

Article

Conformal Gauge Transformations in Thermodynamics

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Abstract: In this work, we show that the thermodynamic phase space is naturally endowed with a non-integrable connection, defined by all of those processes that annihilate the Gibbs one-form, *i.e.*, reversible processes. We argue that such a connection is invariant under re-scalings of the connection one-form, whilst, as a consequence of the non-integrability of the connection, its curvature is not and, therefore, neither is the associated pseudo-Riemannian geometry. We claim that this is not surprising, since these two objects are associated with irreversible processes. Moreover, we provide the explicit form in which all of the elements of the geometric structure of the thermodynamic phase space change under a re-scaling of the connection one-form. We call this transformation of the geometric structure a conformal gauge transformation. As an example, we revisit the change of the thermodynamic representation and consider the resulting change between the two metrics on the thermodynamic phase space, which induce Weinhold's energy metric and Ruppeiner's entropy metric. As a by-product, we obtain a proof of the well-known conformal relation between Weinhold's and Ruppeiner's metrics along the equilibrium directions. Finally, we find interesting properties of the almost para-contact structure and of its eigenvectors, which may be of physical interest.

Keywords: thermodynamic geometry; contact geometry; gauge transformations

1. Introduction

The geometry of equilibrium thermodynamics and thermodynamic fluctuation theory is extremely rich. In particular, equilibrium thermodynamics is based on the first law, which for reversible processes can be written in the internal energy representation as:

$$\eta_U = dU - TdS + p dV - \sum_{i=1}^{n-2} \mu_i dN_i = 0, \quad (1)$$

where the variables have their usual meaning. From the point of view of the theory of differential equations, this is a Pfaffian system in a space of $2n + 1$ variables (n extensive quantities, n intensities and a potential), for which there is no $2n$ -dimensional sub-manifold whose tangent vectors all satisfy Condition (1) (*cf.* [1]). In fact, for this to be the case, the one-form η_U should satisfy the Frobenius integrability condition, $\eta_U \wedge d\eta_U = 0$, whereas in thermodynamics, η_U is as far as possible from being integrable. That is, it satisfies:

$$\eta_U \wedge (d\eta_U)^n \neq 0. \quad (2)$$

This implies that the solutions to Equation (1) have at most n independent variables. Therefore, thermodynamic systems are n -dimensional sub-manifolds of a $(2n + 1)$ -dimensional phase space, which are completely defined as the graph of the “fundamental relation”, *i.e.*, a solution of (1) expressing the dependence of the thermodynamic potential on n independent variables. As an example, for a closed thermodynamic system, the fundamental relation is usually expressed in the form $u(s, v)$, where u is the molar internal energy and s and v are the molar entropy and volume, respectively. The equations of state for the temperature and the pressure then follow from (1). This was already realized by Gibbs and Carathéodory [2,3], who started to study the geometric properties of state functions and relate them to thermodynamic properties of systems. In a geometric language, we can rephrase the above statements by saying that the thermodynamic phase space (TPS) is a contact manifold, and thermodynamic systems are Legendre sub-manifolds of the TPS [4–8].

A Riemannian metric can be introduced on the Legendre sub-manifold representing a thermodynamic system by means of the Hessian of a thermodynamic potential. Weinhold [9–12] was the first to realize this fact and proposed the metric defined as the Hessian of the internal energy. For example, for a closed system:

$$g^W = \frac{\partial^2 u}{\partial s^2} ds \otimes ds + 2 \frac{\partial^2 u}{\partial s \partial v} ds \overset{s}{\otimes} dv + \frac{\partial^2 u}{\partial v^2} dv \otimes dv, \quad (3)$$

where the symbol $\overset{s}{\otimes}$ denotes the symmetric tensor product (*cf.* Section 2, Equation (19)). Weinhold used the inner product induced by this metric in order to recover geometrically most of the thermodynamic relations. Later, Ruppeiner [13] introduced a related metric starting from thermodynamic fluctuation theory. In fact, the Gaussian approximation for the probability of a fluctuation [14]:

$$w = w_0 \exp \left(- \frac{\Delta T \Delta s - \Delta p \Delta v}{2T} \right) \quad (4)$$

depends on the Hessian of the entropy with respect to the fluctuating (extensive) variables. This enables one to equip the Legendre sub-manifold corresponding to a thermodynamic system with a different Hessian metric to that of Weinhold, namely [15]

$$g^R = \frac{\partial^2 s}{\partial u^2} du \otimes du + 2 \frac{\partial^2 s}{\partial u \partial v} du \overset{s}{\otimes} dv + \frac{\partial^2 s}{\partial v^2} dv \otimes dv. \tag{5}$$

The two metrics are related by a conformal re-scaling [16]:

$$g^R = -\frac{1}{T} g^W, \tag{6}$$

which is exactly the same re-scaling between the two one-forms defining the first law in the energy and in the entropy representation, *i.e.*,

$$\eta_s = ds - \frac{1}{T} du - \frac{p}{T} dv = -\frac{1}{T} \eta_u. \tag{7}$$

In this way, Legendre sub-manifolds (defining thermodynamic systems undergoing reversible processes) are equipped naturally with two different Riemannian structures that are related by a conformal transformation. Notice that this fact also implies that Legendre sub-manifolds in thermodynamics are also Hessian manifolds (see, e.g., [17,18]).

The study of Metrics (3) and (5) has been very fruitful. It was found in particular that the thermodynamic length corresponding to g^W (respectively, g^R) implies a lower bound on the dissipated availability (respectively, to the entropy production) during a finite-time thermodynamic process [19] and that the scalar curvature of these geometries is a measure of the stability of the system, since it diverges over the critical points of continuous phase transitions with the same critical exponents as for the correlation volume [20–22]. Moreover, these geometries are related naturally to the Fisher–Rao information metric, and therefore, the investigation of their geometric properties can be extended (*mutatis mutandis*) to the statistical manifold [23] and to microscopic systems, which are characterized by working out of equilibrium [24–26]. As such, the intrinsic geometric perspective of Legendre sub-manifolds of the thermodynamic phase space has given new physical insights for thermodynamics itself, with direct interest for applications in realistic processes, outside the realm of abstract reversible thermodynamics.

So far, the geometric properties of the thermodynamic phase space itself have remained less investigated. Mrugala *et al.* [27] proved that one can endow naturally the TPS with an indefinite metric structure derived from statistical mechanics, which for a closed system can be defined either as:

$$G_u = \eta_u \otimes \eta_u + ds \overset{s}{\otimes} dT - dv \overset{s}{\otimes} dp \tag{8}$$

or as:

$$G_s = \eta_s \otimes \eta_s + du \overset{s}{\otimes} d\left(\frac{1}{T}\right) + dv \overset{s}{\otimes} d\left(\frac{p}{T}\right), \tag{9}$$

depending on the thermodynamic representation being considered. These metrics reduce to Weinhold’s and Ruppeiner’s metrics, respectively, on Legendre sub-manifolds. It was proven [28] that such structures are as perfectly well adapted to the contact structure as they can be, and that in fact, one can introduce also a linear endomorphism in the tangent space to the TPS, so that the manifold is

equipped with a very peculiar geometry, defining a para-Sasakian manifold [29–31]. This, in turn, is the odd-dimensional analogue of the well-known Kähler geometry [32]. Moreover, such a definition implies that the TPS contains a Kähler manifold along the $2n$ directions identified with reversible processes. The important point to notice here is that the thermodynamic phase space has a very rich geometric structure, with elements stemming from the reversible relation (Equation (1)) and others arising from irreversible fluctuations (Equations (8) and (9)). Furthermore, a related, although at first sight slightly different, geometrical approach to thermodynamic fluctuations was also recently pursued. It was shown in [33] that generalized complex structures, a completely new mathematical area, can be introduced in thermodynamic fluctuation theory, especially in order to consider thermal and quantum fluctuations on the same footing, which seems to be the case in the presence of a gravitational field.

An additional physical motivation for our study comes from previous results, where it has also been proved, by means of contact Hamiltonian dynamics, that the lengths computed using Metrics (8) and (9) in the thermodynamic phase space give a measure of the entropy production along irreversible processes identified with fluctuations [34] (see also [35]).

In this work, we revisit these ideas from a different point of view, namely that of the theory of connections. In this manner, we present a novel aspect of the geometric structure of thermodynamics and thermodynamic fluctuation theory. In particular, we study the transformations preserving the connection defined by reversible processes, which we call the equilibrium connection. In fact, it is known that the physical content of the first law resides in those processes that annihilate the connection one-form η_u , and therefore, at the level of an equilibrium (reversible) description, we are presented with the physical freedom of rescaling such a form through multiplication by any non-vanishing function. This operation, known as contactomorphism [36,37], does not change the results of equilibrium thermodynamics. One usually encounters such transformations as the change of thermodynamic representation, e.g., from the energy to the entropy representation (*cf.* Equation (7)). Here, we consider the class of contactomorphisms in the thermodynamic phase space and derive the induced transformations for any object defining its geometric structure. We call these conformal gauge transformations [38]. We prove that the equilibrium connection thus defined is necessarily non-integrable, meaning that its associated curvature (not to be confused with the Riemannian curvature associated with the various thermodynamic metrics) is non-vanishing and not invariant under contactomorphisms. Hence, it follows that, albeit that the equilibrium thermodynamics of reversible processes is independent of the representation used, the description of irreversible fluctuations along such processes does change depending on the choice of a particular representation. We show that the metric structure of the TPS is intimately related to the curvature of the equilibrium connection. Since the connection is non-integrable, it follows that the metric changes under contactomorphisms. We further show that this reduces to the well-known relation (6) between Weinhold's and Ruppeiner's geometries in the appropriate case, but our result is valid for a general transformation. This shows that the induced thermodynamic lengths are not invariant with respect to using different potentials or representations (see also [41–43] for the definition of inequivalent thermodynamic metrics based on the Hessian of other potentials). Finally, we argue that our results can shed light on the physical significance of these geometric objects, highlighting the ones related to a reversible situation and the ones associated with irreversible evolution. Hopefully, this description will help in the identification of geometric properties of potentials that are relevant in irreversible situations.

2. The Equilibrium Connection

In this section, we will recall some formal developments of thermodynamic geometry. The interested reader is referred to [28] and [34] for a detailed discussion about the statistical origin of the structures presented here.

Let us consider a thermodynamic system with n degrees of freedom. As we have argued in the Introduction, the TPS, denoted by \mathcal{T} , is the $(2n + 1)$ -dimensional ambient space of possible thermodynamic states of any system.

The laws of thermodynamics are universal statements (applicable to every thermodynamic system) about the nature of the processes that take place when a system evolves from a particular thermodynamic state to another. Thus, we believe that such laws are better identified in a geometric perspective with the properties of the TPS. In order to accommodate such laws, it is convenient to consider the TPS to be a differentiable manifold. This will make the evolution meaningful in terms of vector fields and their corresponding integral curves.

Our central point is that the first law of thermodynamics (1) is equivalent to defining a $2n$ dimensional connection Γ over the TPS, which we call the equilibrium connection. This is a smooth assignment of $2n$ horizontal directions for the tangent vectors at each point of \mathcal{T} . We express this schematically by:

$$\{\text{First law of thermodynamics at } p\} \equiv \{\Gamma : p \in \mathcal{T} \longrightarrow \Gamma_p \subset T_p\mathcal{T}\}, \tag{10}$$

where we use the standard notation $T_p\mathcal{T}$ for the tangent space at a given point. At first sight, such an assignment seems to be rather abstract. However, we will shortly see that it takes the same local form independently of the thermodynamic system under consideration, reflecting the universality of the first law.

Let us agree that a curve on \mathcal{T} represents a possible process. We say that a curve joining two points in the TPS is an equilibrium (reversible) process if its tangent vector lies in the horizontal subspace Γ_p with respect to the first law. This statement acquires a definite meaning with the aid of a connection one-form η . Recall that a one-form is just a linear map acting on tangent vectors. In the case of the first law, the horizontal directions of $T_p\mathcal{T}$ are given by the vectors annihilated by η , that is,

$$X \in \Gamma_p \iff \eta(X) = 0. \tag{11}$$

From Equation (1), we see that the above condition on X is just the requirement that the corresponding process be a reversible process. In fact, from a geometric point of view, since η is a contact form (see the Introduction), then a theorem by Darboux ensures that around each point on the TPS, one can assign a set of local coordinates (w, p_a, q^a) , where a takes values from one to n , in which η reads:

$$\eta = dw + \sum_{a=1}^n p_a dq^a. \tag{12}$$

It can also be justified from statistical mechanical arguments (*cf.* [34]) that such coordinates are the ones that enter in the equilibrium description of the process. These are known in the literature as Darboux coordinates. For example, for a closed system, as in (7), in the molar entropy representation, the coordinates q^a are naturally associated with the extensive variables u and v ; the p_a are (minus) the intensities T^{-1} and p/T , and w is the molar entropy s .

Note that the horizontal directions in the TPS are uniquely defined by (11), and any particular thermodynamic system at equilibrium has a tangent space, which is a subspace of Γ_p at every point. Therefore, Definition (11) encodes the universality of the first law of thermodynamics.

Now, let us find a coordinate expression for the equilibrium directions around every point of the TPS. These are simply the tangent vectors satisfying (11). In Darboux coordinates, a direct calculation reveals that the vectors:

$$P^a = \frac{\partial}{\partial p_a} \quad \text{and} \quad Q_a = \frac{\partial}{\partial q^a} - p_a \frac{\partial}{\partial w}, \tag{13}$$

generate $2n$ linearly-independent horizontal directions, that is,

$$\eta(P^a) = 0 \quad \text{and} \quad \eta(Q_a) = 0, \tag{14}$$

for every value of a ; thus, every equilibrium direction around each thermodynamic state of a given system, *i.e.*, every element of Γ_p , is a linear combination of the vectors (13).

An interesting fact is that equilibrium directions are not propagated along equilibrium processes. To see this, note that the change of the Q_b 's along the integral curves of P^a does not vanish identically, that is, for any smooth function f on \mathcal{T} ,

$$\begin{aligned} [P^a, Q_b](f) &= \left[\frac{\partial}{\partial p_a}, \frac{\partial}{\partial q^b} - p_b \frac{\partial}{\partial w} \right] (f) \\ &= -\frac{\partial}{\partial p_a} \left(p_b \frac{\partial f}{\partial w} \right) - p_b \frac{\partial}{\partial w} \left(\frac{\partial f}{\partial p_a} \right) \\ &= -\delta_b^a \frac{\partial f}{\partial w} = -\delta_b^a \xi(f). \end{aligned} \tag{15}$$

Here, δ_b^a is a Kronecker delta, and we have introduced the vector field $\xi = \partial/\partial w$, which is known in contact geometry as the Reeb vector. It is straightforward to see that ξ is a “purely vertical” vector at each point of the TPS in the sense of Definition (11). In fact, it is the unique vector field satisfying:

$$\eta(\xi) = 1 \quad \text{and} \quad d\eta(\xi) = 0, \tag{16}$$

and, thus, can be thought of as indicating the “maximally non-equilibrium” direction at each point of the TPS.

Let us observe a crucial consequence of Equation (15). Since the set (13) generates Γ_p at each point in the TPS, then any non-vanishing Lie-bracket of vectors in Γ_p will be necessarily vertical. This means that the equilibrium connection Γ is non-integrable [44]. We will return to this point in the next section when we discuss its relevance on conformal gauge invariance.

Now, we have a basis for the tangent space $T_p\mathcal{T}$, composed by the Reeb vector ξ and the horizontal basis in (13). Notice, however, that we do not have yet a notion of orthogonality for the vector fields ξ , P^a and Q_a . The only information available thus far is that every tangent vector to any point in the TPS can be uniquely decomposed into a vertical part and its equilibrium (horizontal) directions, namely:

$$X \in T_p\mathcal{T} \iff X = X_\xi \xi + \sum_{a=1}^n (X_a^p P^a + X_a^q Q_a), \tag{17}$$

thus the tangent space at each point of the TPS is split into a vertical direction and $2n$ horizontal directions defined by the first law, namely:

$$T_p\mathcal{T} = V_\xi \oplus \Gamma_p. \tag{18}$$

In order to introduce the notion of orthogonality between the horizontal and vertical directions, one can introduce a metric structure on the TPS. It was found by Mrugala *et al.* [27] (see also [28]) that there is a natural choice for such a metric based on statistical mechanical arguments, that is:

$$G = \eta \otimes \eta - \sum_{a=1}^n dp_a \overset{s}{\otimes} dq^a \quad \text{where} \quad dp_a \overset{s}{\otimes} dq^a \equiv \frac{1}{2} [dp_a \otimes dq^a + dq^a \otimes dp_a] \tag{19}$$

Introducing a metric at this stage raises several questions about its possible significance, e.g., if there is a physical quantity associated with the length of a curve, the interpretation of the curvature of its Levi–Civita connection, Killing symmetries, *etc.* None of these issues will be addressed in this work. We will limit ourselves to using the metric as an inner product for the tangent vectors of $T_p\mathcal{T}$ (see [34] for a physical interpretation of the length of particular curves on the TPS corresponding to irreversible fluctuations).

A word of warning is warranted. It can be directly verified that the metric (19) is not positive definite, that is there are non-zero tangent vectors whose norm vanishes identically. To see this, remember that a metric tensor is a bi-linear map (linear in its two arguments), and hence, it is completely determined by its action on a set of basis vectors. Thus, using the decomposition (18) together with the horizontal basis (13), it follows that:

$$G(\xi, \xi) = 1, \quad G(P^a, Q_b) = -\frac{1}{2}\delta_b^a \quad \text{and} \quad G(\xi, P^a) = G(\xi, Q_a) = 0. \tag{20}$$

Interestingly, the remaining combinations vanish identically, that is:

$$G(Q_a, Q_b) = G(P^a, P^b) = 0. \tag{21}$$

There are two important things to be noticed in the above expressions. On the one hand, the metric G makes the splitting of the tangent spaces (18) orthogonal. On the other hand, the vectors generating the horizontal basis, Equation (13), form a set of null vectors (whose norm is zero) at every point of \mathcal{T} . In general, the norm of a vector in $T_p\mathcal{T}$ (*cf.* Equation (17)) is simply given by:

$$G(X, X) = X_\xi^2 - \sum_{a=1}^n X_q^a X_a^p, \tag{22}$$

and thus, we can immediately see that a linear combination of null vectors is not necessarily null.

Now, we want to express the metric tensor in (19) in a coordinate-free manner putting into play the role of η and $d\eta$ as the connection one-form and the curvature two-form, respectively. In terms of the geometry of contact Riemannian manifolds, the result of this derivation means that the metric (19) is associated and compatible with the contact one-form η (*cf.* [36,37]). Since the equilibrium connection Γ is non-integrable, the action of the curvature [45] of the connection one-form (12) on pairs of horizontal vectors $U, V \in \Gamma_p$,

$$d\eta = \sum_{a=1}^n [dp_a \wedge dq^a](U, V) = \frac{1}{2} \sum_{a=1}^n [dp_a(U)dq^a(V) - dp_a(V)dq^a(U)], \tag{23}$$

does not necessarily vanish. In this case, one can observe a similarity of such action with the second term in the right-hand side of (19). Let us exhibit this fact with a short calculation. Consider the coordinate expression of the two horizontal vectors U and V , namely:

$$U = \sum_{a=1}^n [U_a^p P^a + U_q^a Q_a] \quad \text{and} \quad V = \sum_{a=1}^n [V_a^p P^a + V_q^a Q_a]. \tag{24}$$

Their inner product is given by:

$$\begin{aligned} G(U, V) &= \eta(U)\eta(V) - \frac{1}{2} \sum_{a=1}^n [dp_a(U) dq^a(V) + dq^a(U) dp_a(V)] \\ &= -\frac{1}{2} \sum_{a=1}^n [U_a^p V_q^a + V_a^p U_q^a], \end{aligned} \tag{25}$$

where the contribution from the first term vanishes identically, since we are assuming $U, V \in \Gamma_p$. Now, a similar calculation using the exterior derivative of the connection one-form yields:

$$\begin{aligned} -d\eta(U, V) &= -\frac{1}{2} \sum_{a=1}^n [dp_a(U) dq^a(V) - dq^a(U) dp_a(V)] \\ &= -\frac{1}{2} \sum_{a=1}^n [U_a^p V_q^a - V_a^p U_q^a]. \end{aligned} \tag{26}$$

There is an obvious sign difference due to the fact that the metric is a symmetric tensor, whereas $d\eta$ is anti-symmetric. However, we can use here the same argument used in Kähler geometry and introduce a linear transformation of the tangent space at each point, namely $\Phi : T_p\mathcal{T} \rightarrow T_p\mathcal{T}$, such that:

$$\begin{aligned} -d\eta(\Phi U, V) &= -\frac{1}{2} \sum_{a=1}^n [dp_a(\Phi U) dq^a(V) - dq^a(\Phi U) dp_a(V)] \\ &= -\frac{1}{2} \sum_{a=1}^n [U_a^p V_q^a + V_a^p U_q^a] = G(U, V). \end{aligned} \tag{27}$$

The map Φ is known in para-Sasakian geometry as the almost para-contact structure [28]. Since Φ is a linear map, it is uniquely determined by its action on the basis vectors. Thus, one can quickly verify that the desired transformation has to satisfy:

$$\Phi\xi = 0, \quad \Phi P^a = P^a \quad \text{and} \quad \Phi Q_a = -Q_a. \tag{28}$$

Thus, P^a and Q_a are eigenvectors of Φ with eigenvalues one and -1 , respectively, and a local expression for $\Phi : T_p\mathcal{T} \rightarrow \Gamma_p$ in this adapted basis is simply:

$$\Phi = dp_a \otimes P^a - dq^a \otimes Q_a. \tag{29}$$

Now, we can replace the coordinate dependent part in Equation (19) with an equivalent purely geometric (coordinate independent) expression. Furthermore, since $d\eta$ “kills” the vertical part of any tangent vector (*cf.* Equation (16)), our expressions are carried to any tangent vector. Therefore, for any pair of tangent vectors in $T_p\mathcal{T}$, their inner product is given by:

$$G(X, Y) = \eta(X)\eta(Y) - d\eta(\Phi X, Y), \tag{30}$$

that is, we can use a short-hand notation to re-write Equation (19) as:

$$G = \eta \otimes \eta - d\eta \circ (\Phi \otimes \mathbb{I}), \tag{31}$$

where \circ stands for composition and \mathbb{I} is the identity map on $T_p\mathcal{T}$.

Our final expression for the metric poses a compelling geometric structure, expressed as the sum of the equilibrium connection one-form η and its associated field strength $d\eta$, respectively. This was made with the aid of an intermediate quantity Φ , whose role is revealed by means of its “squared” action on any vector $X \in T_p\mathcal{T}$,

$$\Phi^2 X = \Phi (\Phi X) = \Phi \left(\sum_{a=1}^n [X_a^p P^a - X_a^q Q_a] \right) = \sum_{a=1}^n [X_a^p P^a + X_a^q Q_a], \tag{32}$$

returning its purely horizontal part. This can be easily expressed by:

$$\Phi^2 = \mathbb{I} - \eta \otimes \xi. \tag{33}$$

Finally, Φ can be independently obtained as the covariant derivative of ξ with respect to the Levi–Civita connection of G , closing the hard-wired geometric circuit associated with the first law of thermodynamics [28].

Thus far, we have re-formulated the first law as the definition of a connection whose horizontal vector fields are reversible processes (*cf.* Equations (10) and (11)). This sets up a suitable framework to work out the local symmetries shared by every thermodynamic system, that is the various points of view in which a thermodynamic analysis can be made without changing its physical conclusions. In the present case, such conclusions are restricted to the directions in which a system can evolve and the possible interpretation (not analyzed here) of the thermodynamic length of a generic process, not necessarily an equilibrium one, by means of Metric (31). In the next section, we will analyze an important class of such local symmetries, *i.e.*, conformal gauge symmetries.

3. Conformal Gauge Transformations in Thermodynamics

In the previous section, we presented the first law of thermodynamics as a connection over the TPS, that is the assignment of $2n$ equilibrium directions at each point of the tangent space. Such directions were explicitly obtained as the ones that annihilate a one-form whose local expression is the same for every thermodynamic system. There is, however, a whole class of one-forms generating exactly the same connection, each obtained from the other through multiplication by a non-vanishing function. This is referred to here as a conformal gauge freedom. Thus, the central point of this section is to present the class of transformations that leave the equilibrium connection Γ invariant (*cf.* Equation (10)), together with its corresponding effect on the whole intertwined geometric structure of thermodynamic fluctuation theory, namely the para-Sasakian structure $(\mathcal{T}, \eta, \xi, \Phi, G)$.

Consider the thermodynamic connection one-form η . It is easy to see that any re-scaling $\eta' = \Omega\eta$ defines the same equilibrium directions at each point as the original η , that is:

$$X \in \Gamma_p \iff \Omega\eta(X) = 0. \tag{34}$$

here, Ω is any smooth and non-vanishing function on \mathcal{T} . This means we can use indistinctly η or η' to indicate the equilibrium directions at each point of \mathcal{T} [47]. This, however, does change the associated metric structure. In particular, for an arbitrary re-scaling, the curvature of the thermodynamic connection η is not preserved, as can be immediately confirmed by considering a generic pair of horizontal vectors $U, V \in \Gamma_p$ (cf. Equation (24)) and making:

$$d\eta'(U, V) = \Omega d\eta(U, V) + \frac{1}{2} [d\Omega(U)\eta(V) - d\Omega(V)\eta(U)] = \Omega d\eta(U, V). \tag{35}$$

Moreover, the directions annihilated by $d\eta$ do not coincide with those of $d\eta'$. That is, while $d\eta(\xi) = 0$, we have:

$$d\eta'(\xi) = \Omega d\eta(\xi) + [d\Omega \wedge \eta](\xi) = \frac{1}{2} [d\Omega(\xi)\eta - d\Omega], \tag{36}$$

where in the last equality, we have used the two expressions in (16). In general, the last term does not vanish, and therefore, the orthogonality of the equilibrium split of the tangent space (18) is not trivially preserved. This is a consequence of the non-integrability of the equilibrium connection Γ . In the following lines, we will obtain the way in which the various objects introduced in the previous section change when using a different gauge.

Let us take the defining properties of the Reeb vector field, Equation (16), as our starting point. We need a new vertical vector field satisfying:

$$\eta'(\xi') = 1 \quad \text{and} \quad d\eta'(\xi') = 0. \tag{37}$$

The first condition is easily met if we define the new vertical vector field as:

$$\xi' \equiv \frac{1}{\Omega} (\xi + \zeta) \tag{38}$$

where we have introduced an arbitrary horizontal vector field $\zeta \in \Gamma_p$ whose exact form will be determined shortly.

The second condition in Equation (37) is not as trivial. A direct evaluation yields:

$$\begin{aligned} d\eta'(\xi') &= \Omega d\eta(\xi') + \frac{1}{2} [d\Omega(\xi')\eta - \eta(\xi')d\Omega] \\ &= d\eta(\zeta) + \frac{1}{2\Omega} [\xi(\Omega)\eta + d\Omega(\zeta)\eta - d\Omega], \end{aligned} \tag{39}$$

where we have used the fact that $d\Omega(\xi) = \xi(\Omega)$. Now, we are demanding that Equation (39) must vanish identically, that is:

$$d\eta(\zeta) + \frac{1}{2\Omega} [\xi(\Omega)\eta + d\Omega(\zeta)\eta - d\Omega] = 0. \tag{40}$$

Evaluating the above expression on ξ and recalling that $d\eta$ annihilates ξ , we obtain that:

$$d\Omega(\zeta) = 0. \tag{41}$$

Now, recalling that Ω is fixed by the change of the gauge (34), we have obtained the desired equation for ζ . Moreover, substituting (41) back into (40), we obtain the expression for the derivative of the scaling factor:

$$d\Omega = 2\Omega d\eta(\zeta) + \xi(\Omega)\eta. \tag{42}$$

From these calculations, we see that the auxiliary equilibrium (horizontal) vector field ζ plays a central geometric role. Note that in the new gauge η' , the fundamental vertical vector field ξ' is tilted with respect to its unprimed counterpart, that is it has a horizontal component. However, the equilibrium directions are unaltered and, therefore, are generated by the same basis vectors (13). Thus, we write the equilibrium split at each point as:

$$T_p\mathcal{T} = V_\xi \oplus \Gamma_p = V_{\xi'} \oplus \Gamma_p. \tag{43}$$

Note that the expression for ξ' was obtained by requiring that its geometrical properties be the same as those of ξ in the new gauge (cf. Equations (16) and (37)). From the same reasoning, in analogy to (31), we require the new metric to be given by:

$$G' = \eta' \otimes \eta' - d\eta' \circ (\Phi' \otimes \mathbb{I}). \tag{44}$$

The task is to find an expression for G' solely in terms of unprimed objects, and just as in deriving (31), this reduces to obtaining an expression for the new map Φ' . Since Φ' is just a linear transformation of each tangent space and the horizontal directions were not changed by the new gauge, its action on the horizontal basis must be the same as that of Φ (cf. Equation (29)). Therefore, in order to preserve the properties (28), we only have to guarantee that its action on ξ' vanishes. The most general linear expression capturing these observations is $\Phi' = \Phi + \eta \otimes Z$, where the vector field Z is easily determined by the requirement $\Phi'(\xi') = 0$. Thus, a straightforward calculation reveals that:

$$\Phi' = \Phi - \eta \otimes \Phi(\zeta). \tag{45}$$

This implies that Φ and Φ' coincide on horizontal vectors, as has to be the case.

Consider two vector fields $X, Y \in T_p\mathcal{T}$ and their inner product in terms of the new gauge. This is expressed by the action of (44) as:

$$G'(X, Y) = \Omega^2 \eta(X)\eta(Y) - \left[\Omega d\eta(\Phi'X, Y) + \frac{1}{2} d\Omega(\Phi'X)\eta(Y) - \frac{1}{2} d\Omega(Y)\eta(\Phi'X) \right]. \tag{46}$$

We work out each individual term inside the brackets separately. Let us do this in reverse order and start with the last term. One can immediately see that:

$$\eta(\Phi'X) = \eta[\Phi X - \eta(X)\Phi(\zeta)] = 0 \tag{47}$$

since both ΦX and $\Phi\zeta$ are, by construction, horizontal. Now, using the expression we obtained for the differential of the scaling factor (cf. Equation (42), above), combined with the action of Φ' , we can re-write the next term as:

$$\begin{aligned} d\Omega(\Phi'X)\eta(Y) &= 2\Omega d\eta(\zeta, \Phi'X) + \xi(\Omega)\eta(\Phi'X) \\ &= -2\Omega d\eta(\Phi'X, \zeta) \\ &= -2\Omega [d\eta(\Phi X, \zeta) - \eta(X)d\eta(\Phi\zeta, \zeta)] \\ &= -2\Omega [d\eta(\Phi X, \zeta) + \eta(X)G(\zeta, \zeta)]. \end{aligned} \tag{48}$$

Finally, a simple expansion of the first term yields:

$$\Omega d\eta(\Phi'X, Y) = \Omega d\eta(\Phi X, Y) - \Omega \eta(X) d\eta(\Phi \zeta, Y). \tag{49}$$

To conclude, note that both expressions, $d\eta(\Phi X, \zeta)$ in (48) and $d\eta(\Phi \zeta, Y)$ in (49), correspond to inner products involving at least one equilibrium vector. Thus, we can re-write them as $G(\zeta, X)$ and $G(\zeta, Y)$, respectively. Substituting (47) to (49) back into (46), adding the null term $\Omega [\eta(X)\eta(Y) - \eta(X)\eta(Y)]$ and collecting the various resulting expressions, we obtain:

$$G'(X, Y) = \Omega [\Omega - 1 + G(\zeta, \zeta)] \eta(X)\eta(Y) + \Omega [G(X, Y) + \eta(X)z(Y) + \eta(Y)z(X)], \tag{50}$$

where we used the shorthand $z \equiv G(\zeta)$. Hence, our final expression for the primed metric reads:

$$G' = \Omega \left[G + 2\eta \overset{s}{\otimes} z \right] + \Omega [\Omega - 1 + G(\zeta, \zeta)] \eta \otimes \eta. \tag{51}$$

The only ambiguity left is an exact expression for ζ . However, this can be easily obtained recalling once again that $\zeta \in \Gamma_p$. Thus, using the horizontal basis (13), we can write it as:

$$\zeta = \sum_{a=1}^n [\zeta_a^p P^a + \zeta_a^q Q_a] \implies \Phi \zeta = \sum_{a=1}^n [\zeta_a^p P^a - \zeta_a^q Q_a]. \tag{52}$$

Now, a straightforward calculation reveals that:

$$G^{-1} [d\eta(\zeta)] = G^{-1} \left[\sum_{a=1}^n dp_a \wedge dq^a \left(\sum_{b=1}^n [\zeta_b^p P^b + \zeta_b^q Q_b] \right) \right] = - \sum_{a=1}^n [\zeta_a^p P^a - \zeta_a^q Q_a], \tag{53}$$

where the inverse metric is given by:

$$G^{-1} = \xi \otimes \xi - 4 \sum_{a=1}^n P^a \overset{s}{\otimes} Q_a. \tag{54}$$

Finally, using (42) to obtain the coordinate independent expression:

$$\Phi \zeta = -G^{-1} [d\eta(\zeta)] = -\frac{1}{2\Omega} [G^{-1}(d\Omega) - \xi(\Omega)\xi], \tag{55}$$

and recalling the action of Φ^2 (cf. Equations (32) and (33) in the previous section), it follows that:

$$\zeta = -\frac{1}{2\Omega} \Phi [G^{-1}(d\Omega)]. \tag{56}$$

Thus, we have completely determined the new structures in terms of the old ones and the scaling factor relating them. Let us summarize the action of a change of gauge $(\mathcal{T}, \eta, \xi, \Phi, G) \longrightarrow (\mathcal{T}, \eta', \xi', \Phi', G')$, that is:

$$\eta' = \Omega \eta, \tag{57}$$

$$\xi' = \frac{1}{\Omega} (\xi + \zeta), \tag{58}$$

$$\Phi' = \Phi + \frac{1}{2\Omega} \eta \otimes [G^{-1}(d\Omega) - \xi(\Omega)\xi], \tag{59}$$

$$G' = \Omega \left(G + 2\eta \overset{s}{\otimes} G(\zeta) \right) + \Omega [\Omega - 1 + G(\zeta, \zeta)] \eta \otimes \eta, \tag{60}$$

where ζ is given by (56). We call the transformation (57) to (60) a conformal gauge transformation of the thermodynamic phase space [48]. Here, a gauge choice corresponds to a choice of η defining the equilibrium connection.

To close this section, we shall make a few remarks on conformal gauge invariance in equilibrium thermodynamics, that is the mathematical structures that are indistinguishable along equilibrium processes when we make a change of gauge. Firstly, notice that the curvature of the thermodynamic connection one-form is not a conformally gauge-invariant object, as opposed to a standard gauge theory. This is because the equilibrium connection Γ is, by construction, non-integrable (cf. Equations (15) and (16)). This can be interpreted physically by saying that thermodynamic fluctuations are not gauge invariant. Secondly, note that in spite of the rather non-trivial expression for the transformed metric, Equation (60), its action on equilibrium vectors, say $U, V \in \Gamma_p$, is remarkably simple, that is:

$$G'(U, V) = \Omega G(U, V). \tag{61}$$

Thus, in the primed gauge, the inner product between the basis vectors (13) for the horizontal space Γ_p is:

$$G'(P^a, Q_b) = -\Omega \delta^a_b, \quad G'(P^a, P^b) = 0 \quad \text{and} \quad G'(Q_a, Q_b) = 0. \tag{62}$$

Notoriously, one can immediately see that the null equilibrium directions at each point of the TPS are exactly the same. Thus, the null structure is gauge invariant. Thirdly, the linear transformation Φ that we introduced on the tangent space at each point of \mathcal{T} to obtain a coordinate-free expression for the metric tensor is also a gauge invariant object with respect to equilibrium processes,

$$\Phi'U = \Phi U \quad \text{for every} \quad U \in \Gamma_p. \tag{63}$$

Thus, combining the statistical origin of the metric [27,28] and the fact that its null directions are eigenvectors of Φ suggests that there is a physical role played by this structure. This will be the subject of future investigations. We believe that quantities that can be directly linked to gauge-invariant structures for equilibrium thermodynamics will be of great interest, since, on the one hand, their meaning will have a universal scope (valid for every thermodynamic system) and, on the other, their values are independent of the thermodynamic representation one decides to use.

4. Change of Thermodynamic Representation as a Gauge Transformation

In the previous sections, we explored some of the consequences of the geometrization of the first law as a connection of the TPS. In this section, we will study a particular example and observe that the various thermodynamic representations are all related by conformal gauge transformations. It follows that, albeit the directions in which a state can evolve through an equilibrium path are independent of the thermodynamic representation, the fluctuations associated with the path will be different when using a different gauge.

Consider the conformal gauge transformation defined by:

$$\eta' = \frac{1}{p_1} \eta = \frac{1}{p_1} dw + dq^1 + \sum_{a=2}^n \frac{p_a}{p_1} dq^a, \tag{64}$$

where it is assumed that the Darboux neighborhood does not contain points where p_1 vanishes. Now, let us follow the prescription for a gauge transformation given by Equations (56)–(60). We start by computing the horizontal vector field ζ in the definition of ξ' . Using (56) together with the expression for the inverse metric (54) and recalling the action of Φ on the horizontal basis (28), we have that:

$$\zeta = -\frac{1}{2}p_1\Phi G^{-1} \left[d \left(\frac{1}{p_1} \right) \right] = \frac{1}{p_1}Q_1. \tag{65}$$

Thus, the fundamental primed vertical vector field is given by:

$$\xi' = p_1(\xi + \zeta) = p_1 \left(\xi + \frac{1}{p_1}Q_1 \right) = \frac{\partial}{\partial q^1}, \tag{66}$$

where we have used the definition of the horizontal basis (13) and the fact that in these coordinates, $\xi = \partial/\partial w$. Indeed, it can be directly verified that:

$$\eta'(\xi') = \frac{1}{p_1}dw \left(\frac{\partial}{\partial q^1} \right) + dq^1 \left(\frac{\partial}{\partial q^1} \right) + \sum_{a=2}^n \frac{p_a}{p_1}dq^a \left(\frac{\partial}{\partial q^1} \right) = 1, \tag{67}$$

whereas, noting that $\partial/\partial q^1 = Q_1 + p_1\partial/\partial w$,

$$\begin{aligned} d\eta' \left(Q_1 + p_1 \frac{\partial}{\partial w} \right) &= \left[\frac{1}{p_1}d\eta + d \left(\frac{1}{p_1} \right) \wedge \eta \right] \left(Q_1 + p_1 \frac{\partial}{\partial w} \right) \\ &= \frac{1}{p_1}d\eta(Q_1) - \frac{1}{2}\eta \left(Q_1 + p_1 \frac{\partial}{\partial w} \right) d \left(\frac{1}{p_1} \right) \\ &= -\frac{1}{2p_1}dp_1 + \frac{1}{2p_1}dp_1 = 0. \end{aligned} \tag{68}$$

The transformation for Φ is just a straightforward calculation, whose result is:

$$\Phi' = \Phi + \frac{p_1}{2}\eta \otimes \left[G^{-1} \left(d \frac{1}{p_1} \right) \right] = \Phi - \frac{1}{p_1}\eta \otimes Q_1. \tag{69}$$

Finally, in order to obtain the expression for the transformed metric, note that for this gauge, ζ is a re-scaling of a null vector (*cf.* Equation (65) together with (21)). Hence, its squared norm, $G(\zeta, \zeta)$, is identically zero. Thus, it only remains to evaluate the expression:

$$G(\zeta) = -\sum_{a=1}^n \left[dp_a \overset{s}{\otimes} dq^a \right] (\zeta) = -\frac{1}{2} \sum_{a=1}^n [dq^a(\zeta)dp_a] = -\frac{1}{2p_1}dp_1. \tag{70}$$

Therefore, the primed metric takes the form:

$$G' = \frac{1}{p_1} \left[G - \frac{1}{p_1}\eta \overset{s}{\otimes} dp_1 \right] + \left[\frac{1-p_1}{p_1^2} \right] \eta \otimes \eta, \tag{71}$$

whose restriction on vectors belonging to the equilibrium connection Γ at any point of the neighborhood is simply:

$$G'|_{\Gamma} = \frac{1}{p_1} G|_{\Gamma}. \tag{72}$$

The relevance of this exercise is that the conformal gauge transformation presented here corresponds to a change of thermodynamic representation. To see this, let us consider a closed system with the

change of gauge defined in (7). It is clear that the equilibrium directions for both η_s and η_u are the same, as shown in the previous section. Hence, they both annihilate the vectors in Γ_p . Moreover, noticing that $p_1 = -T$ in this case and that by Equation (29):

$$\Phi_u = -(T ds - p dv) \otimes \frac{\partial}{\partial u} - ds \otimes \frac{\partial}{\partial s} - dv \otimes \frac{\partial}{\partial v} + dT \otimes \frac{\partial}{\partial T} + dp \otimes \frac{\partial}{\partial p}, \tag{73}$$

we can use Equations (66), (69) and (71) to obtain:

$$\xi'_u = -T \left[\frac{\partial}{\partial u} - \frac{1}{T} \left(\frac{\partial}{\partial s} + T \frac{\partial}{\partial u} \right) \right] = \frac{\partial}{\partial s} = \xi_s, \tag{74}$$

$$\begin{aligned} \Phi'_u &= \Phi_u - \frac{1}{T} \eta_u \otimes Q_1 = \Phi_u + \left(ds - \frac{1}{T} du - \frac{p}{T} dv \right) \otimes \left(\frac{\partial}{\partial s} + T \frac{\partial}{\partial u} \right) \\ &= -(T ds - p dv) \otimes \frac{\partial}{\partial u} - ds \otimes \frac{\partial}{\partial s} - dv \otimes \frac{\partial}{\partial v} + dT \otimes \frac{\partial}{\partial T} + dp \otimes \frac{\partial}{\partial p} \\ &= - \left(\frac{1}{T} du + \frac{p}{T} dv \right) \otimes \frac{\partial}{\partial s} - du \otimes \frac{\partial}{\partial u} - dv \otimes \frac{\partial}{\partial v} + dT \otimes \frac{\partial}{\partial T} + dp \otimes \frac{\partial}{\partial p} = \Phi_s, \end{aligned} \tag{75}$$

$$\begin{aligned} G'_u &= -\frac{1}{T} \left(G_u + \frac{1}{T} \eta_u \overset{s}{\otimes} dT \right) + \frac{1}{T} \left(\frac{1}{T} + 1 \right) \eta^U \otimes \eta^U \\ &= -\frac{1}{T} \left(\eta_u \otimes \eta_u + ds \overset{s}{\otimes} dT - dv \overset{s}{\otimes} dp + \frac{1}{T} \eta_u \overset{s}{\otimes} dT \right) + \frac{1}{T} \left(\frac{1}{T} + 1 \right) \eta_u \otimes \eta_u \\ &= \eta_s \otimes \eta_s + du \overset{s}{\otimes} d \left(\frac{1}{T} \right) + dv \overset{s}{\otimes} d \left(\frac{p}{T} \right) = G_s. \end{aligned} \tag{76}$$

Equation (76) means that the metrics G_u and G_s on \mathcal{T} are related to each other by the precise conformal gauge transformation that corresponds to a change in the thermodynamic representation (cf. Equations (6) and (7)). Moreover, it follows that on the equilibrium connection Γ , we obtain:

$$\Phi_u|_\Gamma = \Phi_s|_\Gamma \quad \text{and} \quad G_u|_\Gamma = -\frac{1}{T} G_s|_\Gamma. \tag{77}$$

Thus, we see explicitly that the restriction of Φ to Γ is invariant under conformal gauge transformations, whereas we obtain a conformal relationship between G_u and G_s when they are restricted to Γ , which exactly induces the re-scaling between Weinhold and Ruppeiner’s metrics on each Legendre sub-manifold (cf. (6)).

5. Closing Remarks

In thermodynamics, equilibrium (*i.e.*, reversible) processes are defined by the first law (1). In this work, we have given a general geometric statement of the first law in terms of a connection on the thermodynamic phase space. Indeed, we have shown that (1) defines the equilibrium connection Γ (cf. Equations (10) and (11)). Note that the connection one-form η defining Γ is not unique. Indeed, any non-vanishing re-scaling $\eta' = \Omega \eta$ shares the same kernel with η and, thus, defines the same equilibrium connection. Therefore, we call a fixing of a particular one-form determining Γ a conformal gauge choice. The name conformal is in place to denote a difference with gauge theories, such as electromagnetism, where one demands gauge invariance on the curvature of the connection, also referred to as field strength. There, a choice of gauge refers to selecting a one-form generating the same field, whereas in our case, a

choice of conformal gauge refers to selecting a one-form generating the same connection. An interesting property of the equilibrium connection is that it is always non-integrable, which means that its curvature does not vanish, independently of the choice of the conformal gauge.

To introduce a further notion of orthogonality between the horizontal (*i.e.*, reversible) and vertical (*i.e.*, irreversible) directions with respect to the equilibrium connection Γ , we followed the work of Mrugala *et al.* [27] and equipped the thermodynamic phase space with the indefinite metric structure (19). One can justify such a choice by means of the statistical mechanical arguments contained in [27] and [28]. Interestingly, the null directions of such a metric correspond precisely to the basis elements generating the horizontal directions (13). The physical significance of such directions remains to be explored and will be the subject of future work. Here, we have given a coordinate invariant formulation (31) of the metric (19), which highlights the role played by the connection one-form η , as well as by the curvature $d\eta$ in the definition of the distance and explicitly shows that this is an associated metric in the sense of contact Riemannian geometry [36,37].

The main use of presenting equilibrium thermodynamics as a connection theory relies on the notion of gauge invariance, *i.e.*, those geometric objects that are independent of the particular gauge choice. From the mathematical point of view, the conformal gauge transformations presented here are relevant because they preserve the para-Sasakian structure [29]. As we have argued, in thermodynamics, the curvature of the equilibrium connection is not a gauge-invariant object, nor is the metric. Here, we found the explicit transformations relating the various geometric objects defining the thermodynamic phase space under a conformal gauge transformation. The explicit formulas are summarized by Equations (57)–(60). We observed that the null directions of the metric are gauge invariant. Additionally, when restricted to horizontal directions, the tensor field Φ is also gauge invariant, and the metric structures are conformally related. As an example, we have shown that Metrics (8) and (9), which induce Weinhold and Ruppeiner's metrics on Legendre sub-manifolds, respectively, are precisely related by the conformal gauge transformation that corresponds to the change in the thermodynamic representation from energy to entropy. This in turn implies that the restriction of such metrics to the equilibrium connection Γ yields the well-known conformal relation (6).

Finally, let us close this work with some comments on the geometry of the equilibrium connection, its conformal gauge transformations and their physical relevance in various prospect applications. Firstly, the construction presented here exhibits the principal bundle nature of the thermodynamic phase space. That is, we readily have a $2n$ -dimensional (symplectic) base manifold together with a one-dimensional fiber isomorphic to the real line. Such a construction might be suitable to make use of the theory of characteristic classes to formulate universal statements about the nature of thermodynamic processes. Secondly, from the fact that the curvature form of the connection is not preserved by a change of thermodynamic representation together with its statistical origin, one can conclude that thermodynamic fluctuations are not gauge invariant. This is interesting, because thermodynamic fluctuations enter the description of irreversible processes. Therefore, our results can provide new geometric insights on the different extremization problems that one encounters in non-equilibrium thermodynamics, *e.g.*, minimizing dissipation *versus* maximizing work.

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Author Contributions

Each author made an equally valuable contribution in preparing this manuscript. All authors have read and approved the final manuscript.

Conflicts of Interest

The authors declare no conflict of interest.

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15. Actually, Ruppeiner defines his metric for an open system at fixed volume, and therefore, it is defined in terms of densities variables rather than molar ones. However, it has become common in the literature to refer to Equation (5) also as Ruppeiner's metric, as we do here. Moreover, notice that the original definition of the metric by Ruppeiner has a global sign difference with the metric considered here. Of course, this difference does not change any physical result, but it is better for us to use the opposite sign convention in order to get the same conformal factor in Equation (6) as in Equation (7).
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44. A connection is called integrable if the Lie-bracket of any pair of horizontal vector fields is horizontal [32].
45. Since the tangent space to the TPS with the equilibrium connection is a line bundle, the curvature form $\Omega = d\eta + \eta \wedge \eta$ coincides with $d\eta$. Notice also that throughout this work, we are using a convention in which the wedge product is defined with the numerical pre-factor 1/2, as in [32], while other references define such a product without such a pre-factor [46]. Therefore, some formulas can look different by a factor of 1/2 with respect to other references, as, e.g., in (26) and (27) (for instance, with respect to [28]). Here, we choose this convention in order to make evident the relation between the second term in the metric and the curvature of the equilibrium connection and to match with standard references in contact geometry [36,37].
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47. Usually, in contact geometry, η is called the contact form, and infinitesimal transformations generating a re-scaling of η as in (34) are known as contact transformations or contactomorphisms [36,37].
48. In contact geometry, (57) to (60) are known simply as a gauge transformation [36], but we decide here to add the adjective conformal as in [29] in order to distinguish such transformations from those of gauge theories.