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Metric Thermodynamic Phase Space and Stability Problems

Nicolas Hudon * **Martin Guay** * **Denis Dochain** **

* *Department of Chemical Engineering, Queen's University, Kingston, ON, Canada* ({nicolas.hudon, martin.guay}@queensu.ca)
** *ICTEAM, Université catholique de Louvain, Louvain-la-Neuve, Belgium* (denis.dochain@uclouvain.be)

Abstract: In this note, we study thermodynamic systems described in the Thermodynamic Phase Space (TPS), commonly referred as the contact geometry approach to thermodynamics. Following classical and recent contributions in the field, we try to fill a gap between the contact geometry endowed with a metric and stability problems considered in the literature. This examination leads to new interpretations of previously obtained results, and highlights new problems and avenues for research.

Keywords: Thermodynamic phase space, Contact geometry, Metric geometry, Stability and feedback stabilization

1. INTRODUCTION

One classical approach to study thermodynamics is through contact geometry, as an analogue of symplectic geometry for classical mechanics, reported for example in (Hermann, 1973) and (Mrugala et al., 1991), but dating back to the work by Gibbs and later, by Caratheodory. In the context of control systems analysis and feedback design for thermodynamic systems, contact geometry was considered, through a lift of a given control system, in (Eberard et al., 2007), (Favache et al., 2009), (Favache et al., 2010), (Ramirez et al., 2013), and more recently in (Wang et al., 2015). Stability analysis and feedback stabilization problems were successfully addressed for control systems using the contact geometry approach. As discussed in (Favache et al., 2010), both the energy and entropy functions can serve as the generating potential of the contact lift. The aforementioned results are key to understand stability and stabilization problems for thermodynamic systems: By lifting the n-dimensional controlled dynamics to a $(2n+1)$-dimensional dynamical systems endowed with a contact structure, *i.e.*, a differential one-form encoding thermodynamics evolution constraints, it is possible to restrict stability and stabilization problems to admissible evolutions in an extended vector field. A related point of view on admissible evolution criteria, developed independently in (Hoang and Dochain, 2013), can be related to the contact geometry point of view, see for example the exposition in (Haslach Jr., 1997). The difficulty however, to study stability and stabilization problem, resides in the construction of suitable Lyapunov stability arguments in an extended phase space.

From a more general perspective, the contact geometric, also known as the Thermodynamic Phase Space (TPS), approach has its importance in the field of nonequilibrium thermodynamics, relating classical thermodynamics and dynamic systems far from equilibrium, see for example the contribution proposed in (Grmela, 2002), built on material from (Arnold, 1989), that shows that the thermodynamic reciprocity relations are encoded within this framework. Contact geometry also serves as the basis for the geometrothermodynamics approach to nonequilibrium thermodynamics, see for example the original contribution (Quevedo, 2007) and applications presented in (Quevedo and Tapias, 2014), where the TPS is endowed with a metric, in the spirit of Weinhold and Ruppeiner (Quevedo, 2007), *i.e.*, by using the Hessian of the thermodynamic potential as a metric. An indefinite Riemannian metric was also introduced on the TPS in (Mrugala, 1996), a construction later used in (Preston and Vargo, 2008) to study geometric properties of constitutive surfaces defined for different thermodynamical potentials.

Leaving for further discussions the full review of geometrothermodynamics proposed in (Quevedo, 2007), and in particular the interpretation of phase transitions in terms of the metric on the TPS, the present contribution seeks to consider key problems studied in the aforementioned contributions, namely stability and feedback stabilization by using a metric on the TPS. As such, we follow the discussion in (Preston and Vargo, 2008), referring the interested reader to (Mrugala, 1996) for the technical details about almost-contact structures in this context. The objective is show that by complementing the "classical" contact geometry construction with a suitable choice of metric, it is possible to simplify the stability analysis. Our focus is mainly about stability, and for the time being, we assume that the Hessian of the generating potential is non-degenerated. Using the decomposition construction proposed in (Guay and Hudon, 2016), and introducing the notion of a Riemannian within that context, as done previously in (Bennett et al., 2015), conditions for stability are derived, assuming that the metric, constructed using the Hessian of the generating potential, is non-degenerated. In essence, the proposed approach seeks to identify, in the extended phase space, the dissipative gradient structure with respect to a given metric.

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This note is organized as follows. Necessary background on the TPS endowed with a metric is given in Section 2. In Section 3, the lift of controlled dynamical systems and stability results from the literature are considered using the metric on the TPS. An example is given in Section 4. Conclusions and future areas for investigation are discussed in Section 5.

2. BACKGROUND

We first briefly summarize the formalism of contact geometry for thermodynamics. We follow the exposition given in (Preston and Vargo, 2008), complemented by material from the expositions in (Grmela, 2002) and (Ramirez et al., 2013). A complete exposition of contact geometry can be found in (Arnold, 1989) and (Libermann and Marle, 1987).

We denote the n extensive variables by x^i, $i = 1, \ldots, n$, and the thermodynamical potential by x^0, for example the energy $x^0 = E(\boldsymbol{x})$ or the Entropy $x^0 = S(\boldsymbol{x})$. The n intensive variables are denoted by p_i and are dual to the extensive variables by the relations $p_i = \frac{\partial E}{\partial x^i}$ or $p_i = \frac{\partial S}{\partial x^i}$, depending on the choice of thermodynamical potential [1]. The thermodynamic phase space (TPS) is the $(2n+1)$-dimensional vector space endowed with the canonical contact structure

$$\theta = dx^0 + \sum_{i=1}^{n} p_i dx^i.$$

Definition 1. A one-form θ on a $2n+1$-dimensional manifold $\mathcal{T}$ is a contact form if $\theta \wedge (d\theta)^n \neq 0$ is a volume form. Then the pair $(\mathcal{T}, \theta)$ is called a contact manifold.

For a given set of canonical coordinates and any partition I and J of the set of indices $\{1, \ldots, n\}$, for any differentiable function $\phi(x^I, p_J)$ of n variables, $i \in I$, $j \in J$, the formulas

$$\begin{aligned} x^0 &= \phi - \sum_{i \in I} p_i \frac{\partial \phi}{\partial p_i} \\ x^i &= -\frac{\partial \phi}{\partial p_i}, i \in I, \\ p_j &= \frac{\partial \phi}{\partial x^j}, j \in J, \end{aligned} \tag{1}$$

define a Legendre submanifold Σ_ϕ of $\mathbb{R}^{2n+1}$.

Let the function of chosen extensive variables $F(\boldsymbol{x})$ be a thermodynamical potential and let Σ_ϕ be the corresponding Legendre submanifold defined by the relations (1). The thermodynamic metric on the Legendre submanifold Σ_ϕ is defined as

$$\eta_F = \text{Hess }(F) d\boldsymbol{x} \otimes d\boldsymbol{x}, \tag{2}$$

with elements

$$(\eta_F)_{ij} = \frac{\partial^2 F}{\partial x^i \partial x^j} dx^i \otimes dx^j. \tag{3}$$

Historically, as related in (Quevedo, 2007) and (Preston and Vargo, 2008), the Weinhold metric η_U corresponds to the metric obtained when the chosen thermodynamical potential is the internal energy U, while the choice of the entropy leads to the Ruppeiner metric η_S. The choice of a metric to study properties of contact manifold leads to interesting investigations, for example: Compatibility; Metric Invariance; Curvature properties; Symplectization. Here, we focus on the used of a metric for stability studies in the sense given by (Favache et al., 2009). As such, our interest lies in the study of the dynamics of the contact vector field associated with the contact structure $(\mathcal{T}, \theta)$.

Definition 2. A vector field $\mathcal{X}$ on $(\mathcal{T}, \theta)$ is a contact vector field if and only if there exits a differentiable function ρ such that

$$\mathcal{L}_{\mathcal{X}} \theta = \rho \theta. \tag{4}$$

To every contact vector field $\mathcal{X}$, one associates the function $K(x_0, \boldsymbol{x}, \boldsymbol{p})$, called the contact Hamiltonian. Conversely, to every function K, there corresponds the contact vector field $\mathcal{X}_K$ given as

$$\begin{aligned} \mathcal{X}_K = &\left(K - \sum_{i=1}^{n} p_i \frac{\partial K}{\partial p_i} \right) \frac{\partial}{\partial x^0} + \frac{\partial K}{\partial x^0} \left(\sum_{i=1}^{n} p_i \frac{\partial}{\partial p_i} \right) \\ &+ \sum_{j=1}^{n} \left(\frac{\partial K}{\partial x^j} \frac{\partial}{\partial p_j} - \frac{\partial K}{\partial p_j} \frac{\partial}{\partial x^j} \right). \end{aligned} \tag{5}$$

The corresponding dynamical system in the contact phase space is given as

$$\begin{aligned} \dot{x}^0 &= K - \sum_{i=1}^{n} p_i \frac{\partial K}{\partial p_i} \\ \dot{x}^i &= -\frac{\partial K}{\partial p_i} \\ \dot{p}_i &= p_i \frac{\partial K}{\partial x_0} + \frac{\partial K}{\partial x^i}. \end{aligned} \tag{6}$$

For a given controlled dynamical system

$$\dot{x} = f(x) + g(x)u,$$

with $x \in \mathbb{R}^n$, a lift of a n-dimensional vector field to the contact phase space was introduced in the context of control irreversible systems in (Eberard et al., 2007), and extended in the contributions (Favache et al., 2009, 2010; Ramirez et al., 2013; Wang et al., 2015). In particular, in (Ramirez et al., 2013), the drift part of the dynamics $f(x)$ was given by

$$\dot{x} = f\left(x, \frac{\partial U}{\partial x}\right),$$

and the contact lift was generated by the contact Hamiltonian function

$$K = \left(\frac{\partial U}{\partial x} - p \right)^T f\left(x, \frac{\partial U}{\partial x}\right).$$

The key argument to suggest such form of contact Hamiltonian is that a contact Hamiltonian defined this way

[1] Generally speaking, any thermodynamic potential could be used, internal energy, entropy, Helmholtz free energy, or the Gibbs free energy. Those representations are related by Legendre transformations (Callen, 1985). The proper choice of a potential depends on the particular problem at hand. We do not make a particular choice here and in the sequel, and the thermodynamic potential is denoted by $F(\boldsymbol{x})$.