Curvature as a Measure of the Thermodynamic Interaction

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(January 2010)

Abstract

We present a systematic and consistent construction of geometrothermodynamics by using Riemannian contact geometry for the phase manifold and harmonic maps for the equilibrium manifold. We present several metrics for the phase manifold that are invariant with respect to Legendre transformations and induce thermodynamic metrics on the equilibrium manifold. We review all the known examples in which the curvature of the thermodynamic metrics can be used as a measure of the thermodynamic interaction.

PACS numbers: 05.70.-a, 02.40.-k

Keywords: Thermodynamics, Contact geometry, Harmonic maps

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I. INTRODUCTION

Differential geometry is a very important tool of modern science, especially mathematical physics, and it has many applications in physics, chemistry and engineering. In particular, the four known interactions of nature can be described in terms of geometrical concepts. Indeed, Einstein proposed the astonishing principle “field strength = curvature” to understand the physics of the gravitational field (see, for instance, Refs. 1 and 2). In this case, curvature means the curvature of a Riemannian manifold. In general relativity, the connection involved is unique as a consequence of the assumption that the torsion tensor vanishes. The idea of this construction can be represented schematically as

\[
\text{metric} \rightarrow \text{Levi-Civita connection} \rightarrow \text{Riemann curvature} = \text{gravitational field strength}.
\]

The second element of general relativity is Einstein’s field equation \( R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = 8\pi T_{\mu\nu} \), which established for the first time the amazing principle “geometry = energy.” The conceptual fundamentals of this principle were very controversial; however, experimental evidence has shown its correctness, and even modern generalizations of Einstein’s theory follow the same principle. On the other hand, because the field strength can be considered as a measure of the gravitational interaction, we conclude that the entire idea of general relativity can be summarized in the principle “interaction = curvature.”

The discovery by Yang and Mills that the theory of electromagnetism can be described geometrically in terms of the elements of a principal fiber bundle constitutes an additional major achievement. The base manifold is in this case the Minkowski spacetime, the standard fiber is the gauge group \( U(1) \), which represents the internal symmetry of electromagnetism, and the connection across the fibers is a local cross-section, which takes values in the algebra of \( U(1) \). This has opened the possibility of fixing the background metric in accordance with the desired properties of the base manifold and selecting different connections as local cross-sections of the principal fiber bundle. This interesting geometrical approach constitutes the base for constructing the modern gauge theories that are used to describe the physics of the electromagnetic, the weak, and the strong interactions. This construction can be represented

\[
\text{metric} \rightarrow \text{Levi-Civita connection} \rightarrow \text{Riemann curvature} = \text{gravitational field strength}.
\]
schematically as

\[ U(1) - \text{connection} \rightarrow U(1) - \text{curvature} = \text{electromagnetic interaction} \]

\[ \uparrow \]

Minkowski metric \( \rightarrow \) \( SU(2) \) - connection \( \rightarrow \) \( SU(2) \) - curvature = weak interaction

\[ \downarrow \]

\( SU(3) \) - connection \( \rightarrow \) \( SU(3) \) - curvature = strong interaction.

We conclude that the principle “curvature = interaction” holds for all known forces of nature.

Consider now the case of a thermodynamic system. In very broad terms, one can say that in a thermodynamic system, all the known forces act among the particles that constitute the system. Due to the large number of particles involved in the system, only a statistical approach is possible, from which average values for the physical quantities of interest are derived. The question arises whether it is also possible to find a geometric construction for which the principle “curvature = thermodynamic interaction” holds. We will see in the present work that the formalism of geometrothermodynamics (GTD) [4] satisfies this condition. First, we must mention that our interpretation of the thermodynamic interaction is based upon a statistical approach to thermodynamics in which all the properties of the system can be derived from the explicit form of the corresponding Hamiltonian [5], and in which the interaction between the particles of the system is described by the potential part of the Hamiltonian. Consequently, if the potential vanishes, we say that the system has a zero thermodynamic interaction.

In this work, we present the formalism of GTD by using Riemannian contact geometry for the definition of the thermodynamical phase manifold and harmonic maps for the definition of the equilibrium manifold. We will see that this approach allows us to interpret any thermodynamic system as a hypersurface in the equilibrium space completely determined by the field theoretical approach of harmonic maps. This paper is organized as follows: In Section III we introduce the main concepts of Riemannian contact geometry that are necessary to define the phase manifold. Section IV is dedicated to the application of harmonic maps to obtain different aspects of GTD, like the equilibrium manifold and its geodesics. Furthermore, in Section V we present a series of thermodynamic systems described by Riemannian manifolds whose curvature can be interpreted as a measure of thermodynamic interaction. Finally, Section VI is devoted to discussions of our results and suggestions for further research. Throughout this paper, we use units in which \( G = c = k_B = h = 1 \).
The main element of GTD is the thermodynamic phase manifold, which is a Riemannian contact manifold whose contact structure and metric are invariant with respect to Legendre transformations. First, we consider a \((2n + 1)\)-dimensional differential manifold \(\mathcal{T}\) and its tangent manifold \(T\mathcal{T}\). Let \(\mathcal{V} \subset T\mathcal{T}\) be a field of hyperplanes on \(\mathcal{T}\). It can be shown that \(\mathcal{V} = \ker \Theta\), i.e., the kernel of a non-vanishing differential 1-form \(\Theta\). If the Frobenius integrability condition \(\Theta \wedge (d\Theta)^n \neq 0\) is satisfied, the hyperplane field \(\mathcal{V}\) is completely integrable. On the other hand, if \(\Theta \wedge (d\Theta)^n = 0\), then \(\mathcal{V}\) is non-integrable. In the limiting case \(\Theta \wedge (d\Theta)^n \neq 0\), the hyperplane field \(\mathcal{V}\) becomes maximally non-integrable and is said to define a contact structure on \(\mathcal{T}\). The pair \((\mathcal{T}, \mathcal{V})\) is usually known as a contact manifold \([6]\) and is sometimes denoted as \((\mathcal{T}, \Theta)\) to emphasize the role of the contact form \(\Theta\).

Let \(G\) be a non-degenerate metric on \(\mathcal{T}\). The set \((\mathcal{T}, \Theta, G)\) defines a Riemannian contact manifold. Notice that the contact manifold \((\mathcal{T}, \Theta)\) is (almost) uniquely defined in the following sense: The condition \(\Theta \wedge (d\Theta)^n \neq 0\) is independent of \(\Theta\); in fact, it is a property of \(\mathcal{V} = \ker \Theta\). If another 1-form \(\Theta'\) generates the same \(\mathcal{V}\), it must be of the form \(\Theta' = f\Theta\), where \(f : \mathcal{T} \to \mathbb{R}\) is a smooth non-vanishing function. The Riemannian metric \(G\), instead, is completely arbitrary. We will use this freedom to select only those metrics that are invariant under Legendre transformations.

To introduce Legendre transformations in a general fashion, let us choose the coordinates of \(\mathcal{T}\) as \(Z^A = \{\Phi, E^a, I^a\}\) with \(a = 1, \ldots, n\), and \(A = 0, 1, \ldots, 2n\). Here, \(\Phi\) represents the thermodynamic potential used to describe the system whereas the coordinates \(E^a\) correspond to the extensive variables and \(I^a\) to the intensive variables. Notice that in the manifold \(\mathcal{T}\), all the coordinates \(\Phi, E^a\) and \(I^a\) must be completely independent; thus, thermodynamic systems cannot be described in \(\mathcal{T}\). A Legendre transformation is defined as \([7]\)

\[
\{Z^A\} \longrightarrow \{\tilde{Z}^A\} = \{\tilde{\Phi}, \tilde{E}^a, \tilde{I}^a\},
\]

\[
\Phi = \tilde{\Phi} - \delta_{kl} \tilde{E}^k \tilde{I}^l, \quad E^i = -\tilde{I}^i, \quad E^j = \tilde{E}^j, \quad I^i = \tilde{E}^i, \quad I^j = \tilde{I}^j,
\]

where \(i \cup j\) is any disjoint decomposition of the set of indices \(\{1, \ldots, n\}\), and \(k, l = 1, \ldots, i\). In particular, for \(i = \{1, \ldots, n\}\) and \(i = \emptyset\), we obtain the total Legendre transformation and the
identity, respectively. In these particular coordinates, the contact 1–form can be written as

$$\Theta = d\Phi - \delta_{ab} I^a dE^b, \quad \delta_{ab} = \text{diag}(1, 1, \ldots, 1),$$

an expression that is manifestly invariant with respect to the Legendre transformations in Eq. (2). Consequently, the contact manifold \((\mathcal{T}, \Theta)\) is a Legendre invariant, as will be the Riemannian contact manifold \((\mathcal{T}, \Theta, G)\), if we demand Legendre invariance of the metric \(G\).

Any Riemannian contact manifold \((\mathcal{T}, \Theta, G)\) whose components are Legendre invariant is called a thermodynamic phase manifold and constitutes the starting point for a description of thermodynamic systems in terms of geometric concepts. We would like to emphasize the fact that Legendre invariance is an important condition that guarantees that the description does not depend on the choice of the thermodynamic potential, a property that is essential in ordinary thermodynamics.

As mentioned before, the only freedom in the construction of the phase manifold is in the choice of the metric \(G\). Legendre invariance implies a series of algebraic conditions for the metric components \(G_{AB}\), and it can be shown that these conditions are not trivially satisfied. For instance, a straightforward computation shows that the flat metric \(G = \delta_{AB} dZ^A dZ^B\) is not invariant with respect to the Legendre transformations in Eq. (2). It then follows that the phase space is necessarily curved. We performed a detailed analysis of the Legendre invariance conditions and found that the metric

$$G = \left( d\Phi - I_a dE^a \right)^2 + \Lambda \left( E_a I_a \right)^{2k+1} dE^a dI^a, \quad E_a = \delta_{ab} E^b, \quad I_a = \delta_{ab} I^b,$$

where \(\Lambda\) is an arbitrary real constant and \(k\) is an integer, is invariant with respect to partial and total Legendre transformations. To our knowledge, this is the most general metric satisfying the conditions of Legendre invariance. The corresponding scalar curvature

$$R = \frac{2}{\Lambda^2} \left\{ \left[ \sum_{a=1}^n (E_a I_a)^{-2k-1} \right]^2 - 3 \sum_{a \neq b}^n (E_a I_a E_b I_b)^{-2k-1} \right\}$$

shows that the manifold is curved in general.

Furthermore, the phase manifold metric

$$G = \left( d\Phi - I_a dE^a \right)^2 + \Lambda (E_a I^a)^{2k+1} (\chi_{bd} E^b dI^c),$$

where \(\Lambda\) is constant, \(k\) is an integer, and \(\chi_{ab}\) is a constant diagonal tensor, satisfies the conditions that follow from a total Legendre transformation, Eq. (2). The corresponding
curvature is rather cumbersome and cannot be written in a compact form; however, an inspection of its explicit form shows that it is always different from zero.

The metrics in Eqs. (1) and (2) are the most general Legendre invariant metrics we have found so far and contain other known metrics as particular cases [4]. Legendre transformations impose, in general, very strong conditions on the components $G_{AB}$; indeed, Eq. (2) shows that such a transformation can change an extensive variable to the negative of the corresponding intensive variable. This implies that only very specific combinations of extensive and intensive variables can be invariant under Legendre transformations.

III. HARMONIC MAPS

Consider two (pseudo)-Riemannian manifolds $(M, \gamma)$ and $(M', \gamma')$ of dimension $m$ and $m'$, respectively. Let the base manifold $M$ be coordinatized by $x^\alpha (\alpha, \beta, \gamma, ... = 1, 2, ..., m)$, and $M'$ by $x'^\mu (\mu, \nu, \lambda, ... = 1, 2, ..., m')$, so that the metrics on $M$ and $M'$ can be, in general, smooth functions of the corresponding coordinates, i.e., $\gamma = \gamma(x)$ and $\gamma' = \gamma'(x')$. A harmonic map is a smooth map $\varphi : M \to M'$, or in coordinates $\varphi : x \mapsto x'$ so that $x'$ becomes a function of $x$. The $x'$s satisfy the field equations following from the action [8]

$$ S = \frac{1}{2} \int d^m x \sqrt{|\det(\gamma)|} \gamma^{\alpha\beta}(x) \frac{\partial x'^\mu}{\partial x^\alpha} \frac{\partial x'^\nu}{\partial x^\beta} \gamma'_{\mu\nu}(x') , $$

which sometimes is called the “Dirichlet energy functional” of the harmonic map $\varphi$. The straightforward variation of $S$ with respect to $x'^\mu$ leads to the field equations

$$ \frac{1}{\sqrt{|\det(\gamma)|}} \frac{\partial}{\partial x^\beta} \left( \sqrt{|\det(\gamma)|} \gamma^{\alpha\beta}(x) \frac{\partial x'^\mu}{\partial x^\alpha} \right) \Gamma^\mu_{\nu\lambda} \gamma^{\alpha\beta} \frac{\partial x'^\nu}{\partial x^\alpha} \frac{\partial x'^\lambda}{\partial x^\beta} = 0 , $$

where $\Gamma^\mu_{\nu\lambda}$ are the Christoffel symbols associated with the metric $\gamma'_{\mu\nu}$ of the target manifold $M'$. If $\gamma'_{\mu\nu}$ is a flat metric, one can choose Cartesian-like coordinates such that $\gamma'_{\mu\nu} = \chi_{\mu\nu} = \text{diag}(\pm 1, ..., \pm 1)$, the field equations become linear, and the harmonic map is linear. In the following subsections, we will show that harmonic maps are the correct mathematical tool to investigate the properties of the phase manifold and its submanifolds, which contain information on the physical states of thermodynamic systems.
A. Geodesics of the Phase Manifold

Consider a base manifold with $\dim(M) = 1$ and identify the target manifold with the thermodynamic phase manifold $(\mathcal{T}, \Theta, G)$. Then, the field equations, Eqs. (8), reduce to the geodesic equations

$$\frac{d^2 Z^A}{d\lambda^2} + \Gamma^A_{BC} \frac{dZ^B}{d\lambda} \frac{dZ^C}{d\lambda} = 0,$$

where $\lambda$ is an affine parameter and $\Gamma^A_{BC}$ are the Christoffel symbols of the phase manifold metric $G$. Since any Legendre invariant $G$ has a non-zero curvature, these geodesic equations are highly non-linear and difficult to solve in general. Even special cases of the known metrics in Eqs. (4) and (6) require a detailed analysis that is beyond the scope of the present work. Preliminary results indicate that the geodesics of the phase manifold represent families of thermodynamic systems that can be investigated in the context of GTD.

B. Equilibrium Manifold

Consider the harmonic map $\varphi : \mathcal{E} \to \mathcal{T}$, where $\mathcal{E}$ is a subspace of the phase manifold $(\mathcal{T}, \Theta, G)$ and $\dim(\mathcal{E}) = n$. For the sake of concreteness, let us assume that the extensive variables $\{E^a\}$ are the coordinates of $\mathcal{E}$. Then, in terms of coordinates, the harmonic embedding map reads $\varphi : \{E^a\} \mapsto \{Z^A(E^a)\} = \{\Phi(E^a), E^a, I^a(E^a)\}$. Moreover, the pullback $\varphi^*$ of the harmonic map induces canonically a metric $g$ on $\mathcal{E}$ by means of

$$g = \varphi^*(G), \quad \text{i.e.} \quad g_{ab} = \frac{\partial Z^A}{\partial E^a} \frac{\partial Z^B}{\partial E^b} G_{AB} = Z^A_{,a} Z^B_{,b} G_{AB} .$$

If we assume that the metric $\gamma$ of the base manifold coincides with the induced metric $g$, the action in Eq. (7) reduces to

$$S = \frac{n}{2} \int d^nE \sqrt{|\det(g)|} ,$$

and the field equations become

$$\frac{1}{\sqrt{|\det(g)|}} \left( \sqrt{|\det(g)|} g^{ab} Z^A_{,a} \right)_{,b} + \Gamma^A_{BC} Z^B_{,b} Z^C_{,c} g^{bc} = 0 .$$

The action in Eq. (11) corresponds to the volume element of the submanifold $\mathcal{E} \subset \mathcal{T}$; consequently, the field equations in Eqs. (12) represent the condition for $\mathcal{E}$ to be an extremal
hypersurface in the phase manifold \[9\]. If, furthermore, the harmonic map satisfies the condition \(\varphi^*(\Theta) = 0\), the pair \((\mathcal{E}, g)\) is called an equilibrium manifold. The last condition is equivalent to

\[ d\Phi = I_a dE^a, \quad \frac{\partial \Phi}{\partial E^a} = I_a. \]

(13)

The first of these equations corresponds to the first law of thermodynamics whereas the second one is usually known as the condition for thermodynamic equilibrium \[10\]. We conclude that the harmonic map \(\varphi : \mathcal{E} \to \mathcal{T}\) defines the equilibrium manifold \((\mathcal{E}, g)\) as an extremal submanifold of the phase manifold \((\mathcal{T}, \Theta, G)\) in which the first law of thermodynamics and the equilibrium conditions for a given system with fundamental equation \(\Phi = \Phi(E^a)\) hold.

C. Geodesics of the Equilibrium Manifold

Consider a base manifold with \(\dim(M) = 1\) and identify the target manifold \(M'\) with the equilibrium manifold \((\mathcal{E}, g)\) defined above. Then, the field equations reduce to the geodesic equations in the equilibrium manifold:

\[ \frac{d^2 E^a}{d\tau^2} + \Gamma^a_{bc} \frac{dE^b}{d\tau} \frac{dE^c}{d\tau} = 0, \]

(14)

where \(\Gamma^a_{bc}\) are the Christoffel symbols of the thermodynamic metric \(g\), and \(\tau\) is an arbitrary affine parameter along the geodesic. Because the points of the equilibrium manifold represent equilibrium states in which the thermodynamic system can exist, a geodesic in \((\mathcal{E}, g)\) represents a quasi-static process along which the system can evolve. This has been shown explicitly in the case of an ideal gas \[11\].

IV. EXAMPLES

The harmonic maps presented in the last sections allow us to define geometric structures in an invariant way. In particular, the curvature of the thermodynamic metric \(g\) should represent the thermodynamic interaction independently of the thermodynamic potential. In fact, this is not a trivial condition from a geometric point of view. In particular, a geometric analysis of black–hole thermodynamics by using metrics introduced \(\textit{ad hoc}\) in the equilibrium manifold leads to contradictory results \[12–14\]. Using the induced thermodynamic metric \(g\)
as defined in Section III B, by means of the pullback of the harmonic map, the results are consistent and invariant. For instance, in the particular case of the phase metric in Eq. (6) with $k = 0$ and $\chi_{ab} = \eta_{ab} = \text{diag}(-1, 1, \ldots, 1)$, the induced thermodynamic metric

$$g = \varphi^*(G) = \left( E^c \frac{\partial \varphi}{\partial E^c} \right) \left( \eta_{ab} \delta^{bc} \frac{\partial^2 \varphi}{\partial E^c \partial E^d} dE^a dE^d \right)$$

has been applied to a large class of black–hole configurations in the following theories [15–20]: 2–dimensional dilaton gravity, 3–dimensional Einstein gravity, 4– and higher–dimensional Einstein-Maxwell theory with a cosmological constant, and 5–dimensional Einstein-Gauss-Bonnet theory with electromagnetic and Yang-Mills fields. As a general result, we find that the curvature of the equilibrium manifold is non-vanishing, that it can be used as a measure of the thermodynamic interaction, and that it diverges at those points where second–order phase transitions occur.

From the phase manifold metric in Eq. (4), we obtain the thermodynamic metric

$$g = \Lambda \left( E^a \frac{\partial \Phi}{\partial E^a} \right)^{2k+1} \frac{\partial^2 \Phi}{\partial E^b \partial E^c} \delta^{ab} dE^a dE^c ,$$

which has been used to describe GTD of ordinary thermodynamic systems, like an ideal gas and its non-interacting generalizations, a van der Waals gas, and a 1–dimensional Ising model. We have shown that the arbitrary constant $k$ can be chosen such that the field equations are satisfied. Moreover, we found that the curvature of the equilibrium manifold vanishes only in the case of non-interacting systems, that it is non-zero for interacting systems, and that it diverges at those points where first–order phase transitions occur.

V. CONCLUSIONS

In this paper, we showed that harmonic maps play an important role in the formalism of geometrothermodynamics (GTD). They can be used to derive geodesic equations in different spaces and to introduce in a consistent and invariant way the concept of an equilibrium manifold. It turns out that for a given fundamental equation of the form $\Phi = \Phi(E^a)$, GTD provides an invariant approach to construct the corresponding equilibrium manifold whose points represent equilibrium states. The harmonic map, which determines the equilibrium manifold, also generates a system of differential equations that determine extremal hypersurfaces in the phase manifold. This construction allows us to investigate the properties
of the curvature of the equilibrium manifold and to propose it as an invariant measure of
the thermodynamic interaction. We presented all the examples for which we have shown
that the thermodynamic curvature not only measures the interaction of the thermodynamic
system but also becomes singular at those points where phase transitions occur. Thus, GTD
represents an invariant geometric formalism of standard thermodynamics that resembles the
famous principle “curvature = interaction,” which is valid for all known forces of nature.

Acknowledgments

H. Quevedo and S. Taj would like to thank ICRANet for support.

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