Let us consider transformations multiplying the 1-form $\eta$ by a conformal factor, i.e. homotheties of the contact 1-form. We say that a mapping $f : \mathcal{T} \to \mathcal{T}$ is a *homothety of $\eta$* if

$$f^*(\eta) = \Omega \eta$$

for some non-vanishing function $\Omega$. From the definition (30) it is clear that the contact structure $\mathcal{D}$ is preserved by any homothety. In particular, we can define a general class of diffeomorphisms that leave the contact structure $\mathcal{D}$ invariant. We say that a diffeomorphism $f : \mathcal{T} \to \mathcal{T}$ is a *contactomorphism* if

$$\mathcal{L}_X f \eta = \tau \eta,$$

(31)

where $\tau : \mathcal{T} \to \mathbb{R}$ is a non-vanishing function and $\mathcal{L}_X \eta$ is the Lie derivative of $\eta$ along the flow generated by the infinitesimal displacements corresponding to $f$. Contactomorphisms are homotheties of $\eta$ and hence preserve the contact structure $\mathcal{D}$. However, we will distinguish a peculiar class of contactomorphisms: we will say that a contactomorphism is *strict* if and only if $\mathcal{L}_X f \eta = 0$, that is, $f$ not only leaves the contact structure invariant, but also its representative 1-form. In this sense we say that a strict contactomorphism is a *symmetry of the contact form*, while a general contactomorphism can be regarded as a conformal symmetry, or an homothety. Strict contactomorphisms are also called *quantomorphisms* in recent literature on contact Riemannian geometry, c.f. [29].

Given $\mathcal{D}$, we consider now the splitting (5). This splitting is not unique, as $\xi$ depends on the particular choice of $\eta$, as we can see from Eq. (4). In particular, the first condition in (4) just implies that $\xi$ needs to be re-scaled when one changes $\eta$. More complicated is the change due to the second condition in (4), which can also change the direction of $\xi$, as we will shortly see. Therefore the splitting (5) changes in a non-trivial manner. Notice that if the 1-form $\eta$ is transformed by means of a strict contactomorphism, then the splitting of the tangent bundle remains unchanged. That is the reason why we call strict contactomorphisms symmetries of the contact bundle.

As we will show below, the almost contact structure and its associated metric structure change non-trivially with the change of the representative 1-form $\eta$ defining the contact structure.

The notion of a gauge transformation on a contact metric manifold was introduced by Sasaki [33], but it has not received much attention yet [24]. However, we report it here in order to show that the thermodynamic change of representation is a very particular case of this deformation of the contact metric structure.

Let $(\mathcal{T}, \eta, \xi, \phi, G)$ be a contact metric manifold and choose a different 1-form $\tilde{\eta}$ in the same equivalence class of $\eta$. Note that it must be $\tilde{\eta} = \Omega \eta$ where $\Omega$ is an everywhere non-vanishing
function on \( T \). Obviously the contact distribution of the two is the same, equation (1). However the Reeb vector field, the almost contact and the metric structure associated to the contact structure depend on the choice of \( \eta \). In fact, it turns out that the contact metric structure associated to \( \tilde{\eta} \) is obtained by

\[
\tilde{\xi} = \frac{1}{\Omega} (\xi + \zeta),
\]

\[
\tilde{\phi} = \phi + \frac{1}{2\Omega} \eta \otimes \left[ G^{-1}(d\Omega) - \xi(\Omega) \xi \right],
\]

\[
\tilde{G} = \Omega (G - \eta \otimes z - z \otimes \eta) + \Omega (\Omega - 1 + |\zeta|^2) \eta \otimes \eta,
\]

where

\[
\zeta = \frac{1}{2\Omega} \phi \left[ G^{-1}(d\Omega) \right] \quad \text{and} \quad z = G(\zeta).
\]

The change from \((T, \eta, \xi, \phi, G)\) to \((T, \tilde{\eta}, \tilde{\xi}, \tilde{\phi}, \tilde{G})\) is called a gauge transformation of the contact metric structure. When \( \Omega \) is constant it is called a D-homothetic deformation.

Note that if the initial manifold \((T, \eta, \xi, \phi, G)\) is a contact metric manifold (resp. a Sasakian manifold), then the new structure defined as \((T, \tilde{\eta}, \tilde{\xi}, \tilde{\phi}, \tilde{G})\) is still a contact metric manifold (resp. a Sasakian manifold). However, as we see from equations (32)-(34), even though the contact 1-form scales just by a function, the associated Reeb vector field, almost contact structure and Riemannian metric all change by non-trivial transformations.

Let us see an example which is relevant in ordinary thermodynamics. Consider the Gibbs 1-form generating the First Law of thermodynamics in the molar internal energy representation together with its associated Fisher-Rao metric, that is

\[
\eta^U = dU - T \, dS + p \, dV.
\]

and

\[
G_{\text{FR}}^U = \eta^U \otimes \eta^U + dT \otimes dS - dp \otimes dV.
\]

Notice that comparing equations (3) and (36), the coordinates \( \{w, q^1, q^2, p_1, p_2\} \) here are given by \( \{U, S, V, T, -p\} \). It is well-known that we can change to the entropy representation just by multiplying \( \eta^U \) by a conformal factor \( \Omega = -1/T \). Thus one obtains another 1-form in the same equivalence class which reads

\[
\eta^S = -\frac{1}{T} \eta^U = dS - \frac{1}{T} dU - \frac{p}{T} dV.
\]
Moreover, in this case the almost contact structure \( G_{\text{FR}} \) associated to \( G^U_{\text{FR}} \) according to (11) reads

\[
\phi^U = -\hat{\Theta}^2 \otimes \hat{Q}^1 + \hat{\Theta}^1 \otimes \hat{Q}^2 - \hat{P}^2 \otimes \hat{P}_1 + \hat{P}^1 \otimes \hat{P}_2 =
- dV \otimes \left( T \frac{\partial}{\partial U} + \frac{\partial}{\partial S} \right) + dS \otimes \left( -p \frac{\partial}{\partial U} + \frac{\partial}{\partial V} \right) + dp \otimes \frac{\partial}{\partial T} - dT \otimes \frac{\partial}{\partial p},
\]

(39)

where in the second equality we have used the canonical bases (7) and (17). Using \( \phi^U \) and \( G_{\text{FR}} \) we can compute explicitly the gauge transformation (32)-(34) with \( \Omega = -1/T \) to obtain the change in the Sasakian structure associated to the change of representation

\[
\xi^S = - \left( T \xi^U - p \frac{\partial}{\partial U} + \frac{\partial}{\partial V} \right) = -T \xi^U - \hat{Q}^2,
\]

(40)

\[
\phi^S = \phi^U - \frac{1}{T} \eta^U \otimes \left[ T \frac{\partial}{\partial U} + \frac{\partial}{\partial S} \right] = \phi^U - \frac{1}{T} \eta^U \otimes \hat{Q}^1,
\]

(41)

\[
G^S_{\text{FR}} = -\frac{1}{T} \left( G_{\text{FR}} - \frac{1}{T} \eta^U \otimes dp \right) + \frac{1}{T} \left( \frac{1}{T} + 1 \right) \eta^U \otimes \eta^U
\]

(42)

Accordingly, one obtains two different metric structures on the Legendre sub-manifold \( \mathcal{E} \). Let us call such metrics \( g^U = \varphi^*_U(G^U_{\text{FR}}) \) and \( g^S = \varphi^*_S(G^S_{\text{FR}}) \), respectively. Therefore, it is immediate to realize from (42) and (27) that the change in the metric structure from \( G^U_{\text{FR}} \) to \( G^S_{\text{FR}} \) due to the gauge transformation induces a conformal change from the metric \( g^U \) to \( g^S \) given by

\[
g^S = -\frac{1}{T} g^U.
\]

(43)

Such change is the well-known conformal relation between the Weinhold (energy) metric and (minus) the Ruppeiner (entropy) metric on the equilibrium manifold which was first presented in [27]. In the next sub-Section we will consider Legendre transformations and show that they indeed represent a symmetry of the contact bundle of the TPS, in the sense that they leave such structure unchanged.

### B. Legendre Symmetry

Let us consider now transformations leaving the Gibbs 1-form \( \eta \) invariant, i.e. symmetries of the contact 1-form. We say that a mapping \( f : \mathcal{T} \to \mathcal{T} \) is a symmetry of \( \eta \) if

\[
f^*(\eta) = \eta.
\]

(44)

As we have discussed in the preceding sub-Section, strict contactomorphisms leave the 1-form \( \eta \) invariant, therefore they are symmetries of \( \eta \). However this class is in principle larger, because it can include also transformations not generated by an infinitesimal group of diffeomorphisms.
As we have already commented, if $\eta$ is invariant, then the splitting of the contact bundle (5) is unchanged, as well as the Reeb vector field $\xi_\eta$, the almost contact structure $\phi_\eta$ and the associated metric $G$. However, this does not mean that a symmetry of the contact 1-form is also a symmetry of the metric structure, as we discuss below.

As a particular symmetry of the 1-form $\eta$ relevant in thermodynamics, let us consider Legendre transformations. A (discrete) Legendre transformation on the TPS is a change of coordinates on $\mathcal{T}$ given by the relations

$$\begin{align*}
\tilde{w}(i) &\equiv w - q(i)p(i) \\
\tilde{p}(i) &\equiv q(i) \quad \text{and} \\
\tilde{q}(i) &\equiv -p(i),
\end{align*}$$

(45)-(47)

for $i \in I \subseteq \{1, \ldots, n\}$ while leaving the rest of the coordinates unchanged, i.e. $\tilde{q}^j = q^j$ and $\tilde{p}_j = p_j$ for $j \neq i$.

The transformation (45)-(47) is called a partial Legendre transformation (PLT) since it only interchanges the pairs of thermodynamic variables in the subset $I$. The transformation that exchanges every pair of coordinates is called the total Legendre transformation (TLT).

Note that, as well as a change of representation is a (discrete) example of a gauge transformation, a Legendre transformation $f$ is a (discrete) example of a symmetry of the 1-form $\eta$. In fact, it is easy to check that $f^*(\eta) = \eta$. As such, it follows that the contact 1-form $\eta$ and its Reeb vector field $\xi_\eta$ are invariant, and hence the splitting of the tangent bundle (5) is unchanged. We argue here that the basic equilibrium thermodynamics is completely determined by such splitting. Therefore, a Legendre transformation is a symmetry of thermodynamics, as expected.

It is easy to verify that a Legendre transformation is not a symmetry of the metric structure (15). For example, a partial Legendre transformation $f_1$ – exchanging only the first pair of variables $q^1$ with $p_1$ – changes the metric (15) to

$$\tilde{G}_{FR} = f_1^*(G_{FR}) = (dw - \tilde{p}_i dq^i) \otimes (dw - \tilde{p}_i dq^i) - dq^1 \otimes d\tilde{p}_1 + \sum_{i \neq 1} dq^i \otimes d\tilde{p}_i,$$

(48)

where the second term on the right hand side has changed. This means that the metric $G_{FR}$ is not invariant under Legendre transformations. Physically, this is not at all surprising. In fact, one can interpret the metric induced by (15) onto any equilibrium sub-manifold $\mathcal{E}$ as giving a measure of the probability of fluctuations of the unconstrained thermodynamic variables of the corresponding ensemble [10]. Moreover, a Legendre transformation represents the changing from a thermodynamic ensemble to the other, thus changing the constrained variables and the fluctuating ones. Therefore,
a change of the metric structure is completely equivalent to the fact that fluctuating variables and the value of the fluctuations are different in the various ensembles \[34\]. Within this interpretation, the fact that the first law of thermodynamics (represented by the 1-form \(\eta\)) is invariant under a Legendre transformation proves that the mean values of the thermodynamic functions do not change with the ensemble. However, the situation is not the same for the values of the fluctuations of such functions, and thus for the corresponding metric structure in the geometric construction. We comment that in some formulations of the geometry of thermodynamics it has been further required that the metric structure of the TPS should be \textit{invariant} with respect to Legendre transformations (see e.g. \[13, 18\]). However, we will not consider such requirement here, as we are working with the Riemannian structure derived from Gibbs statistical mechanics as in \[21, 22\] and corresponding to thermodynamic fluctuation theory \[10\]. However, it would be worth to explore if different forms of the entropy functional in statistical mechanics (e.g. Rényi or Tsallis entropies \[31, 32\]) can lead to other types of thermodynamic metrics, in the same way as one derives the metric \[15\] directly from the Boltzmann-Gibbs entropy functional \[22\].

In the next Section we will see the physical implications of the Legendre symmetry in ordinary thermodynamics. Before doing that, we close this section by recalling that Legendre transformations in ordinary thermodynamics correspond to a redefinition of the thermodynamic potential by exchanging the role played by conjugate pairs of extensive and intensive variables. Note that in our geometric framework such role is physically relevant while working on the space of equilibrium states \(E\), whilst it is a mere change of coordinates on the phase space \(T\).

**IV. LEGENDRE SYMMETRY AND EQUIVALENCE OF THE ENSEMBLES**

As we have seen in the previous Section, a Legendre symmetry preserves the splitting of the tangent bundle of the TPS. Therefore, it induces a diffeomorphism between its Legendre submanifolds, as we show here. This is the formal cause of the well known fact that we can use the equations of state to perform a Legendre transformation, changing the thermodynamic potential and exchanging the role of the independent variables of the system. Here we show that this is always possible as long as the potential satisfies the global convexity conditions. In ordinary homogeneous thermodynamics this requirement is equivalent to say that the system is in a single phase \[34\].
A. Legendre symmetry as a diffeomorphism

Let us consider now the embedding (26) with two different choices of the thermodynamic potential $w(q^a)$ and $\tilde{w}(p_a)$, where $\tilde{w}(p_a)$ is a Legendre transform of $w(q^a)$. These different choices in principle induce two different Legendre sub-manifolds $E^w$ and $E^{\tilde{w}}$, respectively. We show here that the Legendre symmetry of the TPS induces a diffeomorphism

$$\psi : E^w \rightarrow E^{\tilde{w}}$$

if and only if

$$\frac{\partial^2 w}{\partial q^a \partial q^b} \neq 0 \quad \text{and} \quad \frac{\partial^2 \tilde{w}}{\partial p_a \partial p_b} \neq 0$$

(50)

at every point. For simplicity, let us consider the case in which $\tilde{w}$ is a total Legendre transform of $w$ [c.f. equation (45)]. Such transformation induces – by means of equations (26) and (27) – a diffeomorphism

$$\psi : E^w \rightarrow E^{\tilde{w}}$$

$$\left[w(q^a), q^a, p_a(q^b)\right] \mapsto \left[\tilde{w}(p_a), q^a(p^b), p_a\right]$$

(51)

that transforms the thermodynamic potential from $w(q^a)$ to $\tilde{w}(p_a)$ and at the same time interchanges the role of the independent coordinates from $q^a$ to $p_a$. Remarkably, the explicit expression of the transformation $\psi$ is given by the equations of state

$$p_a(q^b) = \frac{\partial w(q^b)}{\partial q^a}. \quad (52)$$

It is straightforward to calculate the push-forward of such transformation, which is

$$\psi_* : T E^w \rightarrow T E^{\tilde{w}}$$

$$\psi_* (X^a \partial_{q^a}) \equiv \left( \frac{\partial^2 w}{\partial q^a \partial q^b} \right) X^b \partial_{p_a}, \quad (53)$$

where $X = X^a \partial_{q^a}$ is any vector field on $T E^w$. Notice that, had we considered the inverse mapping $\psi^{-1}$, then we would have obtained a similar condition on the Hessian of $\tilde{w}$ with respect to the variables $p_a$. Therefore, we see from equation (53) that, although a Legendre transformation is always a diffeomorphism on the TPS, it induces a diffeomorphism on the equilibrium sub-manifolds if and only if the Hessians of the potential $w(q^a)$ and $\tilde{w}(p_a)$ are both non-degenerate. Therefore, such diffeomorphism between the equilibrium sub-manifolds depends on the particular function $w(q^a)$, i.e. depends on the particular system under exam. Whenever such Legendre symmetry of
the TPS is broken on $\mathcal{E}$, then the transformation on $\mathcal{E}$ corresponding to a Legendre transformation is not a diffeomorphism. In particular, in such case the sub-manifolds $\mathcal{E}^w$ and $\mathcal{E}^{\tilde{w}}$ are not equivalent. The in-equivalence of the information contained on $\mathcal{E}^w$ and $\mathcal{E}^{\tilde{w}}$ in such case reflects geometrically the in-equivalence of ensembles, which is well-known in statistical mechanics and thermodynamics for regions of the phase diagram where the thermodynamic potential does not satisfy the global convexity conditions, that is, where it is not a convex (resp. concave) function of its variables. Notice that in this case the Legendre sub-manifolds are inequivalent, not just their metric structures.

Consider for example the ideal gas. This is a system whose thermodynamic potential $w(q^a)$ globally satisfies the convexity conditions and therefore the ensembles are completely equivalent over the full region of the phase diagram. This is represented in contact geometry by a single, smooth, Legendre sub-manifold $\mathcal{E}$ (up to diffeomorphisms). However, the majority of systems undergo regions of instability and phase coexistence and hence we have different equilibrium sub-manifolds $\mathcal{E}$ corresponding to the different ensembles, that intersect over the regions of coexistence. In ordinary thermodynamics, one recovers the global stability (the convexity requirement) by means of the Maxwell equal area law, but the (local) Legendre symmetry cannot be restored. As we have seen, the breaking of the Legendre symmetry allows for the existence of different ensembles, represented by different sub-manifolds $\mathcal{E}$ whose information over the region of coexistence is inequivalent. Besides the in-equivalence of the ensembles, the intersection of such sub-manifolds implies also that there are processes that can pertain to different phases at the same time. As we will shortly see, such processes represent physically that the system is going from a thermodynamic phase to another through a sequence of equilibrium states, i.e. coexistence processes. In the sub-Section IV C we give a geometric characterization of such processes as curves on the $N$-dimensional sub-manifolds lying in the intersection of $r$ (equilibrium) Legendre sub-manifolds characterizing the $r$ different coexisting phases. The dimension $N$ is calculated by Gibbs phase rule and it turns out that

$$N = C - r + 2,$$

where $C$ is the number of different species in the thermodynamic system. In particular, for most of the cases in classical thermodynamics of simple systems (i.e. $C = 1$), the coexisting region is 1–dimensional, i.e. a curve, in the case of two coexisting phases ($r = 2$) and 0–dimensional, i.e. a point, in the case of three coexisting phases ($r = 3$), as e.g. in the triple point of water.
There is a subtle point to be highlighted here, regarding the non-degeneracy of the Hessian of the potential, equation (50). Whenever we consider an ordinary thermodynamic system for which the entropy (or the internal energy) is a homogeneous function of order one of the extensive variables, then, due to the Gibbs-Duhem relation, the total Legendre transformation is always degenerate, an indication that we are considering more degrees of freedom than needed. Thus, one uses the scaling property of the system to fix one of the extensive variables and divides the rest of them by such a fixed amount. The result of this also divides the potential by the same amount. In practice, one either chooses the particle number or the volume, and works with molar quantities or densities, respectively, for which the Legendre transformation is well-defined.

B. Legendre symmetry as an isometry

Consider now the metric structure induced on $\mathcal{E}$. We have said that different choices of the thermodynamic potential $w(q^a)$ in (26) can induce on $\mathcal{E}$ different and in principle in-equivalent metric structures defined as the Hessian of the corresponding potential. Here we show that the total Legendre transform always induces an isometry between the corresponding induced metric structures. However, this is not true for a partial Legendre transform.

Consider for example the metrics induced on $\mathcal{E}$ by the embedding (26) and corresponding to $w$ and its total Legendre transformation $\tilde{w}$, as defined in (45). For clarity, we write explicitly the corresponding embeddings

$$ \varphi_w : (q^a) \mapsto [w(q^a), q^a, p_a], \quad p_a = \frac{\partial}{\partial q^a} w $$

(55)

and

$$ \varphi_{\tilde{w}} : (p_a) \mapsto [\tilde{w}(p_a), q^a, p_a], \quad q^a = -\frac{\partial}{\partial p_a} \tilde{w}. $$

(56)

The two embeddings (55) and (56) define the two metric structures

$$ g = \varphi_w^* (G_{FR}) = \frac{\partial^2 w}{\partial q^a \partial q^b} dq^a \otimes dq^b $$

(57)

and

$$ \tilde{g} = \varphi_{\tilde{w}}^* (G_{FR}) = -\frac{\partial^2 \tilde{w}}{\partial p_a \partial p_b} dp_a \otimes dp_b. $$

(58)

These two metrics are in principle different. Let us see that a total Legendre transformation on $\mathcal{T}$ induces an isometry between the two. In general, we say that a diffeomorphism $\psi : (\mathcal{E}^w, g) \rightarrow$
$(\mathcal{E}^\tilde{w}, \tilde{g})$ is an isometry if

$$\psi^*(\tilde{g}) = g,$$

that is, if

$$g(X, Y) = \tilde{g}(\psi_\ast X, \psi_\ast Y) \quad \text{for any } X, Y \in T\mathcal{E}.$$

Consider the diffeomorphism of $\mathcal{E}$ induced by a total Legendre transformation, as defined in (51), with $\psi_\ast X$ given by (53). Therefore, after a brief algebraic manipulation, we can write the condition (60) for the metrics (57) and (58) as

$$\frac{\partial^2 w}{\partial q^a \partial q^b} = - \frac{\partial^2 \tilde{w}}{\partial p^c \partial p^d} \frac{\partial^2 w}{\partial q^c \partial q^d} \frac{\partial^2 w}{\partial q^b \partial q^d},$$

which in turn can be re-written, after multiplication on the right by the inverse matrix of $\frac{\partial^2 w}{\partial q^a \partial q^b}$, as

$$\delta^a_b = - \frac{\partial^2 \tilde{w}}{\partial p^c \partial p^d} \frac{\partial^2 w}{\partial q^c \partial q^d}.$$

Equation (62) is therefore the condition for the total Legendre transformation to induce an isometry between $(\mathcal{E}^w, g)$ and $(\mathcal{E}^\tilde{w}, \tilde{g})$. Finally, using equations (55) and (56), we can re-write (62) as

$$\delta^a_b = \frac{\partial q^a}{\partial p^c} \frac{\partial p^c}{\partial q^b},$$

which is an obvious identity. Therefore, we have proved that the diffeomorphism induced by a total Legendre transformation on the equilibrium manifolds is also an isometry. However, the same is not true if we consider a partial Legendre transformation. In fact, the two metric structures induced on the equilibrium manifold are not isometric in this case. For example one can convince himself that it is so by the fact that the scalar curvatures of the two structures are different (see e.g. [19] for their study).

To conclude, let us remark that we have considered here each Legendre sub-manifold $\mathcal{E}$ equipped with the natural induced metric from the metric $G_{\text{FR}}$ on the TPS and we have analyzed the conditions for these metrics to be equivalent. Of course one can decide to fix a priori a particular metric on $\mathcal{E}$ and operate on it only by diffeomorphisms of $\mathcal{E}$ and this would not change the corresponding line element.

C. First order phase transitions

Let us now turn to describe the only region where one encounters ensemble in-equivalence in ordinary thermodynamics, that is the region of coexistence between different phases (for a more
FIG. 3. The coexistence process as it appears on a $P-V$ diagram and on a $P-T$ diagram. Two aspects are of major interest. The first is to note that the process of coexistence (in red in the Figures) is represented by a line on the $P-V$ diagram and a single point on the $P-T$ diagram. Second, in order for the two phases to coexist at equilibrium, the temperatures and the pressures must be the same. More details in the text. Notice that we have also highlighted the spinodal curve (it is depicted in black in the $P-V$ diagram), indicating the points where the local stability conditions fail at any given temperature. Finally, the critical point ($v_c, p_c, T_c$) is depicted in both Figures.

detailed description see e.g. [34]). To this end, we refer to the $P-V$ and $P-T$ diagrams of the liquid-vapour coexistence for a Van der Waals fluid presented in Fig. 3. Above the critical temperature $T_c$, the isotherms on the $P-V$ diagram are decreasing functions of $V$ and, therefore, are stable. On the contrary, below the critical temperature, the isotherms have a region of instability, which is “cut-out” by means of the Maxwell construction (the red horizontal line in the left panel of Fig. 3). Such construction consists in finding the equilibrium value for the pressure at which the two phases coexist at equilibrium. It turns out that such equilibrium value is given by requiring that the two areas indicated by I and II in the $P-V$ diagram be equal. It is crucial for our discussion to note that the way in which Maxwell construction operates to restore equilibrium is by requiring that the intensive quantities be equal between the two phases [34], which is the standard definition of equilibrium between two parts of an ordinary thermodynamic system.

It is worth noting that, when a coexistence of two or more phases is present, already at the level of ordinary thermodynamics, we can see that the description in the variables $q^a$ is not equivalent to that using the variables $p_a$. In fact, by looking at the two diagrams in Fig. 3 one immediately sees that in the $P-V$ coordinates the coexistence process is given by a straight line (in red), whereas in the $P-T$ coordinates it corresponds to the single point, indicated by $(T_q, p_q)$. As
consequence, it is not surprising that the change of coordinates by a Legendre transform in that region is not a diffeomorphism. Indeed, as we have already pointed out, the descriptions using the extensive or the intensive coordinates are equivalent if and only if the Legendre transform is well defined, i.e. when the global convexity conditions are strictly satisfied [34]. From the above observations, we derive the conclusion that the process of coexistence cannot be fully described on a specific equilibrium manifold $E$. This is because the region of coexistence is the intersection of different equilibrium sub-manifolds and the Legendre transformation is not a diffeomorphism along such intersection. However, we can solve this problem in a simple way. More generally, we can parametrize any thermodynamic process as a curve $\gamma(t)$ on the TPS for which the first law $\eta(\dot{\gamma}) = 0$ is satisfied. In particular we can do so for coexistence processes. Therefore from now on we will look at all equilibrium processes as curves on the TPS whose tangent vector annihilates the 1-form $\eta$ (this means that we regard the First Law of thermodynamics as a constraint of motion on the TPS). By this definition, processes of coexistence of different phases are normal equilibrium processes and can be described in the geometric framework.

In the next Section, after a short review of contact Hamiltonian geometry, we will introduce a contact Hamiltonian formulation of thermodynamics which parallels the symplectic Hamiltonian formulation of conservative mechanics. In particular, we will define a contact Hamiltonian function that is the analogue of the Hamiltonian energy for mechanical systems. In fact, the flow of such function defines the evolution of the thermodynamic system, i.e. thermodynamic processes. Contrary to symplectic mechanics, we will see that in this case the Hamiltonian is conserved only on a particular sub-class of processes, i.e. equilibrium processes.

V. CONTACT HAMILTONIAN THERMODYNAMICS

In this Section, after a brief review of the main aspects of contact Hamiltonian dynamics, we use these concepts to introduce a Hamiltonian function on the TPS whose flow defines thermodynamic processes. Such a formulation was intended first by Mrugala (c.f. for instance [35]), but he only presented some special cases, valid only for particular thermodynamic systems. Moreover, Rajeev in [36] has also given a contact Hamiltonian formulation, based on the Hamilton-Jacobi formalism. However, the calculation of the characteristic curves of the generating functions that he considers give the equations of state of the substance and therefore, although the construction is very neat, there is no real ‘time’ evolution of the system. Here we want to propose an approach similar to standard Hamiltonian mechanics, and therefore we demand the flow of the Hamiltonian function
To define thermodynamic processes.

To begin with, let us review quickly some contact Hamiltonian dynamics, following in particular [37]. We start with the contact manifold $\mathcal{T}$ in which the representative contact 1-form $\eta$ is fixed. Therefore, to every differentiable function $h : \mathcal{T} \to \mathbb{R}$, we can associate a vector field $X_h$, called the Hamiltonian vector field generated by $h$, defined through the relation

$$h = \eta(X_h),$$

and we say that $h$ is a contact Hamiltonian. It turns out that

$$\mathcal{L}_{X_h}\eta = \xi(h)\eta. \tag{65}$$

Therefore Hamiltonian vector fields form exactly the Lie algebra $\text{con}(\mathcal{T},\mathcal{D})$ of contactomorphisms, c.f. equation (31). When $h$ is a basic function, i.e. $\xi(h) = 0$ with $\xi$ the Reeb vector field, they reduce to the sub-algebra $\text{con}(\mathcal{T},\eta)$ of strict contactomorphisms, or symmetries of $\eta$. The mapping (64), sending every vector field $X \in \text{con}(\mathcal{T},\mathcal{D})$ to the corresponding function $\eta(X) \in C^\infty(\mathcal{T})$ is an isomorphism of Lie algebras, where the Lie algebra structure of $C^\infty(\mathcal{T})$ is given by the Jacobi brackets

$$\{\eta(X),\eta(Y)\}_\eta = \eta([X,Y]). \tag{66}$$

Notice that both the isomorphism and the definition of the Jacobi brackets depend crucially on the choice of the Gibbs 1-form $\eta$. Note also that for instance the Reeb vector field (4) associated with the contact form $\eta$ is the Hamiltonian vector field generated by the Hamiltonian $h_\xi = 1$ and that the vector field $X_{\text{LT}}$ associated with infinitesimal Legendre transformations is generated by

$$h_{\text{LT}} = \frac{1}{2} \left( \sum a (q^a)^2 + (p_a)^2 \right). \tag{38}$$

Furthermore,

$$\mathcal{L}_{X_{\text{LT}}}\eta = 0 \quad \text{while} \quad \mathcal{L}_{X_{\text{LT}}}G_{\text{FR}} \neq 0, \tag{67}$$

that is, infinitesimal Legendre transformations are symmetries of the contact structure but not of the metric structure of the thermodynamic phase space. Again, this is equivalent to saying that the First Law of thermodynamics is invariant under Legendre transformations, while the fluctuations of the system’s parameters change in the different ensembles. The orbits of the flow of $X_{\text{LT}}$ are given in Fig. 4. A detailed description of this flow is given in [38].

The Jacobi bracket (66) in general does not satisfy the Leibniz rule and one has that $\{g,1\}_\eta = 0$ if and only if $[X_g,\xi] = 0$. Nevertheless, if we restrict our attention to basic functions (resp. to strict contactomorphisms), then the Leibniz rule is satisfied. When the 1-form $\eta$ defining the contact
FIG. 4. Orbits of the infinitesimal Legendre symmetry generator $X_{LT}$ exchanging the $i$th pair of conjugate variables. The height $w$ of the curves along the $p_i$ and $q^i$ axis attains the same value every $\pi/2$ rotations. Notice the different nature of these orbits with those of the isometries of $G_{FR}$ depicted in 1 and 2. See [38] for a more detailed discussion on a class of metrics admitting the Legendre generators as isometries.

structure and the Hamiltonian function $h$ are fixed on $\mathcal{T}$, we say that the quadruple $(\mathcal{T}, D, \eta, h)$ is a Hamiltonian contact structure or a contact Hamiltonian system.

Let $(\mathcal{T}, D, \eta, h)$ be a contact Hamiltonian system. In local Darboux coordinates the Hamiltonian vector field $X_h$ takes the form

$$ X_h = \left( h - p_a \frac{\partial h}{\partial p_a} \right) \frac{\partial}{\partial w} + \left( \frac{\partial h}{\partial q^a} + p_a \frac{\partial h}{\partial w} \right) \frac{\partial}{\partial p_a} - \left( \frac{\partial h}{\partial p_a} \right) \frac{\partial}{\partial q^a}. \quad (68) $$

while in the $\eta$–canonical basis defined in (7) it reads

$$ X_h = h \xi + \hat{Q}^a(h) \hat{P}_a - \hat{P}_a(h) \hat{Q}^a = h \xi + \phi \nabla h, \quad (69) $$

where $\phi$ is the almost contact structure and $\nabla h$ is the gradient of $h$ with respect to an associated metric (c.f. [29]). Finally, in terms of the Jacobi brackets (66), we can express the action of $X_h$ on a function $f$ as

$$ X_h f = \xi(h) f + \{h, f\}_\eta. \quad (70) $$
We say that a function \( f \in C^\infty(T) \) is a first integral of the contact Hamiltonian structure \((T, \xi, \eta, h)\) if \( f \) is constant along the flow of \( X_h \), that is if \( X_h f = 0 \). Notice that by equation (70) this does not coincide with \( \{h, f\}_\eta = 0 \), as in symplectic geometry. From the above equation (70) it follows in general that \( X_h h = \xi(h) \), therefore the Hamiltonian function is not in general a first integral of its flow. Indeed \( h \) is a first integral if and only if it is a basic function. In this case we say that \( h \) is a good Hamiltonian with respect to \( \eta \). Finally, given two first integrals \( f_1 \) and \( f_2 \) of the flow, we say that they are in involution if \( \{f_1, f_2\}_\eta = 0 \) and we say that they are independent if their corresponding Hamiltonian vector fields \( X_{f_1} \) and \( X_{f_2} \) are linearly independent on a dense open subset of \( T \).

According to equation (68), the flow of \( X_h \) can be explicitly written in Darboux coordinates as

\[
\begin{align*}
\dot{w} &= h - p_a \frac{\partial h}{\partial p_a}, \\
\dot{p}_a &= \frac{\partial h}{\partial q^a} + p_a \frac{\partial h}{\partial w}, \\
\dot{q}^a &= -\frac{\partial h}{\partial p_a},
\end{align*}
\]

where its similarity with Hamilton’s equations of classical mechanics is manifest. In fact, these are the contact equivalent to Hamilton’s equations. In particular, when \( h \) is a basic function equations (72) and (73) give exactly Hamilton’s equations \([30]\). Despite this similarity, there is a profound difference with Hamilton’s equations because in general \( h \) is not conserved along the orbits.

A. The Thermodynamic Contact Hamiltonian System and its geometric properties

Let us consider the First Law of thermodynamics as a constraint on the contact Hamiltonian flow (71)-(73). Then, along a process \( \gamma(t) : I \subset \mathbb{R} \rightarrow T \) it takes the form

\[
\dot{w} = p_a(\gamma)q^a.
\]

Then, using equations (71) and (73) this implies that along the integral curves of \( X_h \) that are constrained by the First Law - i.e. along equilibrium processes - we must have \( h(t) \equiv 0 \). It follows that in the contact formulation of thermodynamics we must have a Hamiltonian function that identically vanishes over the orbits representing equilibrium processes. We will now look for the most general form of such function.

One of the basic assumptions in ordinary thermodynamics (sometimes also considered as one of the Laws of thermodynamics) is that the potential be a homogeneous function of order one of
the extensive variables $[34]$, that is
\[ w(\lambda q^a) = \lambda w(q^a), \quad \forall \lambda \in \mathbb{R}^+. \] (75)

Therefore, Euler’s Theorem for homogeneous functions implies
\[ w(q^a) = p_a q^a, \quad p_a = \frac{\partial w}{\partial q^a}. \] (76)

This is a motivation to define the contact Hamiltonian function for thermodynamics $H : \mathcal{T} \to \mathbb{R}$ as follows
\[ H \equiv -w + p_a q^a. \] (77)

Notice that $H = -\tilde{w}$, the total Legendre transform of $w$ [see equation $[45]$, and that Euler’s identity $[76]$ implies that $H$ vanishes on the equilibrium (Legendre) sub-manifolds of $\mathcal{T}$. Therefore $H$ is a good candidate as a contact Hamiltonian function for thermodynamics.

Let us see now how to define equilibrium processes and admissible non-equilibrium processes by means of the flow of the contact Hamiltonian vector field associated to $H$. According to $[68]$, the Hamiltonian vector field associated to $H$ can be written in local Darboux coordinates as
\[ X_H = -w \frac{\partial}{\partial w} - q^a \frac{\partial}{\partial q^a}, \] (78)

which generates the homothety of $\eta$
\[ \mathcal{L}_{X_H} \eta = -\eta. \] (79)

Notice that $X_H H = H$ and therefore $H$ is not a first integral of its flow. Moreover, it follows from $[78]$ that the flow of $H$ reads
\[
\begin{align*}
\dot{w} &= -w, \\
\dot{p}_a &= 0, \\
\dot{q}^a &= -q^a.
\end{align*}
\] (80)-(82)

Now let us first consider the geometrical properties of this flow as a contact Hamiltonian system. Then we will give it a meaning in the thermodynamic context. It is immediate from $[81]$ that the functions $p_a$ are $n$ first integrals of the flow. Moreover, the function 1 provides another (trivial) first integral. Therefore, we have $n + 1$ first integrals of the flow $[80]-[82]$ and it is easy to check that they are in involution and independent. This means that the contact Hamiltonian system $(\mathcal{T}, \mathcal{D}, \eta, H, \{1, p_a\})$ is a completely integrable system of Reeb type.
B. Thermodynamic processes

Let us now turn to a more specific investigation of the integral curves of the flow $\gamma(t) : I \subset \mathbb{R} \to \mathcal{T}$, which read

$$
\begin{align*}
  w(t) &= w_0 e^{-t}, \\
  p_a(t) &= p_0^a, \\
  q^a(t) &= q_0^a e^{-t}.
\end{align*}
$$

From (83)-(85) and the definition of $H$ – equation (77) – it follows that

$$ H(t) = H_0 e^{-t}. $$

This means that we have two types of orbits for the flow:

i) Orbits starting with $H_0 = 0$. Along these orbits $H(t) \equiv 0$ for all $t > 0$.

ii) Orbits starting with $H_0 \neq 0$. Along these orbits $H(t)$ tends exponentially to zero as $t$ increases.

We also know that along equilibrium processes $H(t)$ must be zero, by definition, equation (77). This suggests to define in general thermodynamic processes as the orbits of the flow of $X_H$. In particular, equilibrium processes are the orbits of the flow of $H$ of type i) above and we define $H(t)$ as the entropy production potential along the process. Therefore, with such identifications, we can regard to orbits of type ii) as near-equilibrium processes, since $H(t)$ is not zero but tends to zero quickly.

In fact, let us see why the identification of $H(t)$ with the entropy production potential along a process can make sense. We remind that $H = -w + p_a q^a$. Therefore,

$$ -dH = dw - p_a dq^a - q^a dp_a = \eta - q^a dp_a. $$

and in general on $\mathcal{T}$ the differential of $H$ is different from the Gibbs 1-form $\eta$. However, we have already seen that along the flow of $H$ the $p_a$ are constant. Therefore along the integral curves of $X_H$ we have

$$ -dH(\dot{\gamma}) = \eta(\dot{\gamma}). $$

Equations (87) and (88) give the physical meaning of $H$. It is a function whose differential coincides with the Gibbs 1-form along the orbits of its contact flow, i.e. along all thermodynamic processes.
FIG. 5. Evolution of the entropy production potential $H(t)$ along the orbits of the thermodynamical flow. Solid lines represent thermodynamically admissible processes. As we see, the entropy potential along near-equilibrium processes is a negative concave and monotonically increasing function of $t$ which tends exponentially to zero.

Therefore we understand why the orbits of the flow leaving $H(t) \equiv 0$ coincide with equilibrium processes. Moreover, using standard thermodynamic variables, we can write along the flow

$$-dH(\dot{\gamma}) = \eta(\dot{\gamma}) = \left( dU - T dS + pdV - \sum_i \mu_i dN^i \right) (\dot{\gamma}).$$  \hfill (89)

We know that the right hand side of (89) must vanish for equilibrium processes. Besides, we know that for non-equilibrium processes it must be negative. In fact, this one of the statements of the Second Law of thermodynamics [34]. Therefore, we end up with an additional condition equivalent to the Second Law, that is

$$dH(\dot{\gamma}) \geq 0,$$  \hfill (90)

which, by equation (86), can also be stated as

$$H_0 \leq 0.$$  \hfill (91)
Notice that conditions (90) and (91) imply that $H$ is a Lyapunov function for the system (80)-(82), as entropy production has to be in the local equilibrium regime in order to ensure the damping of fluctuations [40].

According to (91), we now give the definition of an admissible process. A \textit{thermodynamically admissible process} (TAP) is a curve $\gamma: I \subset \mathbb{R} \to \mathcal{T}$ such that

a) $\dot{\gamma} = X_H$ (i.e. $\gamma(t)$ is a thermodynamic process).

b) $H_0 = H(\gamma(0)) \leq 0$ (i.e. $\gamma(t)$ is an equilibrium process or a near-equilibrium process for which the Second Law is valid).

C. The null-cone structure of the thermodynamic phase space

Given the notion of thermodynamic admissible processes, we can give a partial ordering relation on the TPS in the spirit of the Theory of Relativity.

We say that two points $p, q \in \mathcal{T}$ are \textit{thermodynamically related} if there exists a thermodynamic admissible process between the two. Moreover, since $H(t)$ cannot decrease along thermodynamic admissible processes, we can distinguish between past and future over the process. In particular, we say that $p$ is \textit{in the past of} $q$ if there is a thermodynamic admissible process $\gamma$ such that $\gamma(0) = p$ and $\gamma(1) = q$. Since this relation defines a partial ordering on $\mathcal{T}$, we denote it as $p \prec q$. In this way we obtain a \textit{causal structure} on $\mathcal{T}$.

Notice that we have given all the definitions so far without using the metric structure of $\mathcal{T}$. Now let us consider the metric $G_{FR}$ on $\mathcal{T}$ as defined in (15). A direct calculation shows that

$$G_{FR}(X_H, X_H) = H^2$$ (92)

and therefore

$$||\dot{\gamma}(t)|| = \pm H(t)$$ (93)

where we choose the plus sign to ensure that the length of a path coincides with the entropy production along the path. Therefore we can characterize thermodynamically admissible processes in terms of their norm. In fact, it turns out that thermodynamically admissible processes are those for which $||\dot{\gamma}(t)|| \leq 0$ for any $t$. From (93) and (86) we conclude that this is equivalent to requiring that $||\dot{\gamma}(0)|| \leq 0$. It is both unexpected and remarkable that the same causal structure that we have defined in terms of the contact Hamiltonian flow with generating function $H$ can also be given in terms of the cone structure of the metric $G_{FR}$. 
Moreover, given the pseudo-Riemannian structure $G_{FR}$, we can conclude our analysis on the role of $H$. In fact, we can define a functional of the curves defined on $\mathcal{T}$, which is the usual arc length, defined as

$$\tilde{\mathcal{H}} : \mathcal{C}(\mathcal{T}) \to \mathbb{R}$$

$$\gamma(t) \mapsto \int_{0}^{T} ||\dot{\gamma}(t)|| \, dt.$$  

From (93) and (94) it follows that along thermodynamically admissible processes we have

$$\tilde{\mathcal{H}}(\gamma(t)) = \int_{0}^{T} H(t) \, dt = \int_{0}^{T} H_0 e^{-t} \, dt = \left[ -H_0 e^{-t} \right]_{0}^{T} = \left[ -H(\gamma(t)) \right]_{0}^{T}. \tag{95}$$

Thus, since $H_0 \leq 0$ along thermodynamically admissible processes, we get that $\tilde{\mathcal{H}}(\gamma(t)) \leq 0$. We define

$$\mathcal{H}(\gamma(t)) = -\tilde{\mathcal{H}}(\gamma(t)) \geq 0 \tag{96}$$

as the entropy production along the process $\gamma(t)$. Noticeably $\mathcal{H}(\gamma(t))$ has a global minimum $\mathcal{H} = 0$, which is attained if and only if $H(\gamma(t)) \equiv 0$, i.e. if and only if $\gamma(t)$ is an equilibrium process. Hence, we conclude with the result that equilibrium processes are those paths which are thermodynamically admissible and minimize the entropy production. This is something physically expected in the regime of local equilibrium in which we are working here [40]. Incidentally, equilibrium processes are also geodesics of the metric $G_{FR}$, since they maximize the arc length $\tilde{\mathcal{H}}(\gamma(t))$.

VI. DISCUSSION OF THE RESULTS

Let us resume and discuss briefly the new results presented in this work. To the best of our knowledge, the role of contact gauge transformations of the thermodynamic phase space had never been considered before. These transformations were presented here in their generality in III A. We have then considered the particular case of the change of the thermodynamic representation, showing explicitly the related transformation of the Sasakian structure of the thermodynamic phase space. Interestingly, such change in the metric structure induces the well-known conformal equivalence between the Weinhold ‘energy’ metric and the Ruppeiner ‘entropy’ metric on the Legendre sub-manifolds.

In Section IV we have investigated in detail the role of the Legendre symmetry in thermodynamics. We have proved that this symmetry induces a diffeomorphism of the equilibrium sub-manifolds.
and therefore implies ensemble equivalence, as long as the stability conditions are fulfilled. Moreover, we have also proved that a total Legendre transformation is an isometry of the metric structures naturally induced by $G_{FR}$ on the Legendre sub-manifolds by the use of different embeddings, while a partial Legendre transformation is not so. With this respect, it is important to note that our approach differs from previous literature on thermodynamic geometry. In fact, usually in the literature one directly starts with a particular choice of a metric on the Legendre sub-manifold and then operates on it with change of the coordinates of the sub-manifold, which leave the metric unchanged. In our case, we consider $G_{FR}$ as fixed on the thermodynamic phase space and consider the different metrics that can be induced on the Legendre sub-manifolds. We have also presented a digression on first order phase transition as a relevant example of regions of ensemble inequivalence in the context of ordinary thermodynamics.

Finally, in Section V we have given a consistent formulation of thermodynamics in terms of contact Hamiltonian geometry which also permits to define near-equilibrium processes and entropy production in this regime. We have also shown that this construction can be equivalently given in terms of the metric $G_{FR}$. This can be surprising, nevertheless some comments on the microscopic derivation of the contact and geometric structures of the thermodynamic phase space perhaps can clarify the statements. Reminding of the statistical mechanical construction of the contact structure of the thermodynamic phase space, we have $\langle s \rangle_{Gibbs} = w - p_a q^a = -H$. From this point of view, it makes even more sense our identification of $H(t)$ as the entropy production potential. In fact $-dH(t) = \langle ds(t) \rangle_{Gibbs}$ is the first moment of the variation of the microscopic entropy near the equilibrium distribution in the whole phase space $T$, while $\eta$ is just its restriction to thermodynamic processes. This also gives some intuition why the square norm a thermodynamic process computed with respect to the Fisher-Rao metric $G_{FR}$ is exactly $H^2(t)$, equation (92). In fact, by definition $G_{FR} = \langle (ds)^2 \rangle_{Gibbs}$.

Moreover, from the microscopic construction it results that the values of the $p_a$ are the ‘boundary conditions’ of the ensemble, i.e. fixed constraints imposed to maximize the microscopic entropy functional, corresponding to the Lagrange multipliers $q^a$. Therefore, it is not surprising that the corresponding flow (thermodynamic processes) implies that the values of the $p_a$ must be constant. Actually also the additional integral of the contact Hamiltonian system for thermodynamics – the function 1 – arises as a constraint in the maximization of entropy, corresponding to the normalization condition for the probability distributions and related to the Lagrange multiplier $w$. Notice also that changing the number and nature of the $p_a$ we can change the statistical ensemble. Moreover, in each ensemble one should use the appropriate $H$, resulting from the Euler relation...
for the corresponding potential, e.g. \( H^U = -U + TS - pV + \mu N \), whereas \( H^F = -F - pV + \mu N \).

Finally, let us resume schematically the results of the contact Hamiltonian thermodynamics and their connection with the classical Laws of thermodynamics.

- **Zeroth Law.** Notice that we are always working on a specific ensemble, obtained from maximizing the microscopic Boltzmann-Gibbs entropy functional subject to some ‘boundary conditions’ which fix the values of the \( p_a \). Therefore the equilibrium condition is assumed because of the use of the Gibbs distribution corresponding to the ensemble. Accordingly, it turns out that the Hamiltonian flow has the \( p_a \) as first integrals of motion. Changing the character of the variables \( p_a \) we can obtain the different ensembles.

- **First Law.** *Equilibrium processes* of the contact Hamiltonian flow are, by definition, those satisfying \( dH(t) \equiv 0 \), which – by equation (88) – is equivalent to say that the First Law is satisfied along the process.

- **Second Law.** We have seen in equation (90) that the Second Law of thermodynamics is equivalent to requiring that \( dH(t) \geq 0 \) along the process or equivalently that \( ||\dot{\gamma}(t)|| \leq 0 \) when the norm is calculated with respect to the metric \( G_{FR} \) on \( T \). This has served as our definition of thermodynamically admissible processes.

To conclude, in this work we have presented a thorough analysis of some open problems in the geometrization of thermodynamics. In particular, here we have focused on Legendre symmetries, first order phase transitions and on the construction of a comprehensive contact Hamiltonian model for thermodynamics. Nevertheless, several questions remain to be addressed. For example, we have not fully investigated the physical role of gauge transformations and of the other symmetries of the contact structure corresponding to strict contactomorphisms which are not Legendre. From the point of view of contact Hamiltonian thermodynamics, it would be relevant to see whether this formulation can lead e.g. to a kind of quantization of the contact manifold and of the thermodynamic relations, as previously proposed e.g. in [39]. Moreover, we understand that the length of a process in the phase space is related to the entropy production during the process. Therefore it is interesting to perform a detailed analysis of the geodesics, as curves of minimal entropy production, as in [8] and [15, 17]. Finally, equation (87) clearly resembles the transverse deformations of the Sasakian structure recently used in contact geometry to define the Sasaki-Ricci flow [41].
It would be interesting to relate this geometric flow on the thermodynamic phase space to the thermalization of systems. We expect to explore all these topics in future works.

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