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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 $F(\boldsymbol{x})$.

vanishes on the Legendre submanifold generated by $U(x)$. A contact Hamiltonian based on the energy was also used by (Eberard et al., 2007) while an entropy-based lift was employed in (Favache et al., 2010)

The key problem considered in the present note consists in assessing the stability of an isolated equilibrium in the TPS, *i.e.*, to study the stability of an equilibrium of the $(2n+1)$-dimensional dynamical system (6) restricted to the Legendre submanifold. Following the contribution by Favache et al. (2009), we first recall the notion of equilibrium points in the TPS.

Proposition 3. ((Favache et al., 2009)). Consider a contact manifold $(\mathcal{T}, \theta)$ and a contact vector field $\mathcal{X}_K$, generated by the contact Hamiltonian function $K(x^0, \boldsymbol{x}, \boldsymbol{p})$. Consider a state in the extended phase space $(\bar{x}^0, \bar{\boldsymbol{x}}, \bar{\boldsymbol{p}}) \in (\mathcal{T}, \theta)$. Then $(\bar{x}^0, \bar{\boldsymbol{x}}, \bar{\boldsymbol{p}}) \in \{(x^0, \boldsymbol{x}, \boldsymbol{p}) | \mathcal{X}_K(x^0, \boldsymbol{x}, \boldsymbol{p})\}$ if an only if the following conditions are fulfilled:

$$\begin{aligned}
&\frac{\partial K}{\partial p_i}|_{(\bar{x}^0, \bar{\boldsymbol{x}}, \bar{\boldsymbol{p}})} = 0, i = 1, \ldots, n,\\
&K(\bar{x}^0, \bar{\boldsymbol{x}}, \bar{\boldsymbol{p}}) = 0,\\
&\frac{\partial K}{\partial x^i}|_{(\bar{x}^0, \bar{\boldsymbol{x}}, \bar{\boldsymbol{p}})} = -\bar{p}_i \frac{\partial K}{\partial x^0}|_{(\bar{x}^0, \bar{\boldsymbol{x}}, \bar{\boldsymbol{p}})}, i = 1, \ldots, n.
\end{aligned}$$

A sufficient stability result based on a linearization was derived in (Favache et al., 2009). Alternate expressions for Lyapunov stability of contact vector fields were derived or used in (Ramirez et al., 2013) and (Wang et al., 2015) using the concept of availability function, introduced in the control literature by Ydstie and Alonso (1997).

As demonstrated in the study (Favache et al., 2009), deriving a Lyapunov stability argument in the extended phase space might be difficult, as the thermodynamic constraints encoded in the structure of the (6) is not of a gradient form, and involves the computation of the Hessian of the generating function and of the contact Hamiltonian. Following the decomposition approach to study stability proposed in (Guay and Hudon, 2016), we seek in the sequel to identify such gradient structure for the dynamical system (6), using the information given by a metric, in this case the generating potential.

3. STABILITY AND STABILIZATION WITH A METRIC

We consider the problem of studying the stability of dynamical systems of the form

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}), \boldsymbol{x} \in \mathbb{R}^n, \tag{7}$$

to which a thermodynamical potential $F(\boldsymbol{x}) \in \mathbb{R}$ is associated. We assume that the vector field $\boldsymbol{f}(\boldsymbol{x})$ is of class $\mathcal{C}^k$, with $k \geq 2$. We assume that there exists an isolated equilibrium point $\bar{x}$ such that $\boldsymbol{f}(\bar{\boldsymbol{x}}) \equiv 0$. To simplify the exposition, we further assume the following properties for the potential $F(\boldsymbol{x})$:

A1. $F(\boldsymbol{x})$ is convex and positive definite;
A2. $F(\boldsymbol{x})$ reaches a minimum at equilibrium, *i.e.*, $F(\bar{\boldsymbol{x}}) = 0$;
A3. The Hessian of $F(\boldsymbol{x})$ is non-degenerate and positive definite in a neighborhood of an equilibrium $\bar{\boldsymbol{x}}$.

3.1 Lift to the contact space

Following (Eberard et al., 2007; Favache et al., 2009, 2010; Ramirez et al., 2013; Wang et al., 2015), we first define a contact Hamiltonian K to lift the dynamical system (7) with respect to the thermodynamical potential $F(\boldsymbol{x})$. The contact Hamiltonian is hence given by

$$K = \left(\frac{\partial F}{\partial \boldsymbol{x}} - \boldsymbol{p}\right)^T \boldsymbol{f}(\boldsymbol{x}), \tag{8}$$

and we can construct the contact vector field (5)

$$\begin{aligned}
\dot{x}^0 &= \left(\frac{\partial F}{\partial \boldsymbol{x}} - \boldsymbol{p}\right)^T \boldsymbol{f}(\boldsymbol{x}) - \boldsymbol{p}^T \frac{\partial K}{\partial \boldsymbol{p}}\\
\dot{\boldsymbol{x}} &= \boldsymbol{f}(\boldsymbol{x})\\
\dot{\boldsymbol{p}} &= \frac{\partial}{\partial \boldsymbol{x}}\left(\left(\frac{\partial F}{\partial \boldsymbol{x}} - \boldsymbol{p}\right)^T \boldsymbol{f}(\boldsymbol{x})\right).
\end{aligned} \tag{9}$$

This $(2n+1)$ vector field leaves the contact one-form

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

invariant. More importantly in the context of our study, and following Proposition 3 from (Favache et al., 2009), we have the following result characterizing an isolated equilibrium in the extended phase space.

Proposition 4. An isolated equilibrium of the dynamical system (7) $\boldsymbol{f}(\bar{\boldsymbol{x}}) \equiv 0$ coincides with an isolated equilibrium $(\bar{x}^0, \bar{\boldsymbol{x}}, \bar{\boldsymbol{p}})$ on Σ_ϕ of the extended system (9).

Proof. We apply directly the conditions from (Favache et al., 2009) reported in Proposition 3. First, for $\boldsymbol{f}(\bar{\boldsymbol{x}}) \equiv 0$,

$$\frac{\partial K}{\partial p_i}|_{(\bar{x}^0, \bar{\boldsymbol{x}}, \bar{\boldsymbol{p}})} = -f_i(\bar{\boldsymbol{x}}) = 0.$$

Then,

$$K(\bar{x}^0, \bar{\boldsymbol{x}}, \bar{\boldsymbol{p}}) = \left(\frac{\partial F}{\partial \boldsymbol{x}} - \bar{\boldsymbol{p}}\right)^T \cdot \boldsymbol{0} = 0.$$

Finally, since K is not an explicit function of x^0, we must verify that

$$\frac{\partial K}{\partial \boldsymbol{x}}|_{(\bar{x}^0, \bar{\boldsymbol{x}}, \bar{\boldsymbol{p}})} = 0.$$

Expanding K as

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

and taking the derivative with respect to $\boldsymbol{x}$, we have

$$\frac{\partial K}{\partial \boldsymbol{x}} = \frac{\partial^2 F}{\partial \boldsymbol{x}^2} \boldsymbol{f}(\boldsymbol{x}) + \left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right)^T \left(\frac{\partial F}{\partial \boldsymbol{x}} - \boldsymbol{p}\right).$$

By assumption, the Hessian of $F(\boldsymbol{x})$ is non-degenerated, and since $\boldsymbol{f}(\bar{\boldsymbol{x}}) \equiv 0$, the first term vanishes. Since on the Legendre manifold of thermodynamic equilibrium state, by definition, $\boldsymbol{p}$ and $\frac{\partial F}{\partial \boldsymbol{x}}$ coincide, $\frac{\partial K}{\partial \boldsymbol{x}} \equiv 0$, and an equilibrium of (7) coincides with an equilibrium of (9).

3.2 Metric, decomposition, and stability in the contact space

We are now studying stability of the dynamical system X_K

$$\begin{aligned}\dot{x}^0 &= \left(\frac{\partial F}{\partial \boldsymbol{x}} - \boldsymbol{p}\right)^T \boldsymbol{f}(\boldsymbol{x}) - \boldsymbol{p}^T \frac{\partial K}{\partial \boldsymbol{p}} \\ \dot{\boldsymbol{x}} &= \boldsymbol{f}(\boldsymbol{x}) \\ \dot{\boldsymbol{p}} &= \frac{\partial}{\partial \boldsymbol{x}} \left(\left(\frac{\partial F}{\partial \boldsymbol{x}} - \boldsymbol{p}\right)^T \boldsymbol{f}(\boldsymbol{x}) \right),\end{aligned}$$

around the equilibrium $(\bar{x}^0, \bar{\boldsymbol{x}}, \bar{\boldsymbol{p}})$. Developing X_K, we have the dynamics:

$$\begin{aligned}\dot{x}^0 &= \left(\frac{\partial F}{\partial \boldsymbol{x}}\right)^T \boldsymbol{f}(\boldsymbol{x}) \\ \dot{\boldsymbol{x}} &= \boldsymbol{f}(\boldsymbol{x}) \\ \dot{\boldsymbol{p}} &= \frac{\partial^2 F}{\partial \boldsymbol{x}^2} \boldsymbol{f}(\boldsymbol{x}) + \left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right)^T \left(\frac{\partial F}{\partial \boldsymbol{x}} - \boldsymbol{p}\right). \end{aligned} \tag{10}$$

Inspired by the metric proposed in (Preston and Vargo, 2008), but restricted to the Legendre submanifold, we propose the Riemannian metric to be of the form

$$\eta_F = (x^0)^2 dx^0 \otimes dx^0 + \frac{\partial^2 F}{\partial x^i \partial x^j} dx^i \otimes dx^j + dp_i \otimes dp_j.$$

Associated with this metric, we define an extended volume form

$$\mu_{\eta_F} = \sqrt{\det \eta_F} \quad dx^0 \wedge dx^1 \wedge \ldots \wedge dx^n \wedge dp_1 \wedge \ldots \wedge dp_n.$$

For notation sake, we re-label the $2n+1$ state variables as $\boldsymbol{\xi} \in \mathbb{R}^{2n+1}$, such that

$$\boldsymbol{\xi} = \left[x^0 \ x^1 \ \ldots x^n \ p_1 \ \ldots p_n\right]^T,$$

and the volume form is given as

$$\mu_{\eta_F} = \sqrt{\det \eta_F} \quad d\xi_1 \wedge d\xi_2 \wedge \ldots \wedge d\xi_{2n+1}.$$

The elements of the vector field (10) are thus denoted $X_i(\boldsymbol{x}, \boldsymbol{p})$, for $i = 1, \ldots, 2n+1$.

Following the construction given in (Guay and Hudon, 2016), we define a one-form ω by taking the interior product of the volume form with respect to the vector and apply the Hodge star operator (see (Guay and Hudon, 2016) for definitions of those elements):

$$\omega = \star_{\eta_F} (X_K \lrcorner \mu_{\eta_F}). \tag{11}$$

We thus obtain a differential one-form associated to the original $(2n+1)$ dynamical systems parameterized by the metric, given as:

$$\omega = (-1)^{k-1} \sum_{k=1}^{2n+1} \sum_{l=1}^{2n+1} \eta_{kl}(\boldsymbol{\xi}) X_l(\boldsymbol{\xi}, \boldsymbol{p}) d\xi_k. \tag{12}$$

To carry the proposed decomposition locally on a star-shaped region on $\mathbb{R}^{2n+1}$ centered at $\bar{\boldsymbol{\xi}}$, we first define a radial vector field $\mathfrak{X}$, defined in local coordinates by

$$\mathfrak{X}(\xi) = \sum_{i=1}^{2n+1} (\xi_i - \bar{\xi}_i) \frac{\partial}{\partial \xi_i}.$$

We then define two linear operators. For a differential form ω of degree k on a star-shaped region, the **homotopy operator** $\mathbb{H}$ is defined, in coordinates, as

$$(\mathbb{H}\omega)(\xi) = \int_0^1 \mathfrak{X}(\xi) \lrcorner \omega(\bar{\xi} + \lambda(\xi - \bar{\xi})) \lambda^{k-1} d\lambda.$$

On the same star-shaped domain, one can define the **dual homotopy operator** $\mathbb{S}$ as follows:

$$\mathbb{S} = (-1)^{(2n+1)(k+1)+1} \star_\eta \mathbb{H} \star_\eta . \tag{13}$$

We now report the decomposition result given in (Guay and Hudon, 2016):

Proposition 5. Consider a smooth nonlinear dynamical system $\dot{\boldsymbol{\xi}} = \boldsymbol{X}(\boldsymbol{\xi})$ with corresponding one-form, ω. The one-form ω can be decomposed as follows:

$$\omega = d\mathbb{H}\omega + \delta\mathbb{S}\mathbb{H}d\omega + \gamma_{\mathbb{H}}, \tag{14}$$

where the one-form $\gamma_{\mathbb{H}} = Q(\xi)\mathfrak{W}$ is harmonic.

The decomposition of the one-form ω yields an alternative structure of the dynamical system $\boldsymbol{X}(\boldsymbol{\xi})$ of the form

$$\dot{\boldsymbol{\xi}} = -\nabla_{\boldsymbol{\xi}} P^T + \sum_{i \neq j}^{n} J_{ij} \nabla_{\boldsymbol{\xi}} H_{ij}^T + Q(\boldsymbol{\xi})\boldsymbol{\xi},$$

where $P = \mathbb{H}\omega$ and the H_{ij} are computed by the dual homotopy operator. The first term on the right hand side is the gradient part of the flow. The second term provides the anti-symmetric component of the dynamics. The third term takes the form of the gradient of a function $V(\boldsymbol{\xi})$. Using this decomposition for stability analysis of the drift vector field $\boldsymbol{X}(\boldsymbol{\xi})$. We identified a normal form in the extended phase space that is generated by functions $P(bl\xi)$ and $H_{ij}(\boldsymbol{\xi})$ $(i \neq j)$.

Assumption 6. Assume that the functions P and H_{ij} are such that for a neighborhood $\mathcal{D}$ of the equilibrium $\bar{\boldsymbol{\xi}} \in \mathbb{R}^{2n+1}$:

(1) $\nabla_{\boldsymbol{\xi}} P(\bar{\boldsymbol{\xi}}) = \nabla_{\boldsymbol{\xi}} H_{ij}(\bar{\boldsymbol{\xi}}) = 0$, $\forall i, j$, and
(2) $\nabla^2_{\boldsymbol{\xi}} P(\boldsymbol{\xi}) \geq \alpha I$,

for all $\xi \in \mathcal{D}$ and positive constant α.

Under this assumption, the following was proved in (Guay and Hudon, 2016).

Theorem 7. Let the nonlinear system

$$\dot{\boldsymbol{\xi}} = \boldsymbol{X}(\boldsymbol{\xi}) \tag{15}$$

generate a decomposition with potentials that meet Assumption 6. Then the $\bar{\xi}$ is a local exponentially stable equilibrium of the system.

The proof of this theorem can be found in (Guay and Hudon, 2016). Summarizing the result, one notes that by using the above decomposition along a locally defined vector field $\mathfrak{X} = \xi_k \frac{\partial}{\partial \xi_k}$, it is possible to re-write the dynamics (9) as

$$\dot{\boldsymbol{\xi}} = -\nabla_{\boldsymbol{\xi}} P^T + U(\boldsymbol{\xi}) \tag{16}$$

where $U(\boldsymbol{\xi}) = \sum_{i\neq j} J_{ij}\nabla_{\boldsymbol{\xi}} H_{ij}^T + Q(\boldsymbol{\xi})\boldsymbol{\xi}$. It follows by construction that $\boldsymbol{\xi}^T U(\boldsymbol{\xi}) \equiv 0$. Furthermore, it is always possible, by assumption, to re-write the gradient of $P(\boldsymbol{\xi})$ as $\nabla_{\boldsymbol{\xi}} P^T = \Theta(\boldsymbol{\xi})\boldsymbol{\xi}$, where $\Theta(\boldsymbol{\xi}) = \int_0^1 \nabla^2 P(\lambda\boldsymbol{\xi})d\lambda$. Considering the Lyapunov function, $V = \frac{1}{2}\boldsymbol{\xi}^T\boldsymbol{\xi}$, its derivative with respect to t yields:

$$\dot{V} = -\boldsymbol{\xi}^T\nabla_{\boldsymbol{\xi}} P^T + x^T U(\boldsymbol{\xi}) = -\boldsymbol{\xi}^T\nabla_{\boldsymbol{\xi}} P^T. \tag{17}$$

Based on the discussion above, it follows that the second term is identically zero. It follows that, by assumption, one can write:

$$\dot{V} = -\boldsymbol{\xi}^T\Theta(\boldsymbol{\xi})\boldsymbol{\xi}, \tag{18}$$

and for all $\boldsymbol{\xi} \in D$ we have:

$$\dot{V} \leq -\alpha\|\boldsymbol{\xi}\|^2 = -2\alpha V. \tag{19}$$

Local exponential stability of the system over $\mathcal{D}$ is achieved, as required.

Applying this result to the thermodynamic system in the TPS, the key feature is to test if the Hessian of the potential $P(\boldsymbol{\xi})$, computed by homotopy of the one-form ω is positive definite. In our context, the one-form is given in coordinates as

$$\begin{aligned}\omega = x^0\Bigg(&\left(\frac{\partial F}{\partial \boldsymbol{x}}\right)^T \boldsymbol{f}(\boldsymbol{x})dx^0 \\ &+ (-1)^k \sum_{k=1}^n\sum_{l=1}^n \left(\frac{\partial F}{\partial x^k \partial x^l} f_l(\boldsymbol{x})\right) dx^k \\ &+ (-1)^{n+k} \sum_{k=1}^n\sum_{l=1}^n \left(\frac{\partial^2 F}{\partial x^k \partial x^l} f_l(\boldsymbol{x}) + \left(\frac{\partial F}{\partial_k} - p_k\right)\frac{\partial f_l}{\partial x_k}\right) dp_k\Bigg).\end{aligned}$$

By using homotopy integration along a locally-defined vector field $\mathfrak{X}$ centered at the equilibrium $(\bar{x}^0, \bar{\boldsymbol{x}}, \bar{\boldsymbol{p}})$, one obtain a potential of the form

$$P(x^0, \boldsymbol{x}, \boldsymbol{p}) = \mathbb{H}\omega,$$

in terms of the known generating function $F(\boldsymbol{x})$. By restricting the equilibrium to the Legendre submanifold Σ_ϕ, one can verify that $\nabla_{\boldsymbol{\xi}} P(\bar{\boldsymbol{\xi}}) = \nabla_{\boldsymbol{\xi}} H_{ij}(\bar{\boldsymbol{\xi}}) = 0$ for all i, j. The key problem therefore, consists in checking the condition on the Hessian of the computed potential P, *i.e.*,

$$\text{Hess } P(x^0, \boldsymbol{x}, \boldsymbol{p}) > \alpha I_{2n+1}.$$

The full condition, as developed in (Favache et al., 2009), will be stated in a future contribution. For this note, we illustrate the result for a particular class of systems in the next section.

To summarize, the key feature of introducing a metric on the TPS is to yield to a one-form ω that is parameterized by a known metric. Using a previously proposed approach to decompose vector fields, one can identify, under suitable assumptions, the gradient structure of the vector field in the contact phase space and derive suitable stability conditions on a derived potential.

4. EXAMPLE

As an example, we consider the stability of dynamical systems generated using Helmholtz free energy $F(\boldsymbol{x})$ with a constant structure matrix $\mathcal{F}$

$$\dot{\boldsymbol{x}} = \mathcal{F} \cdot \nabla^T F(\boldsymbol{x}). \tag{20}$$

Examples of such dynamical systems are metriplectic systems, derived originally in the work by Morrison (1986), but also gradient systems and Hamiltonian systems. In the present case, we assume that the generating potential is quadratic in its arguments, *i.e.*, we consider the case where $F(\boldsymbol{x})$ is given by

$$F(\boldsymbol{x}) = \sum_{i=1}^n \frac{1}{2}(x^i)^2,$$

and as a result, the convex generating potential vanishes at the origin and the non-degenerated Hessian matrix of $F(\boldsymbol{x})$ is the identity matrix. The key question about stability of the system hence lies in the property of the structure matrix $\mathcal{F}$. By setting the contact Hamiltonian as

$$K = (\boldsymbol{x} - \boldsymbol{p})^T \mathcal{F}\boldsymbol{x},$$

we can construct the contact vector field (5) as:

$$\dot{x}^0 = \boldsymbol{x}^T\mathcal{F}\boldsymbol{x} \tag{21}$$

$$\dot{\boldsymbol{x}} = \mathcal{F}\boldsymbol{x} \tag{22}$$

$$\dot{\boldsymbol{p}} = (\mathcal{F}^T + \mathcal{F})\boldsymbol{x} - \boldsymbol{p}^T\mathcal{F}. \tag{23}$$

At the origin $\bar{\boldsymbol{x}} = \boldsymbol{0}$, we have $\dot{x}^0 = 0$, and $\dot{\boldsymbol{x}} = \boldsymbol{0}$ since $\mathcal{F}\boldsymbol{x} = \boldsymbol{0}$. Furthermore, on the Legendre submanifold Σ_ϕ, $\boldsymbol{p}$ and $\frac{\partial F}{\partial \boldsymbol{x}}$ coincide, hence $\dot{\boldsymbol{p}} = \boldsymbol{0}$.

Since the Hessian of the generating function is the identity matrix, the Riemannian metric on the $(2n+1)$-dimensional contact phase space is given as

$$\eta_F = (x^0)^2 dx^0 \otimes dx^0 + dx^i \otimes dx^i + dp_i \otimes dp_i,$$

for $i = 1, \ldots, n$, and the volume form in the extended space is given as

$$\mu_{\eta_F} = x^0 dx^0 \wedge dx^1 \wedge \ldots \wedge dx^n \wedge dp_1 \wedge \ldots \wedge dp_n.$$

Following the construction given above, and because of the decoupled structure of the potential F, we define a one-form ω as

$$\omega = \star_{\eta_F}(X_K \lrcorner \mu_{\eta_F}),$$

which in this particular case is given by

$$\begin{aligned}\omega = \left(\boldsymbol{x}^T\mathcal{F}\boldsymbol{x}\right)x^0dx^0 &+ \sum_{i=1}^n (-1)^i \left(\mathcal{F}_{i,i}x^i\right)x^0dx^i \\ &+ \sum_{i=1}^n (-1)^{(i+n)} \left(2\mathcal{F}_{i,i}x^i - \mathcal{F}_{i,i}p_i\right)x^0dp_i.\end{aligned}$$

By homotopy integration of this one-form centered at the origin, one obtains a potential $P(x^0, \boldsymbol{x}, \boldsymbol{p})$ of the form

$$P(x^0, \boldsymbol{x}, \boldsymbol{p}) = \mathbb{H}\omega = a(\boldsymbol{x})(x^0)^2 + \sum_{i=1}^{n} b_i(x^i)^2 + \sum_{i=1}^{n} c_i x^i p_i + \sum_{i=1}^{n} d_i p_i^2,$$

from which the condition on the Hessian for stability can be computed and conditions on the structure of $\mathcal{F}$ can be computed.

The opened question is obviously the choice of metric. As argued in (Guay and Hudon, 2016), for a structure as simple and decoupled as the one considered here, there is a simple relation between the Hessian of $P(\cdot)$ and the Jacobian of the vector field (in this case in extended dimensions). As such, to ensure stability, the Jacobian matrix of the vector cannot have zero on its diagonal, which is the case when the contact Hamiltonian is not an explicit function of x^0. In the present context, it leads to a particular choice of metric, in order to perturb the one-form and hope for a full-rank Hessian. It is believed however, that stability analysis using this proposed approach could deal with non-hyperbolic equilibrium points. Further investigations will consider those topics.

5. CONCLUSIONS

In this note, we study the stability problems of thermodynamic systems described in the Thermodynamic Phase Space (TPS) endowed with a metric. Using a specific and known metric and a decomposition approach recently proposed in the literature, stability conditions in the extended phase were developed. This examination leads to new interpretations of previously obtained results, and highlights new problems and avenues for research, in particular, the possibility of using Riemannian geometry to study thermodynamic problems, as proposed in (Preston and Vargo, 2008). It is believed that concrete problems could be considered, following for example the geometrothermodynamic approach proposed by Quevedo (2007), as well as more fundamental problems, using contributions collected in the references (Blair, 2002). In particular, the knowledge of a metric enables one to study the Reeb vector field in the contact phase space, which is believed to be of importance in the computation of admissible (optimal) control for thermodynamic systems.

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