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# Control of irreversible thermodynamic processes using port-Hamiltonian systems defined on pseudo-Poisson and contact structures

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## Résumé de Thèse

Dans cette thèse nous présentons résultats sur l'emploi des systèmes Hamiltoniens à port et des systèmes de contact commandés pour la modélisation et la commande de systèmes issus de la Thermodynamique Irréversible. Premièrement nous avons défini une classe de pseudo-systèmes Hamiltoniens à port, appelée systèmes Hamiltoniens à port irréversibles, qui permet de représenter simultanément le premier et le second principe de la Thermodynamique et inclut des modèles d'échangeurs thermiques ou de réacteurs chimiques. Ces systèmes ont été relevés sur l'espace des phases thermodynamiques muni de une forme de contact, définissant ainsi une classe de systèmes de contact commandés, c'est-à-dire des systèmes commandés non-linéaires définis par des champs de contacts stricts. Deuxièmement, nous avons montré que seul un retour d'état constant préserve la forme de contact et avons alors résolu le problème d'assignation d'une forme de contact en boucle fermée. Ceci a mené à la définition de systèmes de contact entrée-sortie et l'analyse de leur équivalence par retour d'état. Troisièmement, nous avons montré que les champs de contact n'étaient en général pas stable en leur zéros et avons alors traité du problème de la stabilisation sur une sous-variété de Legendre en boucle fermée.

**Mots-clés**: Systèmes Hamiltoniens à ports, systèmes de contact, thermodynamique irréversible, commande non-linéaire

## Thesis Abstract

This doctoral thesis presents results on the use of port Hamiltonian systems (PHS) and controlled contact systems for modeling and control of irreversible thermodynamic processes. Firstly, Irreversible PHS (IPHS) has been defined as a class of pseudo-port Hamiltonian system that expresses the first and second principle of Thermodynamics and encompasses models of heat exchangers and chemical reactors. These IPHS have been lifted to the complete Thermodynamic Phase Space endowed with a natural contact structure, thereby defining a class of controlled contact systems, i.e. nonlinear control systems defined by strict contact vector fields. Secondly, it has been shown that only a constant control preserves the canonical contact structure, hence a structure preserving feedback necessarily shapes the closed-loop contact form. The conditions for state feedbacks shaping the contact form have been characterized and have lead to the definition of input-output contact systems. Thirdly, it has been shown that strict contact vector fields are in general unstable at their zeros, hence the condition for the the stability in closed-loop has been characterized as stabilization on some closed-loop invariant Legendre submanifolds.

**Keywords**: Port Hamiltonian system, contact system, irreversible thermodynamics, nonlinear control.

*a mis padres Enid y Hector*

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## The context

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# Chapter 1

# Introduction

*"Every mathematician knows that it is impossible to understand any elementary course in thermodynamics. The reason is that the thermodynamics is based – as Gibbs has explicitly proclaimed – on a rather complicated mathematical theory, on the contact geometry."*

*Vladimir I. Arnold, 1989*

## 1.1 Motivation and previous work

Energy, as a fundamental property of all physical systems, was the starting point of this work. It was during my master thesis [71] that we first began to explore the possibility of using this property to perform process control. Doing some research on the subject we immediately found that one of the areas where this concept has been widely applied is in mechanics, and more specific in the control of Hamiltonian system [11, 17, 86]. But even more interesting for our purposes was the use for control of an extension of Hamiltonian system, namely port Hamiltonian systems (PHS) [49, 89, 19].

PHS are perfectly suited for the use of control method based on energy shaping, like passivity based control (PBC) [63], or methods that not only shape the energy but also change the structure of the system, like interconnection and damping assignment (IDA)-PBC [89]. The results of using PHS to model and control systems where no thermal interaction occurs are very good and large number of examples confirms it. However, when the objective is to represent some process that posses a non-negligible thermal gradient we find that PHS are no longer so well suited. The PHS structure is actually destroyed in this case, since it is not longer possible to define a true Poisson bracket for the PHS and we are forced to consider some generalised (or pseudo) PHS [22, 72, 42]. This is strongly related to the irreversible production of entropy.

The previous motivated us to look for some extension of PHS that could provide a geometric structure for thermodynamic systems. We found this extension in controlled contact systems [21, 20, 22, 24, 27]. Controlled contact systems offer a

framework where it seems possible to develop an important theory for modelling and control of thermodynamic systems. The framework of contact systems is not new, nor the use of it for modelling reversible and irreversible thermodynamic systems [40, 41, 8, 53, 48, 57, 54, 36, 34], however the definition of controlled contact system to model open systems has only recently been proposed [21, 20, 22]. Furthermore there exists no studies of these systems for control purposes. To our knowledge the only results in this line are presented in [30], where some general properties including conditions for the existence of equilibrium points and local stability of conservative controlled contact systems are given.

The aim of this doctoral thesis was to study the use of controlled contact systems for control purposes and develop results along this line.

## 1.2 Organization and contribution of the thesis

The thesis is divided into three chapters. Chapter 2 is devoted to the modelling of thermodynamic systems. It is through this chapter that we aim to motivate the study of controlled contact systems for modelling and control purposes. We start this chapter by introducing PHS and we propose an extension of PHS, that we call irreversible PHS (IPHS), to model thermodynamic systems. We then introduce contact systems and we use IPHS to define a class of contact systems for modelling thermodynamic processes.

In Chapter 3 we analyse the feedback of controlled contact systems. More precisely characterize the conditions for achieving a structure preserving feedback, i.e., a state feedback such that the closed-loop system is again a contact system. This is done from a system theoretic point of view and thermodynamic systems only motivates the examples of the chapter. Hence Chapter 3 may be read independently of Chapter 2. We present general conditions for structure preserving feedback and we specialise the conditions for strict contact systems. The chapter ends with the study of existence of closed-loop invariant Legendre submanifolds of the closed-loop vector field.

In Chapter 4 the stability properties of controlled contact system are studied. A general analysis is carried out for the existence of zeros of the contact vector field. Most of the results are for controlled contact systems subject to the state feedback proposed in Chapter 3. Conditions for local and partial stability on closed-loop invariant Legendre submanifolds are given. The final section of this chapter presents a control design method based on the contact framework that differs from the preceding results in the sense that it does not define a structure preserving state feedback.

The thesis concludes with some final remarks and perspectives of future work in Chapter 5. The main contributions are:

- ***Chapter 2:*** A class of pseudo PHS that expresses the first and second principle of thermodynamic as a structural property of the system is defined: irreversible PHS (IPHS). It shown that IPHS encompasses a large set of thermodynamic systems, including heat exchangers and chemical reactors. The

IPHS is used to define a class of conservative contact system that are regular on the complete thermodynamic phase space. The continuous stirred tank reactor (CSTR) is modelled using IPHS and contact Hamiltonian formulation.

- ***Chapter 3:*** It has been demonstrated that only a constant control preserves the canonical contact structure, hence a structure preserving feedback necessarily renders the closed-loop system a contact system with respect to a new contact form. The conditions for structure preserving feedback are characterized and specialised for strict contact systems. The relation with feedback of input-output Hamiltonian systems is also addressed. For conservative controlled contact system the feedback invariant Legendre submanifolds have been characterized and it has been suggested to use the invariant Legendre submanifold as a design criteria to define the state feedback.

- ***Chapter 4:*** It is shown that the linearisation of strict contact vector fields has one eigenvalue at zero and $2n$ eigenvalues symmetric with respect to the imaginary axis. Hence, the linearised contact vector field is in general unstable. The existence of stable and unstable submanifolds related with Lagrangian submanifolds of Hamiltonian systems is discussed. The partial stability on a Legendre submanifold is characterized using Lyapunov's direct method and particular results for controlled conservative contact system are presented. The framework of conservative contact systems has been used to propose a control design method that consists of the matching of contact Hamiltonian functions defined by the lift of vector fields.

# Chapter 2

# A geometric representation of thermodynamic systems

## 2.1 Introduction

In the last decade a powerful control theory based on Hamiltonian system representation has been developed for electrical, mechanical and electro-mechanical systems. This control theory is based on the principle of conservation of energy [63, 65, 66] providing a clear physical interpretation of control design problem. Although traditionally Hamiltonian models arise from the Euler-Lagrange equations of motion, these have been extended to deal with network models of physical systems by using the concept of port Hamiltonian systems (PHS) [89, 19, 90, 91]. In network models the system is considered as the interconnection of energy storing elements via basic physical interconnection laws (e.g. Newtons third law or Kirchhof's law) together with energy dissipating elements. PHS theory formalizes the basic interconnection laws together with the power-conserving elements by a geometric structure, and defines the Hamiltonian as the total energy stored in a system. The energy function determines not just the static behaviour, but also, via the energy transfer between subsystems, its transient behaviour. Thus, PHS have direct physical interpretation since they rely on energy balances (not only restricted to energy, balance of mass and "virtual" energy has also been reported), and are directly related with other network models, such as bond-graphs [50, 83, 33, 31, 94, 32].

Irreversible thermodynamic, deals with irreversible processes [12, 47, 10]. An irreversible process is a process that occurs with internal temperature, pressure, and/or velocity gradients so that there are internal flows and/or viscous dissipation [79]. On other hand a reversible process proceed without internal flows or viscous dissipation. In any irreversible process the entropy, and thereby the second law of thermodynamics plays a major role. From a thermodynamic perspective, all natural processes are irreversible.

Irreversibility has been introduced in PHS theory by adding a dissipative term into the dynamical equations [91], however at the expense of losing the conserva-

tion of the Hamiltonian function. In this way, the Hamiltonian function does not represent any more the total energy of the system and the model does not express the first principle of thermodynamics [22]. The use of Hamiltonian formalism to describe the dynamic of a thermodynamic process inevitably leads to the definition of *pseudo PHS*. Indeed, the geometric structure is not longer preserved since the structure matrices depends on states and co-states destroying any possibility of defining the system in term of a Poisson bracket [22, 72, 42]. By using pseudo PHS with dissipation it has been possible to extend this kind of representation and associated control theory to industrial processes, in particular to hydraulic [80, 43, 71, 96], chemical [81, 39, 71, 76, 78, 77] and biological [60, 9, 44] processes.

There have been major efforts searching a dynamical system representation for thermodynamic system. In this context pseudo PHS and Brayton-Moser formulations [82] have been defined with respect to a Hamiltonian function equal to a thermodynamic potential of the system, such as the total enthalpy or the entropy production [42, 28]. However, defining the generating function of the pseudo PHS as a thermodynamic potential does in general not lead to structure matrices with physical interpretation and, furthermore, does in general not express the conservation of energy and the irreversible entropy creation as a consequence of the definition of the system. Other efforts have been centred in providing thermodynamic systems with a geometric structure, just like mechanical systems with the Hamiltonian representation. In this line the "General Equation for the Non-Equilibrium Reversible Irreversible Coupling", or shortly GENERIC [36, 69] propose to "complete" the Hamiltonian (reversible) part of a system with a purely dissipative (irreversible) part. The GENERIC system is expressed with respect to two generating functions: the total energy and the total entropy, and with respect to two geometric structures: a Poisson bracket and a pseudo-Riemannian metric. This representation is capable to express simultaneously the conservation of energy and the irreversible creation of entropy as a geometric property of the system. The GENERIC representation for open system [58, 45] is however not easy to define and has not a "classical" control affine structure since the inputs of the system are expressed in terms of auxiliary variables and form part of the state variables of an extended GENERIC system.

The use of contact geometry and Hamiltonian systems have made possible to model irreversible thermodynamic processes as a mathematical structure that simultaneously expresses the thermodynamic irreversibility of a process and the conservation of energy, i.e., the first and second law of thermodynamics. The fundamental idea behind the use of contact system to model thermodynamic systems is the use of a $2n + 1$ dimensional space for the representation of a $n$ dimensional dynamical system (or control system). This allows to endow the Thermodynamic Phase Space (TPS), the space of extensive and intensive variables, with a contact structure. The first works in this line where done by R. Hermann for reversible thermodynamic systems [40, 41]. Since the work of R. Hermann the introduction of the contact structure for reversible thermodynamic systems was further developed in [8, 53, 57]. This formalism was later used to define contact vector fields to describe reversible [54] and irreversible transformations [36, 34]. In the last years the previous works have been extended to open thermodynamic systems. This has been done by augmenting the contact vector field with an interaction contact vector field

[21, 20, 22]. These systems have been called controlled conservative contact systems and are defined by a contact vector field generated by a contact Hamiltonian function satisfying a compatibility condition with some Legendre submanifold, defined by Gibbs' relation, on a contact manifold. Recently, the conservative contact systems theory have been used to model and analyse several controlled thermodynamic systems [22, 27]. This opens a new frame of research, with big potential in our opinion, for modelling and control of thermodynamic system. Indeed as it has been discussed in [30] the properties of the contact vector fields are entirely determined by the thermodynamic properties of the system, hence an abstract use of the contact geometry for analysis and control is possible.

There are two main contributions in this chapter: the definition of a class of pseudo PHS that encompasses the energy conservation and the entropy creation, and the construction of a lift to the TPS which is well defined in the sense that the generating functions (potentials) are smooth on the whole TPS. This class of pseudo PHS has been called Irreversible port Hamiltonian system (IPHS) and is defined by the thermodynamic properties of the system. This allows to express the conservation of energy and the irreversible entropy creation as a structural property of the system. IPHS encompass a large class of thermodynamic processes, including heat exchangers and the continuous stirred tank reactor (CSTR). The lifts of dynamical systems to the TPS are not always well defined since the contact Hamiltonian function may present singularities on the TPS and thus the generated contact vector field. IPHS are used to define a class of well defined conservative contact systems. The regularity of contact vector fields constructed by using the lift of a dynamical system has not been addressed in previous work. A heat exchange process is used to illustrate the ideas through the chapter, and a complete section is devoted to analyse a complex thermodynamic system, namely the non-isothermal CSTR, using the proposed approaches.

### 2.1.1 Organization of the chapter

The chapter is organized as follows. In Section 2.2 the basics of PHS and the GENERIC formalism are presented to motivate the use of IPHS and contact Hamiltonian systems. In Section 2.2.3 the definition of IPHS is given. Section 2.3 presents the contact Hamiltonian framework and a class of lift of IPHS is defined. In Section 2.4 the CSTR is extensively analysed using the framework of IPHS and contact systems. Finally in Section 2.5 some concluding remarks are given.

### 2.1.2 Main contributions of the chapter

The main contributions of this chapter are the following.

- In Section 2.2.3 a class of pseudo PHS expressing the first and second principle of thermodynamic as a structural property of the system is defined, namely IPHS (Definition 1). The IPHS is defined by: a generating function that for physical systems corresponds to the total energy; a constant skew-symmetric structure matrix that represents the network structure of the system; a non-linear function that depends on the states and co-states, defined by a Poisson

bracket evaluated on the dissipative and conserved quantities of the system. It is interesting to remark for physical systems the non-linear function is actually defined by the thermodynamic driving force. The IPHS is completed with input and output ports. The defined IPHS encompasses a large set of thermodynamic systems, including heat exchangers and chemical reactors.

- The immersion of the IPHS on TPS as a conservative contact system is presented. In particular the issue of well defined contact Hamiltonian functions is addressed. Previous work on the matter did not address this issue. The fact that the contact vector field evolves in the TPS forces the contact Hamiltonians to be well defined in the whole whole TPS, and not only on the Legendre submanifold defining the physical properties of the system. We analyse this matter in detail and suggest a class of well defined lift for IPHS in Subsection 2.3.2.

- In Section 2.4 we apply all the previously exposed concepts on a complex thermodynamic system, namely the CSTR. Two IPHS representation for the CSTR are proposed (Proposition 5 and 6). One uses the total internal energy as Hamiltonian function while the second one uses the total enthalpy. Both of them posses the same structure matrix given by a constant skew-symmetric matrix defined by the stoichiometric coefficients of the chemical reaction network. The non-linear function modulating the constant structure matrix is defined by the thermodynamic driving force: the chemical affinity and the enthalpy of reaction respectively. The IPHS representation of the CTSR is then used to propose a well defined contact Hamiltonian function that expresses the dynamical equation of the CSTR when projecting the contact vector field on the Legendre submanifold defining the physical properties of the system (Proposition 7). The contact Hamiltonian is analysed and a physical interpretation is provided.

## 2.2 Pseudo Hamiltonian formulation of open thermodynamic systems

In this section we define Irreversible port Hamiltonian systems (IPHS). We begin by introducing PHS and showing why they are not sufficient to model irreversible thermodynamic systems. In order to further motivate the definition of IPHS we present briefly an alternative formalism for the modelling of irreversible thermodynamic systems, namely GENERIC. It should be noted that we use the term pseudo PHS to refer to "quasi" PHS formulations of thermodynamic systems. However we do not use the denomination pseudo PHS in the sense of [93], where it has been suggest for PHS associated to Poisson brackets not fulfilling the Jacobi identities.

### 2.2.1 Port Hamiltonian systems

Port Hamiltonian systems (PHS) [49] have been widely used in modelling and passivity-based control (PBC) of mechanical and electro-mechanical system[19, 64].

On the state space $\mathbb{R}^n \ni x$, a PHS is defined by the following state equation,

$$\dot{x} = J(x)\frac{\partial U}{\partial x}(x) + g(x)u(t) \tag{2.1}$$

where $U : \mathbb{R}^n \to \mathbb{R}$ is the Hamiltonian function, $J(x) \in \mathbb{R}^n \times \mathbb{R}^n$ is a skew-symmetric structure matrix, $g(x) \in \mathbb{R}^m \times \mathbb{R}^n$ is the input vector field and $u(t) \in \mathbb{R}^m$ is a time dependent input. For those systems, the Hamiltonian function represents the total electro-mechanical energy of the system and the skew-symmetric structure matrix represents the energy flows between the different energy domains of the system. Furthermore the structure matrix $J(x)$ relates to symplectic geometry as it defines a Poisson bracket, if it satisfies the Jacobi identities, else it is just a pseudo-Poisson bracket (see [93]). If $J$ is constant in some local coordinates then it satisfies the Jacobi identities [89]. In the sequel we will consider only true Poisson brackets (not pseudo-Poisson brackets). The Poisson bracket of two $C^\infty(\mathbb{R}^n)$ functions $Z$ and $G$ is expressed as:

$$\{Z, G\}_J = \frac{\partial Z}{\partial x}^\top (x)J(x)\frac{\partial G}{\partial x}(x). \tag{2.2}$$

The PHS dynamics may be expressed in term of the Poisson bracket:

$$\dot{x} = \{x, U\}_J + g(x)u(t). \tag{2.3}$$

The properties of Poisson brackets such as its skew-symmetry and the Jacobi identities correspond to the existence of conservation laws or balance equations for open systems. For instance the conservation of the energy is the base of the control using PBC methods [66, 64].

For physical systems representing irreversible phenomena, i.e., transformations that involves irreversible entropy creation, it is not sufficient to express only the conservation of energy (first principle of thermodynamic); it is also necessary to express the irreversible entropy creation (second principle of thermodynamic) as a system theoretic property. The first and second principle express, respectively, the conservation of energy and the irreversible transformation of entropy. It is possible to represent this by the following equations

$$\frac{dU}{dt} = 0 \qquad \text{and} \qquad \frac{d\mathfrak{S}}{dt} = \sigma\left(x, \tfrac{\partial U}{\partial x}\right) \geq 0 \tag{2.4}$$

where the Hamiltonian $U$ is the total energy, $\mathfrak{S}$ denotes an entropy like function (that may be equal to the total entropy $S$) and $\sigma\left(x, \frac{\partial U}{\partial x}\right)$ the irreversible entropy creation which in general depends on the state and the gradient of the total energy. By skew-symmetry of the Poisson bracket the total energy of the system satisfies the energy balance equation

$$\frac{dU}{dt} = \frac{\partial U}{\partial x}^\top gu.$$

Indeed, since $g(x)u(t)$ represent the flows through the controlled-ports of the system the only energy variation is due to the interaction with the environment. The entropy variation on other hand is given by

$$\frac{dS}{dt} = \frac{\partial S}{\partial x}^\top J(x)\frac{\partial U}{\partial x} + \frac{\partial S}{\partial x}^\top gu.$$

A consequence of the second principle of thermodynamic is that the entropy variation due to internal transformations is always greater or equal to zero. This actually requires $J(x)$ to explicitly depend on $\frac{\partial U}{\partial x}$,

$$\frac{\partial S}{\partial x}^{\top} J\left(x, \tfrac{\partial U}{\partial x}\right) \frac{\partial U}{\partial x} = \sigma_{int} \geq 0, \tag{2.5}$$

since this should hold for any generating function $U(x)$. In order to include the second principle an alternative geometric structures have to be considered. This is the reason that for physical systems embedding the internal energy and expressing simultaneously the energy conservation and the irreversible entropy creation as it occurs in chemical engineering for instance, the Hamiltonian formulation has to be questioned. In the last years various formulations have been suggested in this line [57, 36, 39, 22, 68, 27, 72]. Several attempts have been made in order to preserve as much as possible of the PH structure, leading to a class of system called *pseudo PHS* [39, 68, 78, 18, 72, 42]. These system retain as much as possible the port Hamiltonian structure, but differ by their structure matrices and input vector fields which depend explicitly on the gradient of the Hamiltonian. An important remark is that, although the forms of PHS (2.1) and pseudo PHS are very similar and both embed, by skew-symmetry of the structure matrix, the conservation of energy, in the latter the drift dynamic is a *nonlinear function* in the gradient $\frac{\partial U}{\partial x}(x)$. In this sense the symplectic structure of the PHS, given by the Poisson tensor associated with the structure matrix $J(x)$, is destroyed. This is our main motivation for considering other geometric structures that may express simultaneously the conservation of energy and the irreversible entropy creation. We will return to the definition and properties of pseudo PHS in Section 2.2.3.

A particularly interesting formulation embedding the energy conservation and the entropy creation is GENERIC. This formulation is an extension of Hamiltonian system to thermodynamic systems. GENERIC divides the system in two parts: a conservative part given by a Hamiltonian system and a dissipative part modelled in terms of a pseudo-Riemannian metric. Its main feature is the use of two different generating functions (the total energy and the total entropy) to express the system dynamics. This formalism, although not used in this work, is briefly presented in the next subsection to illustrate the non-triviality of embedding thermodynamic systems with a geometric structure and as an introduction to the suggested pseudo PHS.

## 2.2.2 The GENERIC formalism

GENERIC is the abbreviation for "General Equation for the Non-Equilibrium Reversible Irreversible Coupling". It was proposed in [36, 69] for isolated systems and extended to open system in [58, 45].

### 2.2.2.1 GENERIC for isolated systems

In this formalism the dynamics of an isolated thermodynamic system is expressed as the sum of a conservative and a dissipative system. The conservative system is

defined as a Hamiltonian system, i.e., it is defined with respect to a Poisson bracket and the Hamiltonian function being the total energy of the system. The dissipative system is defined with respect to a pseudo-Riemannian metric and generated by the total entropy as the potential function. In GENERIC the time evolution of the state variables $x \in \mathbb{R}^n$ is defined as

$$\frac{dx}{dt} = J(x)\frac{\partial U}{\partial x}(x) + M(x)\frac{\partial S}{\partial x}(x) \tag{2.6}$$

where $U(x) \in \mathcal{C}^\infty(\mathbb{R}^n)$ and $S(x) \in \mathcal{C}^\infty(\mathbb{R}^n)$ are respectively the total energy and entropy functions of the system and matrices $J(x)$ and $M(x)$ defining respectively a Poisson bracket and a pseudo-Riemannian metric. This means that the matrix $J(x)$ is skew-symmetric and satisfies the Jacobi identities and $M(x)$ is symmetric and positive semi-definite. The GENERIC dynamic is complemented by the following degeneracy requirements

$$J(x)\frac{\partial S}{\partial x}(x) = 0 \qquad \text{and} \qquad M(x)\frac{\partial U}{\partial x}(x) = 0. \tag{2.7}$$

Hence the entropy function is an invariant of the Hamiltonian dynamics which is generated only by the internal energy function, and the internal energy is an invariant of the pseudo-gradient dynamic which is generated only by the entropy function. The two contributions generated by the energy function $U$ and the entropy function $S$ are called the reversible and irreversible contributions, respectively. The Poisson bracket has already been defined in (2.2). The pseudo-Riemannian metric is expressed by the Ginzburg-Landau dissipative bracket [36], denoted by $[\cdot,\cdot]$ and defined by

$$[Z, G]_M = \frac{\partial Z}{\partial x}^\top (x) M(x) \frac{\partial G}{\partial x}(x), \tag{2.8}$$

with $Z$ and $G$ two $C^\infty(\mathbb{R}^n)$ functions. These brackets and equation (2.6) lead to the following dynamical equation for an arbitrary function $V \in C^\infty(\mathbb{R}^n)$ in terms of the two separate generators $U$ and $S$:

$$\frac{dV}{dt} = \{V, U\}_J + [V, S]_M. \tag{2.9}$$

Using this last expression and the degeneracy conditions (2.7) it is straightforward to verify that for a GENERIC system the energy is a conserved quantity and the entropy is an increasing function.

$$\begin{aligned}
\frac{dU}{dt} &= \{U, U\}_J + [U, S]_M = 0, \\
\frac{dS}{dt} &= \{S, U\}_J + [S, S]_M = [S, S]_M = \sigma_{int} \geq 0.
\end{aligned}$$

where $\sigma_{int}$ is the irreversible internal entropy production [12]. The GENERIC formalism encompasses in its definition simultaneously the first and second principles of thermodynamics: the conservation of internal energy and the creation of entropy associated with irreversible processes.

#### 2.2.2.2 GENERIC for open systems

The extension of GENERIC to open system was originally proposed in [58] and later in [45]. We will use the latest formulation and more specifically, we will present it following the developments presented in [27]. An open GENERIC system on the state space $x \in \mathbb{R}^n$ with the two pairs of external variables, denoted by $(\dot{x}_J, F_J) \in \mathbb{R}^{m_1}$ and $(\dot{x}_M, F_M) \in \mathbb{R}^{m_1}$, is defined by a skew-symmetric and a symmetric positive semi-definite tensor with the following structure matrices respectively

$$\hat{J} = \begin{bmatrix} 0 & 0 & \Gamma(x) \\ 0 & 0 & 0 \\ -\Gamma^\top(x) & 0 & J(x) \end{bmatrix}, \qquad \hat{M} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \Pi(x) \\ 0 & \Pi^\top(x) & M(x). \end{bmatrix}$$

with $\Gamma(x) \in \mathbb{R}^{m_1} \times \mathbb{R}^n$ and $\Pi(x) \in \mathbb{R}^{m_2} \times \mathbb{R}^n$. The dynamic is generated by two functions $U(x)$ and $S(x)$ satisfying the degeneracy condition (2.7) and the differential-algebraic system of equations

$$\begin{bmatrix} -\dot{x}_J \\ \dot{x}_M \\ \frac{dx}{dt} \end{bmatrix} = \hat{J}(x) \begin{bmatrix} F_J \\ 0 \\ \frac{\partial U}{\partial x} \end{bmatrix} + \hat{M}(x) \begin{bmatrix} 0 \\ F_M \\ \frac{\partial S}{\partial x} \end{bmatrix}.$$

Note that from the previous equation the following relations are obtained

$$\dot{x}_J = -\Gamma(x)\frac{\partial U}{\partial x} \quad \text{and} \quad \dot{x}_M = \Pi(x)\frac{\partial S}{\partial x}. \tag{2.10}$$

The balance equations of the energy and the entropy are obtained by evaluating their time derivative along the trajectories of $x$:

$$\begin{aligned} \frac{dU}{dt} =& \frac{\partial U}{\partial x}^\top \left(-\Gamma^\top F_J + \Pi^\top F_M\right) = \dot{x}_J F_J + \left(\Pi \frac{\partial U}{\partial x}\right)^\top F_M, \\ \frac{dS}{dt} =& \frac{\partial S}{\partial x}^\top \left(M\frac{\partial S}{\partial x} - \Gamma^\top F_J + \Pi^\top F_M\right) = \frac{\partial S}{\partial x}^\top M \frac{\partial S}{\partial x} - \left(\Gamma \frac{\partial S}{\partial x}\right)^\top F_J + \dot{x}_M F_M. \end{aligned}$$

where we have used (2.10). In [27] it has been suggested, in order that the entropy variation only through the irreversible (dissipative) ports of the system, that the matrix $\Gamma(x)$ should be in the null space of $\frac{\partial S}{\partial x}(x)$. A similar condition for $\Pi(x)$ with respect to $\frac{\partial U}{\partial x}(x)$ is however not imposed since the energy variation may be due to reversible and irreversible phenomena coupling the system to its environment.

It should be noticed that it is by far not trivial to embed a thermodynamic system with a geometric structure. The GENERIC formalism succeed but presents a drawback when dealing with control systems. The extension of GENERIC to open system is performed in terms of two pairs of auxiliary variables that are included as state variables and embedded in the geometric structure, hence it is not evident how to pose the control problem in a traditional sense. The degeneracy conditions (2.7) are also not trivial to verify for complex systems hence it is not straightforward to find a GENERIC representation for a particular system.

In the following section we suggest a class of pseudo PHS which indeed embeds in its definition both principles of thermodynamics but retains only a skew-symmetric structure matrix which can be constructed uniquely from the physical couplings. We shall then use this class of systems throughout the whole thesis.

### 2.2.3 Irreversible PHS

There is a large class of thermodynamic systems that can be expressed as pseudo PHS if the Hamiltonian function is selected as a thermodynamic potential such as the internal energy or the entropy [22, 27, 72]. We should clarify that we use the term pseudo PHS to refer to "quasi" PHS formulations of thermodynamic systems. Hence we do not use the denomination pseudo PHS in the sense of [93], where it is for PHS with associated Poisson bracket not fulfilling the Jacobi identities. From a control perspective it is usually more complicated to impose a desired closed-loop dynamic on pseudo PHS. Passivity based techniques can be easily applied to PHS, however due to the non-linearity with respect to the gradient of the Hamiltonian, this is not the case for pseudo PHS. In this work we define a class of pseudo PHS to model large class of thermodynamic systems and to embed the first and second principle in the structure of the pseudo PHS.

**Definition 1** *IPHS are defined by the dynamical equation*

$$\dot{x} = R\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right) J \frac{\partial U}{\partial x}(x) + W\left(x, \tfrac{\partial U}{\partial x}\right) + g\left(x, \tfrac{\partial U}{\partial x}\right) u, \tag{2.11}$$

*where*

*i.* $x \in \mathbb{R}^n$ *is the state vector,* $U(x) : \mathcal{C}^\infty(\mathbb{R}^n) \to \mathbb{R}$ *and* $S(x) : \mathcal{C}^\infty(\mathbb{R}^n) \to \mathbb{R}$.

*ii. The structure matrix* $J \in \mathbb{R}^n \times \mathbb{R}^n$ *is a constant skew-symmetric matrix.*

*iii.* $R = R\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right)$ *is composed of a positive definite function and a Poisson bracket evaluated on* $S$ *and* $U$*:*

$$R\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right) = \gamma\left(x, \tfrac{\partial U}{\partial x}\right) \{S, U\}_J, \tag{2.12}$$

*with* $\gamma(x, \frac{\partial U}{\partial x}) = \hat{\gamma}(x) : \mathcal{C}^\infty(\mathbb{R}^n) \to \mathbb{R}$, $\hat{\gamma} \geq 0$, *a non-linear positive function of the states and co-states of the system that may be expressed as a function of the states only.*

*iv.* $W(x, \frac{\partial U}{\partial x}) \in \mathbb{R}^1 \times \mathbb{R}^n$ *and* $g(x, \frac{\partial U}{\partial x})u \in \mathbb{R}^1 \times \mathbb{R}^n$ *are associated with the ports of the system, where the input is* $u(t) \in \mathbb{R}^m$ *a time dependent function.*

The main difference with the definition of a PHS is that $R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right)$ depends on the co-state variables destroying the linearity of any Poisson tensor, considering the mapping $\frac{\partial U}{\partial x}$ to the drift dynamics $R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right) J \frac{\partial U}{\partial x}$ and associated with the matrix $RJ$. Furthermore, the two vector fields $W\left(x, \frac{\partial U}{\partial x}\right)$ and $g\left(x, \frac{\partial U}{\partial x}\right)$ may also depend on states and co-states.

Let us analyse Definition 1 for the particular case of thermodynamic systems. The first principle of thermodynamic states that the energy of the system is conserved. This condition is also true for PHS in mechanics. It is then logical that the Hamiltonian function of IPHS corresponds to the energy (as for PHS). As for PHS, there is sometimes more than one conserved quantity that may be used as Hamiltonian function. For instance in mass balance system a conserved quantity frequently used as Hamiltonian function is the total mass of the system [60, 80, 9, 18]. In the

case of IPHS there may also exist more than one conserved quantity depending on the constraints of the system. For instance in the case of a continuous stirred tank reactor (CSTR) with constant pressure and volume, the enthalpy is a conserved quantity and may be used as Hamiltonian function.

The second item of Definition 1 states that $J$ is a constant skew-symmetric matrix. We will actually see in the following sections that for the case of heat exchangers and chemical reactors this matrix represents the interconnection structure of the system. As it has been clearly exposed in [49, 50, 91], PHS arise systematically from network models of physical systems. In network models of complex physical systems the overall system is seen as the interconnection of energy-storing elements via basic interconnection (balance) laws as Newton's third law in mechanics or Kirchhoff's laws in electrical circuits, as well as power conserving elements, like transformers together, with energy-dissipating elements. PHS formalizes these basic interconnection laws together with the power conserving elements by a geometric structure. In PHS the structure matrix $J(x)$ and the input matrix $g(x)$ are directly associated with the network interconnection structure, while the Hamiltonian is just the sum of the energies of all the energy-storing elements. In thermodynamic there is a similar network relation between different domains. The efforts (intensive variables) of one domain generates the flows in other domains (time evolution of the extensive variables). We expect the IPHS to represent this network-like interconnection, thus we also expect $J$ to be constant with coefficients given by the network structure of the system. We will show that for a simple thermodynamic systems as the heat exchanger $J$ will just indicate the direction of the flows, thus its elements will be $-1$, 0, or 1, while for more complex systems such as chemical reactions it is given by the stoichiometry of the chemical network.

The fact that in our definition of IPHS the structure matrix $J$ is a constant matrix forces the function $R$ to capture all the state and co-state dependent behaviour of the internal interconnection of the system. In order to study the specific form of $R$ we again recall the first and second principle that we have represented with equation (2.4). It is clear that by the skew-symmetry of $J$ the energy of the system is conserved. The entropy balance of the system is given by

$$\frac{dS}{dt} = R\frac{\partial S}{\partial x}^{\top} J\frac{\partial U}{\partial x} + \frac{\partial S}{\partial x}^{\top} W + \frac{\partial S}{\partial x}^{\top} gu.$$

If it is assumed that the system is isolated ($W = 0$ and $g = 0$) the balance becomes

$$\frac{dS}{dt} = R\frac{\partial S}{\partial x}^{\top} J\frac{\partial U}{\partial x}.$$

By the second law of thermodynamic, the entropy balance of an isolated thermodynamic system is always positive and equal to the *internal entropy production*, that will be denote by $\sigma_{int}$. Thus we may write the following relation

$$R\frac{\partial S}{\partial x}^{\top} J\frac{\partial U}{\partial x} = \sigma_{int} \geq 0.$$

Recall that $\frac{\partial S}{\partial x}^\top J \frac{\partial U}{\partial x}(x) = \{S,U\}_J$, this suggest to define $R = \gamma\left(x, \frac{\partial U}{\partial x}\right)\{S,U\}_J$ such that

$$\frac{dS}{dt} = R\frac{\partial S}{\partial x}^\top J\frac{\partial U}{\partial x} = \gamma\left(x, \tfrac{\partial U}{\partial x}\right)\{S,U\}_J^2 = \sigma_{int} \geq 0,$$

with $\gamma\left(x, \frac{\partial U}{\partial x}\right)$ a positive definite function. Recall that the entropy is a state variable and the gradient of the entropy $\frac{\partial S}{\partial x}$ is a vector whose elements are either 1 or 0. Since the Poisson bracket is defined with respect to the constant matrix $J$, the bracket $\{S,U\}_J$ is a linear combination of the co-energy variables (elements of $\frac{\partial U}{\partial x}$) and actually defines the thermodynamic driving force. Finally, computing $\frac{dU}{dt}$ along the trajectories of (2.11) we obtain

$$\frac{dU}{dt} = \frac{\partial U}{\partial x}^\top W + \frac{\partial U}{\partial x}^\top gu,$$

due to the skew-symmetry of $J$. Since the energy of the system is conserved, the only admissible energy variation is through input and output ports (interaction point with the environment) of the system. Hence the sum $W + gu$ represents these ports. Furthermore, since $\frac{\partial U}{\partial x}$ is a vector of efforts, $W$ and $gu$ are vectors of flows.

Despite that we are restricting our work to a specific class of systems, this class is wide enough to encompass several thermodynamic processes of practical importance, notably chemical reactions and heat exchange processes [72, 74, 73, 75]. The specific form the drift dynamic $RJ$ collects all the non-linear terms in the scalar function $R\left(x, \frac{\partial U}{\partial x}\right)$. This will prove to be of practical importance in the design of feedback laws using the contact formulation in Chapter 3.

Along this work two examples will be used to illustrate our ideas: a heat exchange process and the continuous stirred tank reactor (CSTR). The heat exchanger is a simple example that only involves the thermal domain. We consider it the ideal system to clearly and explicitly show the computations of the propositions. The CSTR on other hand is a complex thermodynamic process and involves mass and energy balance. This example will be thoroughly analysed in Section 2.4.

### 2.2.4 Example: the heat exchanger

Consider two simple thermodynamic systems, indexed by 1 and 2 (for instance two ideal gases), which may interact only through a conducting wall. The dynamic of this system is given by the following equation

$$\begin{bmatrix}\dot{S}_1\\ \dot{S}_2\end{bmatrix} = \lambda\begin{bmatrix}\frac{T_2(S_2)}{T_1(S_1)} - 1\\ \frac{T_1(S_1)}{T_2(S_2)} - 1\end{bmatrix} + \lambda_e\begin{bmatrix}0\\ \frac{T_e(t)}{T_2(S_2)} - 1\end{bmatrix}$$

where $S_1$ and $S_2$ are the entropies of subsystem 1 and 2, $T_e(t)$ a time dependent external heat source and $\lambda > 0$ and $\lambda_e > 0$ denotes Fourier's heat conduction coefficients. The temperatures are modelled as exponential functions of the entropies [14] $T(S_i) = T_0 \exp\left(\frac{S_i}{c_i}\right)$, where $T_0$ and $c_i$ are constants.

This system may be written as

$$\begin{bmatrix}\dot{x}_1\\ \dot{x}_2\end{bmatrix} = \lambda\left(\frac{1}{\frac{\partial U}{\partial x_2}} - \frac{1}{\frac{\partial U}{\partial x_1}}\right)\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}\begin{bmatrix}\frac{\partial U}{\partial x_1}\\ \frac{\partial U}{\partial x_2}\end{bmatrix} + \lambda_e\begin{bmatrix}0\\ \frac{1}{\frac{\partial U}{\partial x_2}} - \frac{1}{u}\end{bmatrix}u,$$

where $x = [S_1, S_2]$, $U(x_1, x_2) = U_1(x_1) + U_2(x_2)$ is the internal energy of the overall system composed of the addition of the internal energies of each subsystem, $u(t)$ the controlled input that corresponds to the external heat source $T_e(t)$. Remark that $\frac{\partial U}{\partial x_i} = T_i(x_i)$. This system has been widely studied from a modelling perspective using the contact Hamiltonian framework in [22]. It is possible to write the model of the heat exchanger as a IPHS (2.11) by writing the system explicitly as an affine control system

$$\dot{x} = R(x,T)JT(x) + W + g(T)u(t), \tag{2.13}$$

where $T(x) = [T_1(x_1), T_2(x_2)]$, $R(x, T(x)) = \lambda\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$, $J = \left[\begin{smallmatrix}0 & -1\\ 1 & 0\end{smallmatrix}\right]$, $W = -\lambda_e\left[\begin{smallmatrix}0\\ 1\end{smallmatrix}\right]$ and $g = \frac{\lambda_e}{T_2}\left[\begin{smallmatrix}0\\ 1\end{smallmatrix}\right]$. Let us verify that the IPHS (2.13) fulfils Definition 1. The total entropy of the system is given by the sum of the entropies of each compartments $S = S_1 + S_2$. The Poisson bracket $\{S, U\}_J$ is then simply the difference of temperatures between the compartments

$$\{S,U\}_J = \frac{\partial S}{\partial x}^\top J\frac{\partial U}{\partial x} = \begin{bmatrix}1\\ 1\end{bmatrix}^\top\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}\begin{bmatrix}T_1\\ T_2\end{bmatrix} = T_1 - T_2.$$

And one may then identify the expression of the modulating function

$$R(x,T) = \lambda\left(\frac{1}{T_2} - \frac{1}{T_1}\right) = \lambda\frac{T_1 - T_2}{T_1T2} = \gamma(T_1 - T_2),$$

with $\gamma = \frac{\lambda}{T_1T2}$. Since $\lambda$, $T_1$ and $T_2$ are always greater than zero, $\gamma > 0$. The sum $W + g(T_2)u$ defines entropy flows generated by the interaction of subsystem 2 and the external heat source, hence corresponds to the port of the system. ■

## 2.3 Formulation of open thermodynamic systems in the TPS

In this section the definition of conservative contact systems in terms of IPHS is introduced. The dynamical system is lifted to the Thermodynamic Phase Space (TPS) similarly as it has been suggested in previous work [22, 27]. The special structure of IPHS is used to suggest alternative lifts of dynamical systems that ensure that the contact Hamiltonian functions are regular or well defined, even $C^\infty$ in the complete TPS (i.e. do not posses singularities). Indeed, because of the particular structure IPHS it is possible to identify the parts of the dynamical system that may induce singularities on the contact Hamiltonian function and hence also on the contact vector field. In the following we will define control contact systems in $\mathbb{R}^{2n+1}$ using canonical coordinates. A more geometrical definition of contact systems is presented in Chapter 3.

### 2.3.1 Reminder on control contact systems

Thermodynamic systems are defined by $n+1$ extensive variables and by Gibbs' fundamental equation relating them. In practice $n$ additional variables, namely the intensive variables that may be measured, are also used to model thermodynamic systems. Contact systems are defined in the $2n+1$-dimensional space of extensive and intensive variables, hence they define a sort of redundant system. Using this extended space it is possible to endow the TPS with a geometric structure. We shall in the sequel recall briefly the main definitions and properties of the control contact systems considered in this chapter and the reader is referred to [22, 48, 8] for details. For the sake of simplicity we shall restrict to a presentation in some coordinates and hence identify the thermodynamic phase space with the real vector space $\mathcal{T} = \mathbb{R}^{2n+1}$, $n \in \mathbb{N}$.

According to Darboux's theorem there exists a set of *canonical coordinates* $(x_0, x, p) \in \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n$ of $\mathcal{T}$ where the contact form $\theta$ is given by

$$\theta = dx_0 - \sum_{i=1}^{n} p_i dx_i,$$

where $d$ denotes the exterior derivative. Associated with the contact form there is set of distinguished submanifolds, called *Legendre submanifolds* (since they are closely related to Legendre transformations), denoted by $\mathcal{L}$, which are defined by the Pfaffian equation: $\theta = 0$. The following theorem presented in [8] allows to locally describe Legendre submanifolds by using generating functions.

**Theorem 2** *For any partition $I+J$ of the set of indices $\{1, \ldots, n\}$ into two disjoint subsets and for any function $\mathcal{F}(x_I, p_J)$ of $n$ variables $x_i, i \in I$, $p_j, j \in J$, the $2n+1$ equations*

$$x_0 = \mathcal{F} - p_J^\top \frac{\partial \mathcal{F}}{\partial p_J}, \qquad x_J = -\frac{\partial \mathcal{F}}{\partial p_J}, \qquad p_I = \frac{\partial \mathcal{F}}{\partial x_I}. \tag{2.14}$$

*define a Legendre submanifold $\mathcal{L}$ of $\mathbb{R}^{2n+1}$. Conversely, every Legendre submanifold of $\mathbb{R}^{2n+1}$ is defined in a neighbourhood of every point by these formulas for at least one of the $2^n$ possible choices of the subset $I$.*

The contact geometry may be applied to describe equilibrium thermodynamics [53, 57, 20, 24]. Indeed in thermodynamics $x_0$ is associated with a thermodynamic potential, such as the internal energy, and $(x_i, p_i)$ denotes the pairs of conjugated extensive and intensives variables. In this case the Pfaffian equation $\theta = 0$ is a statement of Gibbs' fundamental relation

$$dU = \sum_{i=1}^{n-2} \mu_i dN_i - pdV + TdS,$$

where the extensive variables $U$, $N_i$, $V$, and $S$, respectively the internal energy, the number of moles of the $i$th chemical specie, the volume and the entropy, and the intensive variables $\mu_i$, $p$ and $T$, respectively the chemical potential of the $i$th chemical specie, the pressure and the temperature, are identified with canonical

coordinate $x_0, x, p$. The canonical coordinates have physical meaning only on a Legendre submanifold of $\theta$. There $x_0$ is a thermodynamic potential function of the independent variables $x$, and $p$ are the corresponding variables conjugated with respect to the potential. On the Legendre submanifold these parameters are related by the equation $p = \frac{\partial x_0}{\partial x}$, which is a special case of theorem 2, where $\mathcal{F}$ is a function of $x$ only. The Legendre submanifold generated by the internal energy $U$ is defined as

$$\mathcal{L}_U = \left\{ x_0 = U(x), x = x, p = \frac{\partial U}{\partial x}(x) \right\}.$$

Note that Gibbs' relation is satisfied on this Legendre submanifold.

Irreversible thermodynamics may be described by using *contact vector fields*. As it will be shown in Chapter 3, these are vector fields which leaves the contact distribution invariant. The vector space of contact vector fields and the space of smooth real functions are isomorphic[48]. More specifically there exists uniquely for each contact vector field a function, called *contact Hamiltonian* and denoted by $K$, that generates the contact vector field, denoted by $X$. In any set of canonical coordinates a contact system is then expressed by the dynamical equation $\frac{d}{dt}\begin{bmatrix} x_0 \\ x \\ p \end{bmatrix} = X$, with

$$X = \begin{bmatrix} K \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & -p^\top \\ 0 & 0 & -I_n \\ p & I_n & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial K}{\partial x_0} \\ \frac{\partial K}{\partial x} \\ \frac{\partial K}{\partial p} \end{bmatrix}, \tag{2.15}$$

where $I_n$ denotes the identity matrix of order $n$.

The following theorem, presented in [57], shows that functions on $\mathbb{R}^{2n+1}$ which vanish on on a Legendre submanifold $\mathcal{L}$ give rise to continuous contact transformations which preserve $\mathcal{L}$, i.e., which map $\mathcal{L}$ into itself.

**Theorem 3** *Let $\mathcal{L}$ be a Legendre submanifold. Then $X_K$ is tangent to $\mathcal{L}$ if and only if $K$ vanishes on $\mathcal{L}$, i.e., $\mathcal{L} \subset K^{-1}(0)$.*

Controlled contact systems have been introduced in [21] and then used for modelling and analysis of simple and complex open thermodynamic systems [22, 20, 24]. They are defined by contact Hamiltonians which depend not only on the state variables $(x_0, x, p)$ but also on a time dependent input function $u(t) \in L_1^{\text{loc}}(\mathbb{R})$. In this chapter we shall consider the following class of controlled contact systems

$$X = X_{K_0} + X_{K_c} \tag{2.16}$$

where $K_0(x_0, x, p) \in C^\infty(\mathcal{T}) \to \mathbb{R}$ is the *internal contact Hamiltonian* that models the internal behaviour of the system, $K_c(x_0, x, p, u) \in C^\infty(\mathcal{T} \times \mathbb{R}) \to \mathbb{R}$ is the *interaction (or control) contact Hamiltonian* that models the ports of the system and where $X_{K_0}$ and $X_{K_c}$ are contact vector fields with respect to the canonical contact form $\theta$.

A *conservative controlled contact system* is defined with respect to a Legendre submanifold. The contact vector field leaves a Legendre submanifold invariant which for physical systems is defined by Gibbs' fundamental relation. This means that conservative contact systems arising from the modelling of physical systems leaves the thermodynamic properties invariant [53, 57].

**Definition 4** *A conservative control contact system is defined as a control contact system with the contact Hamiltonians satisfying the invariance condition*

$$K_0\big|_{\mathcal{L}} = 0, \quad K_c\big|_{\mathcal{L}} = 0,$$

*where* $\cdot|_{\mathcal{L}}$ *denotes the restriction to* $\mathcal{L}$*.*

An important feature of conservative contact systems is that on the invariant Legendre submanifold it is possible to express $n+1$ variables as function of the remaining $n$ variables. The equilibrium properties of a thermodynamic system are defined by the Legendre submanifold, hence on the restriction to the Legendre submanifold the extensive and intensive variables are related by Gibbs' relation an may be expressed as function of each others.

### 2.3.2 Regular lift of IPHS to the TPS

It is possible to define a conservative contact system from a dynamical system by *lifting* it into the TPS [20, 22, 24, 30, 27]. The lift of dynamical systems to the TPS has the interesting property that it may be performed such that the contact vector field leaves invariant the Legendre submanifold where the contact Hamiltonian is zero. This means by theorem 2 that on the Legendre submanifold only $n$ independent variables are required to describe the system dynamic and by theorem 3 that the trajectories will remain on the Legendre submanifold.

A kind of lift of dynamical systems that has been proposed in [20, 22, 24, 30, 27] is defined by pre-multiplication of the vector field expressing the dynamical equation of the system by the vector $\left(\frac{\partial U}{\partial x}(x) - p\right)^\top$. Indeed let us consider the (closed) dynamical system

$$\dot{x} = f(x, \tfrac{\partial U}{\partial x}).$$

A conservative contact Hamiltonian system is then simply defined by the contact Hamiltonian function

$$K_0 = \left(\tfrac{\partial U}{\partial x}(x) - p\right)^\top f(x, \tfrac{\partial U}{\partial x}).$$

The contact vector field $X_{K_0}$ leaves the Legendre submanifold $\mathcal{L}_U$ invariant and it is not difficult using the expression in local coordinates of the contact vector field (2.15) to verify that on the restriction to $\mathcal{L}_U$ the $x$ coordinate of $X_{K_0}$ is equal to $\dot{x}|_{\mathcal{L}_U} = f(x, \frac{\partial U}{\partial x})$. The previous lift is not uniquely defined, and as it has been shown in [30] there are infinite different possibilities to perform the lift of a dynamical system, each one defined by a different contact Hamiltonian function. One possibility is to define the contact Hamiltonian as

$$K_0 = \left(\tfrac{\partial U}{\partial x}(x) - p\right)^\top f(x, p).$$

In this case the intensive variables have been "parametrized" by the $p$ coordinates. This is justified since on the Legendre submanifold $\mathcal{L}_U$ the $p$ coordinates are equal to the intensive variables. In previous works [20, 22, 24, 30, 27] this parametrization has in general been used to define the lift of dynamical systems to the TPS. Once again, the contact vector field $X_{K_0}$ leaves the Legendre submanifold $\mathcal{L}_U$ invariant

and we may verify that on the restriction to $\mathcal{L}_U$ the $x$ coordinate of $X_{K_0}$ is equal to $\dot{x}|_{\mathcal{L}_U} = f(x, \frac{\partial U}{\partial x})$. Although the previous contact Hamiltonians (and hence also the contact vector fields) are different, they generate the same dynamical system on the restriction to $\mathcal{L}_U$.

One may then ask the following question: can a dynamical system be lifted on the TPS with the only restriction that the dynamic of the system is recovered when restricting the contact vector field to $\mathcal{L}_U$? The answer is actually no. Due to regularity properties the contact Hamiltonian should be defined such that it does not present singularities on the complete TPS. In the fundamental works of D. Eberard and co-workers [22] and Favache and co-workers [30, 27] the discussion on regular or well defined lift has not been addressed. Moreover, many of the conservative contact Hamiltonian systems presented in the literature posses singularities in the contact Hamiltonian functions and hence generates contact vector fields with singularities. We will address the concept of regular or well-defined lift of dynamical systems by using IPHS.

As previously mentioned a large class thermodynamic processes, such as the ones modelling chemical reactors [72] and heat exchangers [22] may be represented as IPHS (Definition 1),

$$\dot{x} = R\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right) J \frac{\partial U}{\partial x}(x) + W\left(x, \tfrac{\partial U}{\partial x}\right) + g\left(x, \tfrac{\partial U}{\partial x}\right) u,$$

with $R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right)$ a non-linear scalar function modulating the constant skew-symmetric matrix $J$ and $W\left(x, \frac{\partial U}{\partial x}\right) + g\left(x, \frac{\partial U}{\partial x}\right) u$ the input port. According to the preceding discussion the IPHS may be lifted to the TPS by defining the following conservative contact Hamiltonian

$$K_0 + K_c = \left(\frac{\partial U}{\partial x} - p\right)^\top \left(RJ\frac{\partial U}{\partial x}(x) + gu\right) = -p^\top RJ\frac{\partial U}{\partial x}(x) + \left(\frac{\partial U}{\partial x} - p\right)^\top gu, \tag{2.17}$$

where we have assumed $W = 0$ for simplicity. The Legendre submanifold $\mathcal{L}_U$, generated by the internal energy $U(x)$, is left invariant by the contact vector field. On $\mathcal{L}_U$ the vector field $X$ is equal to the dynamic of the lifted thermodynamic system. The contact Hamiltonian (2.17) is affine in the input, hence generates a vector field affine in the input. The internal contact Hamiltonian is given by $K_0(x,p) = -p^\top RJ\frac{\partial U}{\partial x}$ and the interaction contact Hamiltonian by $K_c(x,p,u) = \left(\frac{\partial U}{\partial x} - p\right)^\top gu$. The contact Hamiltonians are smooth and well defined in the whole TPS since they do not present singularities.

Let us now consider the parametrization of the intensive variables in $R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right)$ by $p$. This leads to consider an internal contact Hamiltonian function of the following form

$$K_0 = -p^\top R(x, p, \tfrac{\partial S}{\partial x}) J \frac{\partial U}{\partial x}. \tag{2.18}$$

As discussed in the previous paragraphs this contact Hamiltonian generates the same vector field on the restriction to $\mathcal{L}_U$ as

$$K_0 = -p^\top R\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right) J \frac{\partial U}{\partial x}. \tag{2.19}$$

Despite that both lifts generate the same dynamic restricted to $\mathcal{L}_U$ there exists a structural problem with (2.18). Consider a closed IPHS and Gibbs' fundamental equation [12], that we will write as

$$dU = \sum_{i=1}^{n-1} \frac{\partial U}{\partial x_i} dx_i + \frac{\partial U}{\partial S} dS.$$

The continuity, differentiability and monotonic property $\left(\frac{\partial S}{\partial U} > 0\right)$ of the entropy imply that the entropy function can be inverted with respect to the energy, hence it is possible to write

$$dS = -\frac{\partial S}{\partial U} \sum_{i=1}^{n-1} \frac{\partial U}{\partial x_i} dx_i + \frac{\partial S}{\partial U} dU.$$

From this last equation, and since $= \frac{\partial S}{\partial U} = \frac{1}{T}$ with $T > 0$, we have that the for the closed IPHS system the time evolution of the entropy will always be of the form

$$\frac{dS}{dt} = \frac{\partial S}{\partial U} \gamma' \left(x, \tfrac{\partial U}{\partial x}\right) \{S, U\}_J^2 ,$$

with $\gamma' \left(x, \frac{\partial U}{\partial x}\right) \geq 0$. Recall from Definition 1 that $R = \gamma \left(x, \frac{\partial U}{\partial x}\right) \{S, U\}_J$, and that for thermodynamic systems $\{S, U\}_J$ is a linear combination of the co-states variables. Hence we may write for a thermodynamic system

$$R \left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right) = \gamma \left(x, \tfrac{\partial U}{\partial x}\right) \{S, U\}_J = \frac{1}{T} \gamma' \left(x, \tfrac{\partial U}{\partial x}\right) \{S, U\}_J,$$

with $\gamma = \frac{1}{T} \gamma' \left(x, \frac{\partial U}{\partial x}\right)$. A complete parametrization of $R$ would lead to

$$R(x, p) = \frac{1}{p_T} \gamma' (x, p) \frac{\partial S}{\partial x} Jp, \tag{2.20}$$

where $p_T$ indicates the parametrization of $T$ in the $p$-coordinates. It is clear from equation (2.20) that it is not possible to arbitrarily replace $\frac{\partial U}{\partial x}$ by $p$ since the inverse of the temperature appears in the definition of $R$. If (2.20) is used to perform the lift then, at least, on the point $p_T = 0$ the contact Hamiltonian possesses a singularity. As mentioned before this issue has never been addressed in previous publications, and unfortunately the lifts proposed in [22, 30, 27] present this particular singularity.

A regular lift of $R$ will depend on the particular form of the function $\gamma \left(x, \frac{\partial U}{\partial x}\right)$. However the simplest way to perform a regular lift of a closed IPHS is by not parametrizing it by $p$. Indeed $R \left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right)$ is in general well-defined for all $x$ and so is the vector $J \frac{\partial U}{\partial x}$. Hence the lift defined by equation (2.19) is in general well defined in the complete TPS.

Nevertheless it may still be desirable to lift the IPHS as in equation (2.18), specifically if we are thinking on control design. It will be shown in Chapter 3 that the special structure of $R$ and an adequate parametrization simplifies some matching conditions when doing control synthesis on the TPS. Using equation (2.20) we can conclude the following.

- The function $\gamma\left(x, \frac{\partial U}{\partial x}\right)$ may be lifted as $\gamma(x,p)$ as long as it does not present singularities in $p$. In particular the term $\frac{1}{T}$ can never be lifted as $\frac{1}{p_T}$ since it possesses a singularity at $p_T = 0$.
- The Poisson bracket $\{S,U\}_J$ may always be lifted as $\frac{\partial S}{\partial x}Jp$ since it is a linear combination of $p$.

If $\gamma(x,p)$ presents singularities at some point it may still be lifted to the TPS as a partially parametrized function $\gamma\left(x, \frac{\partial U}{\partial x}, p\right)$. Let us illustrate this on the heat exchanger.

### 2.3.3 Example: the heat exchanger (continued)

Recall the heat exchanger

$$\begin{bmatrix}\dot{S}_1\\ \dot{S}_2\end{bmatrix} = \lambda\left(\frac{1}{\frac{\partial U}{\partial S_2}} - \frac{1}{\frac{\partial U}{\partial S_1}}\right)\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}\begin{bmatrix}\frac{\partial U}{\partial S_1}\\ \frac{\partial U}{\partial S_2}\end{bmatrix} + \lambda_e\begin{bmatrix}0\\ \frac{1}{\frac{\partial U}{\partial S_2}} - \frac{1}{u}\end{bmatrix}u,$$

and its representation as IPHS

$$\dot{x} = R(x,T(x))J\frac{\partial U}{\partial x}(x) + W + g(T)u$$

where $x = [S_1, S_2]$ is the entropy of subsystem 1 and 2, $U(S_1,S_2) = U_1(S_1) + U_2(S_2)$ is the internal energy of the overall system composed of the addition of the internal energies of each subsystem, $u(t)$ the controlled input that corresponds to an external heat source, $\lambda > 0, \lambda_e > 0$ denote Fourier's heat conduction coefficients, $\frac{\partial U}{\partial x_i} = T_i(x_i)$, $T(x_i) = T_0\exp\left(\frac{x_i}{c_i}\right)$, where $T_0$ and $c_i$ are constants, $R(x,T(x)) = \lambda\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$, $J = \left[\begin{smallmatrix}0 & -1\\ 1 & 0\end{smallmatrix}\right]$, $W = -\lambda_e\left[\begin{smallmatrix}0\\ 1\end{smallmatrix}\right]$ and $g = \frac{\lambda_e}{T_2}\left[\begin{smallmatrix}0\\ 1\end{smallmatrix}\right]$.

As mentioned before, lifting this system to the TPS may be done in infinite number of ways. In previous work [22] this lift has been performed using the following parametrization of $R$ and $g$ as

$$R(p) = \lambda\left(\frac{1}{p_2} - \frac{1}{p_1}\right) = \lambda\left(\frac{p_1 - p_2}{p_1 p_2}\right), \quad g(p) = \frac{\lambda_e}{p_2}\begin{bmatrix}0\\ 1\end{bmatrix}. \tag{2.21}$$

However since $p$ may have any value on the TPS, $R(p)$ and $g(p)$ in (2.21) are undefined at $p = [0,0]^\top$. Hence, the lift using the previously defined parametrization is not defined on the whole TPS. This issue can be overcome by regularizing the parametrizations. Recall from the first part of this example that $R = \lambda\frac{1}{T_1T_2}(T_1 - T_2)$, with $\gamma = \frac{\lambda}{T_1T_2}$ and $\{S,U\}_J = T_1 - T_2$. The only part of $R$ that is parametrizable is the bracket $\{S,U\}_J = T_1 - T_2$. The lift may then be defined as

$$R(x,p) = \lambda\left(\frac{p_1 - p_2}{T_1T_2}\right), \quad g(x) = \frac{\lambda_e}{T_2}\begin{bmatrix}0\\ 1\end{bmatrix}.$$

This parametrization of $R$ and $g$ generates a different contact vector field than the one defined by (2.21), but as previously discussed, it is possible to verify using

equation (2.15) that on the restriction to $\mathcal{L}_U$ the contact vector fields coincide. The lift of the heat exchanger may then be defined as

$$\begin{aligned} K_0(x,p) &= -\,R(x,p)p^\top J_s T(x), \\ K_c(x,p) &= \left(\tfrac{\partial U}{\partial x} - p\right)^\top (W + gu)\,. \end{aligned} \tag{2.22}$$

The thermodynamic properties of the composed system are simply obtained by considering the Legendre submanifold $\mathcal{L}_U$ generated by the potential $U = U_1 + U_2$,

$$\mathcal{L}_U : \left\{ \begin{array}{ll} x_0 & = U \\ x & = [S_1, S_2]^\top \\ p & = \left[\tfrac{\partial U}{\partial S_1}, \tfrac{\partial U}{\partial S_2}\right]^\top = [T_1, T_2]^\top \end{array} \right\}. \tag{2.23}$$

Hence on $\mathcal{L}_U$ the thermodynamic properties of the system are recovered and the extensive variables may be identified with $x_0$ and $x$, and the intensive variables with $p$. ■

## 2.4 On the Hamiltonian formulation of the CSTR

In this section we will apply the previously developed concepts on a complex thermodynamic process, namely the CSTR. We should begin this discussion by distinguish the formulations for the isothermal and non-isothermal CSTR. The isothermal CSTR does not involve energy balance, hence the dynamic is described only by mass balance equations and it is possible to use a PHS to model the system. The non-isothermal CSTR includes in addition to the mass balance equations an energy balance equation, making it no longer possible to propose a (true) PHS to model the system.

Nevertheless, in the last decades big efforts have been made to propose a Hamiltonian structure for the non-isothermal CSTR. Some of these attempts where centred in making the dynamical equation of the CSTR suit in some (pseudo) PHS representation for control purposes [81, 78, 18]. In those works there were no major needs to define a pseudo PHS with physical interpretation and usually the Hamiltonian function was defined as a linear combination or a quadratic function of the state variables. A similar approach but using Brayton-Moser representation [82] for the application of power-shaping control [62] was proposed in [26]. The standard symplectic Hamiltonian structure was used to express the dynamic of chemical reaction networks and the CSTR in [39, 68]. In these works thermodynamic concepts and especially the second principle of thermodynamic are taken into account to define the Hamiltonian system. The passivity of these system is proved following similar arguments to the ones presented in [5, 6]. The Hamiltonian functions in these works are obtained by integration and resembles the potential functions of mechanical systems, hence do not have a physical interpretation.

A different approach was followed in [28] and [42], where the entropy of the system was used to define the generating function of the system. In [28] the entropy production was used to define a Brayton-Moser formulation for a first order

reaction in a CSTR. In this case the existence of a Brayton-Moser representation depends on the solution of a PDE and the authors make emphasis on the difficulty of solving this PDE for higher dimensional systems. Furthermore, the structure matrices of the system are given by the solution of the PDE and do not have physical interpretation. In [42] the negative of the total entropy is used as Hamiltonian function to define a pseudo PHS. Indeed, since the entropy production is an always increasing function the time derivative of the negative of the entropy will be always decreasing and assure the passivity of the system. However, the pseudo PHS do not longer represent the conservation of energy and as in [28] the structure matrices lack physical meaning.

In this section we show that the non-isothermal CSTR may be expressed as an IPHS with clear thermodynamic interpretation. For a CSTR with a single reaction with arbitrary stoichiometry two IPHS representations are proposed (Propositions 5 and 6). One uses the total internal energy as Hamiltonian function while the second one uses the total enthalpy. Both of them posses the same structure matrix defined by the stoichiometric coefficients of the chemical reaction network. The non-linear function modulating the constant structure matrix is defined by the thermodynamic driving force: the chemical affinity and the enthalpy of reaction respectively. The IPHS representation of the CTSR is then used to propose a well defined contact Hamiltonian function that expresses the dynamical equation of the CSTR when projecting the contact vector field on the Legendre submanifold defining the physical properties of the system (Proposition 7). The contact Hamiltonian is analysed and physical interpretation is provided.

### 2.4.1 Formulation of the mass balance equations

Assume a chemical reaction in a continuous stirred tank reactor (CSTR) with the following reaction scheme

$$\nu_1 A_1 + \ldots + \nu_l A_l \rightleftharpoons \nu_{l+1} A_{l+1} + \ldots + \nu_m A_m, \qquad m > l \geq 1.$$

The time variation of the species in the reactor is given by [7]

$$\dot{n}_i = F_{ei} - F_{si} + r_i V \qquad i = 1, \ldots, m \tag{2.24}$$

where $n_i$ is the number of moles of the specie $i$, $F_{ei}$ and $F_{si}$ are respectively the inlet and outlet molar concentrations, $r_i = \bar{\nu}_i r$ where $r$ is the reaction rate composed of two reaction rates, one for the forward reaction $r_f$ and the other for the backward reaction $r_b$, with $r = (r_f - r_b)$ where each reaction rate only depends on the temperature and on the reactant concentration, $\bar{\nu}_i$ is the signed stoichiometric coefficient: $\bar{\nu}_i = -\nu_i$ if it appears on the left hand side of the reaction scheme, $\bar{\nu}_i = \nu_i$ in the other case. Following the usual assumptions [7, 25], $V$ the volume in the reactor is assumed to be constant as well as the pressure. We shall assume a reaction in gas phase, but the developments may be applied identically to a reactor with a reaction in liquid phase. The assumptions of constant volume and pressure impose a constraint over the total outlet flow $F_s = \sum_{i=1}^{m} F_{si}$ as discussed in [14, 16], making the outlet flows $F_{si}$ state dependent.

### 2.4.2 Models based on Gibbs relation

When considering the non-isothermal CSTR it is necessary to introduce an additional state variable to model the energy balance. We have chosen to model the energy balance using the extensive variable internal energy or total entropy, or by using the intensive variable temperature. In the following we will motivate the construction of the IPHS for the CSTR.

A classical construction of the state spaces is based on Gibbs' relation. Assuming once again constant volume and pressure Gibbs' relation reduces to

$$\dot{U} = \sum_{i=1}^{m} \frac{\partial U}{\partial n_i} \dot{n_i} + \frac{\partial U}{\partial S} \dot{S} \tag{2.25}$$

where $U$ denotes the internal energy, $S$ the entropy and the conjugated intensive variables are the chemical potential $\frac{\partial U}{\partial n_i} = \mu_i$ and the temperature $\frac{\partial U}{\partial S} = T$. Gibbs' relation can also be written in the so called entropy formulation

$$\dot{S} = \sum_{i=1}^{m} \frac{\partial S}{\partial n_i} \dot{n_i} + \frac{\partial S}{\partial U} \dot{U} \tag{2.26}$$

where $\frac{\partial S}{\partial n_i} = -\frac{\mu_i}{T}$ and $\frac{\partial S}{\partial U} = \frac{1}{T}$ are the intensive thermodynamic variables conjugated to $n_i$ and the internal energy $U$. In the sequel we shall formulate the dynamic of the CSTR as a control system in the form:

$$\dot{x} = \Theta \frac{\partial H}{\partial x} + gu$$

where $\Theta(x)$ is a matrix which is a function of the state variables and $g(x)$ is the input map. The choice of the generating function $H$ and the matrix $\Theta$ for the CSTR model, has been the matter of several papers [81, 39, 68, 78, 26, 42] and the results encompasses specially the theory of Hamiltonian and Brayton-Moser's [82] systems. In the general case, the manipulated input in the CSTR is the heat flux from the jacket $Q = h(T_e - T)$, where $T_e$ is the temperature of the jacket while the input flows of matter are supposed to be constant. Under the previous assumptions the internal energy of the CSTR is given by

$$U = \sum_{i=1}^{m} n_i [c_{pi}(T - T_0) + u_{0i}],$$

where $c_{pi}$, $u_{0i}$ are respectively the heat capacity and reference molar energy. Assuming constant volume and pressure the reference molar enthalpy $h_{0i} = u_{0i}$ [79], and the balance equation of the internal energy is [14, 25]

$$\dot{U} = \dot{H}_H = \sum_{i=1}^{m} (F_{ei} h_{ei} - F_{si} h_{si}) + Q, \tag{2.27}$$

where $H_H$ is the total enthalpy of the reactor and $h_{ei}, h_{si}$ the inlet and outlet specific molar enthalpies respectively. The entropy function in the CSTR is given by

$$S = \mathcal{C}_p \ln\left(\tfrac{T}{T_0}\right) - R\sum_{i=1}^{m}\left[n_i \ln\left(\tfrac{n_i}{N}\right)\right] + \sum_{i=1}^{m}(n_i s_{0i}), \tag{2.28}$$

where $\mathcal{C}_p = \sum_{i=1}^{m} n_i c_{pi}$, $T_0$, $N$, $s_{0i}$ and $R$ are respectively total heat capacity, reference temperature, total number of moles, reference molar entropy and the ideal gas constant. Hence, the entropy balance equation may be deduced from this expression or from Gibbs' relation

$$\dot{S} = \sum_{i=1}^{m}(F_{ei}s_{ei} - F_s s_i) + \frac{Q}{T_w} + \sigma, \tag{2.29}$$

where

$$\sigma = \sum_{i=1}^{m}\frac{F_{ei}}{T}(h_{ei} - Ts_{ei} - \mu_i) + \frac{Q}{T} - \frac{Q}{T_w} - \sum_{i=1}^{m}\mu_i\nu_i\frac{r}{T}$$

is the entropy creation due to mass transfer, heat transfer and chemical reactions. We may define different dynamical equations representing the CSTR depending on the choice of state variables.

Let us in a first instance consider the following state vector $x = [n_1, \ldots, n_m, S]^\top$, where the entropy is used as state variable to express the energy balance (that is the balance equation associated with the thermal domain). By defining the two following skew-symmetric, respectively symmetric structure matrices:

$$\mathcal{J}_f = \begin{bmatrix} 0 & 0 & 0 & f_{n1} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & f_{nm} \\ -f_{n1} & \ldots & -f_{nm} & 0 \end{bmatrix}, \qquad M = \begin{bmatrix} 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 \\ 0 & \ldots & 0 & \theta \end{bmatrix}, \tag{2.30}$$

with $f_{ni} = \dot{n}_i$, $j = 1, 2$ and

$$\eta = \frac{1}{T}\sum_{i=1}^{m}(F_{ei}h_{ei} - F_{si}h_{si}).$$

By combining the mass balance relation (2.24) with Gibbs' relation (equation (2.25) and defining the vector $g = [0, \ldots, 0, 1]^\top$ of dimension $m+1$ we define the following dynamical system

$$\dot{x} = \frac{1}{T}\left(\mathcal{J}_f(x) + M(x)\right)\frac{\partial U}{\partial x}(x) + \frac{1}{T}gQ. \tag{2.31}$$

Now, if the internal energy is used to model the energy balance of the system we chose the following state variable $x_2 = [n_1, \ldots, n_m, U]^\top$. By defining

$$\eta = T\sum_{i=1}^{m}\left(F_{ei}s_{ei} - F_{si}s_i - \mu_i\frac{r_i V}{T}\right), \tag{2.32}$$

we may once again use (2.30) and combine them with the mass balance relation and Gibbs' relation (2.26) to obtain the dynamical system

$$\dot{x} = T\left(\mathcal{J}_f(x) + M(x)\right)\frac{\partial S}{\partial x}(x) + gQ. \tag{2.33}$$

While the internal energy balance depends only on the energy carried in or out to the system by external interactions (inlet, outlet flows and heat transfer) the entropy balance depends in addition on the entropy production due to the chemical reaction. This immediately gives some insight on the consequences of entropy creation in a chemical system: not only it produces nonlinear relations destroying the Poisson brackets of the Hamiltonian formulation [22] but also introduces additional source terms due to the entropy creation.

It is possible to obtain an alternative formulation using the temperature to express the energy balance equation. Using as state variable the temperature one has to consider as thermodynamic potential, the Legendre transformation with respect to the entropy of the internal energy, the total enthalpy. Furthermore in a CSTR with constant volume and pressure, the change of enthalpy in time equals the time variation of the internal energy (2.27). The total enthalpy is given by

$$H_H = \sum_{i=1}^{m} n_i h_i(T). \tag{2.34}$$

By considering the state vector $x = [n_1, \ldots, n_m, T]^\top$, and noting that $c_{pi} = \frac{\partial h_i}{\partial T}$, the gradient of $H_H$ is

$$\frac{\partial H_H}{\partial x} = [h_1(T), \ldots, h_m(T), \mathcal{C}_p(n)]^\top.$$

The following system can then be defined to represent the CTSR

$$\dot{x} = \frac{1}{\mathcal{C}_p}\left(\mathcal{J}_f(x) + M(x)\right)\frac{\partial H_H}{\partial x}(x) + \frac{1}{\mathcal{C}_p} gQ, \tag{2.35}$$

where $M$ is as in (2.30) with $\eta = \frac{1}{\mathcal{C}_p}\sum_{i=1}^{m}(F_{ei}h_{ei} - F_{si}h_{si})$. The time variation of the temperature can be obtained from (2.31), (2.33) or (2.35):

$$\mathcal{C}_p\dot{T} = \sum_{i=1}^{m} F_{ei}c_{pi}(T - T_{in}) - \sum_{i=1}^{m} h_i r_i V + Q. \tag{2.36}$$

### 2.4.3 IPHS formulation of the CTSR

In the previous subsection we started from Gibbs' relation to derive a dynamical equation expressed in terms of a thermodynamic potential of the system. In this subsection we are going to be more specific and represent the CSTR as a IPHS according to Definition 1. In order to proceed we have to take into account two things. Firstly we would like to express the conservation of energy through a constant structure matrix $J$. We know from the PHS and GENERIC formalism that

this has to be done using a conservative quantity as generating function, hence we discard the entropy as Hamiltonian function. Secondly, we want to identify the ports of the system and separate them from the internal dynamics. When dealing with open systems, as for instance control, it is necessary to explicitly define the port variables of the system, i.e. the variables that interconnects the process with its environment. In the case of the CSTR this variables are given by: the heat flow from the jacket $Q$ and the inlet and output molar flows of each specie, $F_{ei}$ and $F_{si}$ respectively.

**Proposition 5** *The dynamical equation of the CSTR may be expressed as the IPHS*

$$\dot{x} = R\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right) J \frac{\partial U}{\partial x}(x) + W(x, F_e) + g\frac{Q}{T} \tag{2.37}$$

*with state vector* $x = [n_1, \ldots, n_m, S]^\top$*, the internal energy* $U(x)$ *as Hamiltonian function,*

$$J = \begin{bmatrix} 0 & \ldots & 0 & \bar{\nu}_1 \\ 0 & \ldots & 0 & \vdots \\ 0 & \ldots & 0 & \bar{\nu}_m \\ -\bar{\nu}_1 & \ldots & -\bar{\nu}_m & 0 \end{bmatrix}$$

*a constant skew-symmetric matrix whose elements are the stoichiometric coefficient of the chemical reaction mapping the network structure of the reaction, and*

$$R = \gamma\left(x, \tfrac{\partial U}{\partial x}\right)\{S, U\}_J = \left(\frac{rV}{T\mathcal{A}}\right)\mathcal{A}$$

*with* $\gamma = \frac{rV}{T\mathcal{A}}$ *and* $\{S, U\}_J = \mathcal{A}$*, where* $\mathcal{A} = -\sum_{i=1}^{m} \bar{\nu}_i \mu_i$ *is the chemical affinity of the reaction and corresponds to thermodynamic driving force of the chemical reaction. The port of the IPHS is given by* $W + gQ$ *and is composed by the extended input and output flow vector and the thermal interaction vector defined respectively as*

$$W = \begin{bmatrix} F_{e1} - F_{s2} \\ \vdots \\ F_{em} - F_{sm} \\ \omega \end{bmatrix}, \qquad g = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix} \frac{Q}{T}$$

*with* $\omega = \frac{1}{T}\sum_{i=1}^{m}(F_{ei}s_{ei} - F_{si}s_i)$*.*

**Proof.** Let us analyse (2.37) in the sense of Definition 1. As previously mentioned $J$ is constant and skew-symmetric, moreover, it represents the chemical reaction network.

It is interesting that the bracket $\{S, U\}_J$ is exactly the thermodynamic driving force of the chemical reaction. Indeed

$$\{S, U\}_J = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}^\top \begin{bmatrix} 0 & \ldots & 0 & \bar{\nu}_1 \\ 0 & \ldots & 0 & \vdots \\ 0 & \ldots & 0 & \bar{\nu}_m \\ -\bar{\nu}_1 & \ldots & -\bar{\nu}_m & 0 \end{bmatrix} \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_m \\ T \end{bmatrix} = -\sum_{i=1}^{m} \bar{\nu}_i \mu_i = \mathcal{A}.$$

Here $\mathcal{A}$ is the chemical affinity [47], that corresponds to the thermodynamic driving force of the chemical reaction. From the expression of the previous bracket we have that

$$R = \gamma\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right)\{S, U\}_J = \gamma\left(x, \tfrac{\partial U}{\partial x}\right)\mathcal{A},$$

which implies that

$$\gamma = \frac{rV}{T\mathcal{A}}. \tag{2.38}$$

It is not evident from (2.38) but $\gamma$ is a well defined positive definite function. Indeed, from De Donder's fundamental equation [70]

$$\sigma_r = \frac{rV}{T}\mathcal{A} \geq 0, \tag{2.39}$$

with $\sigma_r$ the entropy creation due to the chemical reaction. From this last equation we have

$$\begin{array}{lll} \mathcal{A} > 0 & \text{if} & \frac{rV}{T} \geq 0, \\ \mathcal{A} < 0 & \text{if} & \frac{rV}{T} \leq 0, \\ \mathcal{A} = 0 & \text{if} & \frac{rV}{T} = 0. \end{array}$$

The case $\mathcal{A} \neq 0$ if $\frac{rV}{T} = 0$ is physically impossible, since it would imply to have a chemical reaction proceeding at a finite rate in a reversible manner, i.e., it follows from the assumption that the reactions are irreversible processes. Hence, from De Donder's fundamental equation $\gamma = \frac{rV}{T\mathcal{A}}$ is positive definite. It remains to check if $\gamma$ is a well defined function. Since $T > 0$ the only possible singularity is when $\mathcal{A} = r = 0$. The affinity may be decomposed into a forward affinity and a reverse affinity [67, 14, 15]

$$\mathcal{A} = \mathcal{A}_f - \mathcal{A}_r \tag{2.40}$$

and the reaction rate may expressed in terms of the forward and reverse affinities as

$$r(\mathcal{A}_f, \mathcal{A}_r, T) = k_f(T)e^{\frac{\mathcal{A}_f}{RT}} - k_r(T)e^{\frac{\mathcal{A}_r}{RT}}, \tag{2.41}$$

where $k_f(T)$ and $k_r(T)$ are positive functions depending solely on the temperature. Using this relations it is possible to rewrite $\gamma$ in terms of the forward and reverse affinities

$$\gamma = \frac{V}{T}\frac{k_f e^{\frac{\mathcal{A}_f}{RT}} - k_r e^{\frac{\mathcal{A}_r}{RT}}}{\mathcal{A}_f - \mathcal{A}_r}. \tag{2.42}$$

To verify that $\gamma$ is well defined we study its limit when $\mathcal{A} = 0$, i.e., when $\mathcal{A}_f = \mathcal{A}_r$. We may study this limit applying l'Hôpital's rule.

$$\lim_{\mathcal{A}_f \to \mathcal{A}_r} \frac{V}{T}\frac{k_f e^{\frac{\mathcal{A}_f}{RT}} - k_r e^{\frac{\mathcal{A}_r}{RT}}}{\mathcal{A}_f - \mathcal{A}_r} = \frac{V}{RT^2}k_f e^{\frac{\mathcal{A}_f}{RT}} = \frac{V}{RT^2}k_r e^{\frac{\mathcal{A}_r}{RT}}. \tag{2.43}$$

The last limit is well defined since $T > 0$ and always positive. Hence we have that

$$R = \gamma\left(x, \tfrac{\partial U}{\partial x}\right)\{S, U\}_J = \left(\frac{rV}{T\mathcal{A}}\right)\mathcal{A}.$$

To complete the analysis of the proposed IPHS (2.37) it just remain to check that the vectors $W$ and $\frac{1}{T}gQ$ corresponds to input/output ports. The elements of vector $W$ are composed of the inlet and outlet flows of matter. For the coordinates modelling mass balance they are just the ratio of mass exchange with the environment. Similarly, the element corresponding to the last coordinate represents the ratio of entropy exchange due to mass transfer with the environment. Hence, $W$ is the input/output port related with mass transfer of the IPHS. If the CSTR is connected with another CSTR (as for reactors in series) the connection is performed through this port. The vector $\frac{1}{T}gQ$ has only the element corresponding to the entropy balance different from zero. This element models the interaction of the reactor with the cooling jacket and represents the entropy flow due to the temperature difference between the reactor and the jacket. Hence the vector $\frac{1}{T}gQ$ is the input/output port related with the thermal interaction not due to mass transfer. ■

It is possible to define another pseudo PH representation of the CSTR by using the temperature as state variable to model the energy balance. In this case the enthalpy is used as the Hamiltonian function of the system. In this case the systems has the structure of a IPHS but do not express the second principle.

**Proposition 6** *The dynamical equation of the CSTR may be formulated as the following pseudo PHS*

$$\dot{x} = R\left(x, \tfrac{\partial H_H}{\partial x}, \tfrac{\partial S}{\partial x}\right) J \frac{\partial U}{\partial x}(x) + W(x, F_e) + g\frac{Q}{\mathcal{C}_p} \tag{2.44}$$

*with state vector* $x = [n_1, \ldots, n_m, T]^\top$*, the total enthalpy* $H_H(x)$ *as Hamiltonian function,* $J$ *as in Proposition 5,*

$$R = \gamma\left(x, \tfrac{\partial H_H}{\partial x}\right)\{S, H_H\}_J = \left(\frac{rV}{T(-\Delta_r H_H)}\right)(-\Delta_r H_H)$$

*with* $\gamma = \frac{rV}{T(-\Delta_r H_H)}$ *and* $\{S, U\}_J = -\Delta_r H_H$*, where* $-\Delta_r H_H = -\sum_{i=1}^m \bar{\nu}_i h_i$ *is the reaction enthalpy. The port of the pseudo PHS is given by* $W + gQ$ *and is composed by the extended input and output flow vector and the thermal interaction vector, respectively* $W$ *and* $g$ *as in Proposition 5 with* $\omega = \frac{1}{\mathcal{C}_p}\sum_{i=1}^m (F_{ei}h_{ei} - F_{si}h_i)$*.*

Both (2.37) and (2.44) are pseudo PHS, however only the representation that uses the internal energy as Hamiltonian function is a IPHS fulfilling Definition 1. This is due to the fact that the temperature is not a conserved quantity, hence function $\gamma\left(x, \frac{\partial H_H}{\partial x}\right)$ of Proposition 6 is not a positive definite function.

### 2.4.4 Example: a closed chemical reaction

Consider for simplicity the following closed reaction

$$\nu_1 A_1 + \nu_2 A_2 \rightleftharpoons \nu_3 A_3. \tag{2.45}$$

Using the internal energy as Hamiltonian of the system the following IPHS can be formulated to model the CSTR:

$$\begin{bmatrix}\dot{n}_1\\ \dot{n}_2\\ \dot{n}_3\\ \dot{S}\end{bmatrix} = \left(\frac{rV}{T\mathcal{A}}\right)\mathcal{A}\begin{bmatrix}0 & 0 & 0 & -\nu_1\\ 0 & 0 & 0 & -\nu_2\\ 0 & 0 & 0 & \nu_3\\ \nu_1 & \nu_2 & -\nu_3 & 0\end{bmatrix}\begin{bmatrix}\mu_1\\ \mu_2\\ \mu_3\\ T\end{bmatrix} + \frac{1}{T}\begin{bmatrix}0\\ \vdots\\ 0\\ 1\end{bmatrix}Q. \tag{2.46}$$

Here the thermodynamic driving force is

$$\{S,U\}_J = \nu_1\mu_1 + \nu_2\mu_2 - \nu_3\mu_3 = \mathcal{A}.$$

We may also use the total enthalpy as Hamiltonian to write the following pseudo PHS

$$\begin{bmatrix}\dot{n}_1\\ \dot{n}_2\\ \dot{n}_3\\ \dot{T}\end{bmatrix} = \left(\frac{rV}{\mathcal{C}_p\left(-\Delta_r H_H\right)}\right)\left(-\Delta_r H_H\right)\begin{bmatrix}0 & 0 & 0 & \nu_1\\ 0 & 0 & 0 & \nu_2\\ 0 & 0 & 0 & \nu_3\\ -\nu_1 & -\nu_2 & -\nu_3 & 0\end{bmatrix}\begin{bmatrix}h_1\\ h_2\\ h_3\\ \mathcal{C}_v\end{bmatrix} + \frac{1}{\mathcal{C}_v}\begin{bmatrix}0\\ \vdots\\ 0\\ 1\end{bmatrix}Q.$$

The thermodynamic driving force is here given by

$$\{S,H_H\}_J = \nu_1 h_1 + \nu_2 h_3 - \nu_3 h_3 = -\Delta_r H_H.$$

If the reaction occurs in an open reactor, then the port of the system must be completed with the input-output flow vector $W$.

### 2.4.5 Lift of the IPHS

In the previous section it has been shown that by using the internal energy it is possible to define a IPHS for the CSTR according to Definition 1. We may proceed as for the heat exchanger in order to define a class of lift for the CSTR. Let us consider the IPHS defined in Proposition 5. We define the Legendre submanifold generated by the internal energy

$$\mathcal{L}_U : \begin{cases} x_0 = U \\ x = [n_1,\ldots,n_m,S,V]^\top \\ p = [\mu_1,\ldots,\mu_m,T,-P]^\top \end{cases}$$

A regular lift may be defined according to the procedure discussed in Section 2.3. We start by looking more closely on the function $R$ of the IPHS representation of the CSTR

$$R = \gamma\left(x,\tfrac{\partial U}{\partial x}\right)\{S,U\}_J = \left(\frac{rV}{T\mathcal{A}}\right)\mathcal{A}.$$

with $\gamma = \left(\frac{rV}{T\mathcal{A}}\right)$ and $\{S,U\}_J = \mathcal{A}$. Now, $r\left(x,\frac{\partial U}{\partial x}\right)$ is a function of extensive and intensive variables and $r\left(x,p\right)$ is well defined for all values of $(x,p) \in \mathbb{R}^{2n}$. The affinity $\mathcal{A} = -\sum_{i=1}^m \bar{\nu}_i\mu_i = -\sum_{i=1}^m \bar{\nu}_i\frac{\partial U}{\partial x_i}$ is a linear combination of the elements of the gradient with 0 in the image of $\mathcal{A}$. From Proposition 5 we have that

$$\frac{r\left(x,\frac{\partial U}{\partial x}\right)}{\mathcal{A}\left(\frac{\partial U}{\partial x}\right)}$$

is well defined for all $\left(x, \frac{\partial U}{\partial x}\right) \in \mathbb{R}^{2n}$. Hence it is possible to parametrize $R$ as

$$R = \frac{r(x,p)V}{T(x)\mathcal{A}(p)}\mathcal{A}(p) \tag{2.47}$$

or as

$$R = \frac{r(x, \frac{\partial U}{\partial x})V}{T(x)\mathcal{A}\left(\frac{\partial U}{\partial x}\right)}\mathcal{A}(p). \tag{2.48}$$

Both (2.47) and (2.48) are well defined. Another possible well defined lift is given by $R = \frac{V}{T} r\left(x, \frac{\partial U}{\partial x}\right)$. The lift of the port of the system cannot be performed arbitrarily as discussed in Section 2.3. Let us analyse the two components of the port $W + gQ$. The vector corresponding to the mass exchange is

$$W = \begin{bmatrix} F_{e1} - F_{s2} \\ \vdots \\ F_{em} - F_{sm} \\ \omega \end{bmatrix},$$

with $\omega = \frac{1}{T}\sum_{i=1}^{m}(F_{ei}s_{ei} - F_{si}s_i)$. Note that the inlet flows and partial molar entropies of each species at the input are not state dependent and may be modelled, respectively, as $F_{ei}(t)$ and $s_{ie}(t)$, $i = 1 \dots m$. Considering this we may characterize the terms of $W$ that may be parametrized by $p$.

- The outlet flows are state dependent [7, 14, 25]: $F_{si}\left(x, \frac{\partial U}{\partial x}\right), i = 1, \dots, m$, and the parametrization $F_{si}(x,p), i = 1, \dots, m$ is well defined for all $(x,p) \in \mathbb{R}^{2n}$.
- The partial molar entropies of each specie in the reaction are state dependent $s_i\left(x, \frac{\partial U}{\partial x}\right), i = 1, \dots, m$, and have a logarithmic dependence on the temperature [14]. Thus the parametrization $s_i(x,p)$ is not possible and the lift should be performed considering the parametrization $s_i\left(x, \frac{\partial U}{\partial x}, p\right)$.
- Finally the term $\frac{1}{T}$ in $\omega$ can not be replaced by $\frac{1}{p_T}$ since it is not defined at $p_T = 0$.

The second component of the port of the process is due to the interaction with the external cooling jacket. it is given by

$$g = \begin{bmatrix} 0 & \vdots & 0 & 1 \end{bmatrix}^\top \frac{Q}{T}.$$

The only element different from zero is $\frac{Q}{T}$. This term is due to heat transfer, and as for the heat exchanger it is given by $\frac{Q}{T} = \lambda\frac{(T_e(t)-T)}{T}$, where $T_e(t)$ is the time dependent temperature of the cooling jacket. This term may be parametrized by $p$ as $\lambda\frac{(T_e(t)-p_T)}{T}$. However in controlled CSTR's this term is frequently written as $\frac{u}{T}$, and $u = Q$ is considered as the controlled input of the system. In that case it is not parametrized at all. Finally we have the following Proposition for regular lift of a CSTR.

**Proposition 7** *A well defined lift of the IPHS formulation of the CSTR is given by*

$$K = \underbrace{-p^\top R\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}, p\right) J \frac{\partial U}{\partial x}(x)}_{K_0} + \underbrace{\left(\frac{\partial U}{\partial x} - p\right)^\top W\left(x, \tfrac{\partial U}{\partial x}, p\right) + \left(\frac{\partial U}{\partial x} - p\right)^\top g\frac{Q}{T}}_{K_c}, \quad (2.49)$$

*with $R$ given by (2.47) or (2.48) and*

$$W = \begin{bmatrix} F_{e1} - F_{s2}(x,p) \\ \vdots \\ F_{em} - F_{sm}(x,p) \\ \omega\left(x, \tfrac{\partial U}{\partial x}, p\right) \end{bmatrix},$$

*where* $\omega\left(x, \tfrac{\partial U}{\partial x}, p\right) = \tfrac{1}{T}\sum_{i=1}^{m}\left(F_{ei}s_{ei} - F_{si}(x,p)s_i\left(x, \tfrac{\partial U}{\partial x}, p\right)\right)$.

Let us analyse each term of the contact Hamiltonian (2.49). While the Hamiltonian of the IPHS representation of the CSTR has the dimension of energy, the contact Hamiltonian has the dimension of power. Hence $K$ defines a kind of virtual power as it has already been addressed in [22]. From equation (2.49) we identify three different power products, given by $K_0$ and the two terms of $K_c$, that represent the power contribution due to the chemical reaction, the inlet and outlet flows and the heat transfer through the jacket respectively. $K_0$ represents the power contribution of the chemical reaction that is related with a pseudo-Poisson bracket. We may decompose the interaction contact Hamiltonian $K_c$ in two main terms: the term

$$\sum_{i=1}^{m}\left(\mu_i - p_i\right)\left(F_{ei} - F_{si}\left(x,p\right)\right)$$

is the power generated by the mass exchange between the reactor and its environment; the term

$$\left(T - p_T\right)\left(\sum_{i=1}^{m}(F_{ei}s_{ei} - F_{si}\left(x,p\right)s_i\left(x, \tfrac{\partial U}{\partial x}, p\right)) + \frac{Q}{T}\right)$$

represents the power generated by the energy exchange. It is important to note that the vector field generated by the contact Hamiltonians will be different depending on the choice of the lift. For instance, let us consider the vector field generated by $K_0$. If we define

$$K_0 = -p^\top R\left(x, \tfrac{\partial U}{\partial x}\right) J\frac{\partial U}{\partial x}(x)$$

the corresponding vector field (2.15) is given by

$$X_{K_0} = \begin{bmatrix} \frac{dx_0}{dt} \\ \frac{dx}{dt} \\ \frac{dp}{dt} \end{bmatrix} = \begin{bmatrix} 0 \\ R\left(x, \tfrac{\partial U}{\partial x}\right) J\frac{\partial U}{\partial x}(x) \\ -\frac{\partial R}{\partial x}\left(x, \tfrac{\partial U}{\partial x}\right) p^\top J\frac{\partial U}{\partial x}(x) + R\left(x, \tfrac{\partial U}{\partial x}\right)\frac{\partial^2 U}{\partial x^2}(x)Jp \end{bmatrix}.$$

On other hand, if the internal contact Hamiltonian is defined using (2.47) or (2.48),

$$K_0 = -p^\top R\left(x, \tfrac{\partial U}{\partial x}, p\right) J \frac{\partial U}{\partial x}(x),$$

then the generated contact vector field is

$$X_{K_0} = \begin{bmatrix} \frac{dx_0}{dt} \\ \frac{dx}{dt} \\ \frac{dp}{dt} \end{bmatrix} = \begin{bmatrix} p^\top \frac{\partial R}{\partial p}\left(x, \frac{\partial U}{\partial x}, p\right) J \frac{\partial U}{\partial x}(x) \\ \frac{\partial R}{\partial p}\left(x, \frac{\partial U}{\partial x}, p\right) J \frac{\partial U}{\partial x}(x) \\ -\frac{\partial R}{\partial x}\left(x, \frac{\partial U}{\partial x}, p\right) p^\top J \frac{\partial U}{\partial x}(x) + R\left(x, \frac{\partial U}{\partial x}, p\right) \frac{\partial^2 U}{\partial x^2}(x) J p \end{bmatrix}.$$

The contact vector fields are different since the generating functions are different. Now let us consider the complete contact Hamiltonian of the CSTR. Independently of which well defined lift is used, when restricting the vector field generated by $K$ to the invariant Legendre submanifold $\mathcal{L}_U$ the dynamic of the CSTR is obtained [22, 29, 30]

$$\begin{aligned} \left.\frac{dx_0}{dt}\right|_{\mathcal{L}_U} &= \frac{dU}{dt} = \frac{\partial U}{\partial x}^\top(x) W\left(x, \tfrac{\partial U}{\partial x}\right) + \frac{\partial U}{\partial x}^\top(x) g \frac{Q}{T(x)}, \\ \left.\frac{dx}{dt}\right|_{\mathcal{L}_U} &= R\left(x, \tfrac{\partial U}{\partial x}\right) J \frac{\partial U}{\partial x}(x) + g\frac{Q}{T(x)} + W\left(x, \tfrac{\partial U}{\partial x}\right), \\ \left.\frac{dp}{dt}\right|_{\mathcal{L}_U} &= \frac{\partial^2 U}{\partial x^2}(x)\left(R\left(x, \tfrac{\partial U}{\partial x}\right) J \frac{\partial U}{\partial x}(x) + W\left(x, \tfrac{\partial U}{\partial x}\right) + g\frac{Q}{T(x)}\right). \end{aligned} \tag{2.50}$$

Note that the contact vector fields are different only *outside* the Legendre submanifold. The Hessian of the Hamiltonian (internal energy) is given by $\frac{\partial^2 U}{\partial x^2}(x)$ Since this matrix is the Hessian of a scalar function it is symmetric and it is possible to identify Maxwell relations, which indicate the relationships between the thermodynamic properties of this system [3, 79]. The time evolution of the thermodynamic variables is obtained from (2.50). We may for instance obtain the dynamic of the intensive variables directly from (2.50).

### 2.4.6 Example: a closed chemical reaction (continued)

Consider the closed ($W = 0$) chemical reaction (2.45) and its IPHS representation (2.46). We may obtain the time evolution of the intensive variables by restricting the lift of (2.46) to the Legendre submanifold generated by the internal energy

$$\begin{aligned} \dot{\mu_i} &= \frac{s_i}{C_v}\left(\sum_{j=1}^{3}(\nu_j r V h_j) - Q\right) + RT\left(\frac{\nu_i r V h_i}{n_i} - \frac{\sum_{j=1}^{3}\nu_j r V h_j}{N}\right) \\ \dot{T} &= \frac{-1}{T}\sum_{j=1}^{3}\nu_j r V h_j + \frac{Q}{C_v}. \end{aligned}$$

where $i = 1, 2, 3$. ■

## 2.5 Conclusion

In this chapter the modelling of thermodynamic systems using the IPHS formalism has been presented. Firstly, we have a defined a class of pseudo PHS (Definition 1) that encompasses a large set of thermodynamic systems, including heat exchangers and continuous stirred tank reactors (CSTR). The IPHS includes as a structural property the conservation of energy and the irreversible production of entropy. Furthermore, the structure of the IPHS resembles classical PHS since the constant structure matrix maps the network structure of the system (direction of flows for the heat exchanger and stoichiometric chemical network for the CSTR). The Hamiltonian is, as for PHS, the energy of the system. The irreversible entropy creation is expressed through a non-linear function of states and co-states, $R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right)$, that modulates the constant structure matrix. This non-linear function is composed of a positive definite function in the states and co-states and a Poisson bracket defined by the structure matrix of the system evaluated on the entropy and the energy; hence $R$ is actually defined by the the thermodynamic structure of the process.

Secondly, we have explored the lift of the defined IPHS to the TPS by using the framework of contact geometry building upon the works of D. Eberard [20] and A. Favache [24]. We have remarked that the issue of well defined lifts have not been previously addressed, hence we have suggested a constructive method to performed the lifts of IPHS. It is important to point out that a contact Hamiltonian that is not everywhere defined in the TPS will not only generate contact vector fields with singularities, but will also not be useful for control design in the TPS. This point will be further discussed in Chapter 3.

Finally, we have extensively illustrated the proposed modelling approach on the CSTR. IPHS and contact Hamiltonian representations for the dynamical equation of the CSTR have been proposed (Propositions 5, 6 and 7) and physical interpretation of the system have been provided.

# Chapter 3

# Structure preserving feedback of controlled contact systems

## 3.1 Introduction

Find and characterize the natural structure of physical systems has been the matter of study for many decades. The abstract representation of a physical system permits to find general methods for obtaining the dynamical equation of the system and investigate, in a generalized framework, their solutions. In this aspect the geometric structure arising in Hamiltonian systems has proved to be particularly powerful [8, 2, 48]. Not only for describing the dynamic behaviour and studying the systems properties have the geometric structure of Hamiltonian system been most useful, but also for prescribing the dynamic behaviour. In the past years great efforts have been made to study Hamiltonian system from a control perspective, i.e., as open systems interacting with their environment. Of particular importance are the works of R. Brockett [11], A. van der Schaft [84, 85, 92, 86] and P.Crouch [17]. These works were the starting point for the study of Hamiltonian control system from a system theoretic point of view and the development of general geometric control theory for these class of systems. Today it is well known that the symmetries arising from the symplectic structure of Hamiltonian systems can be used to characterize the properties and solve control problems of physical systems. A fruitful generalization of input-output Hamiltonian systems to non-Hamiltonian input vector fields was later proposed and called port-Hamiltonian systems (PHS) [49, 50, 89]. PHS are well suited for network type of coupling and have been widely used in control of physical systems using energy shaping methods [65, 66, 89].

The aim of this chapter is to extend the results of structure preserving feedback of input-output Hamiltonian systems defined on symplectic manifolds to control contact systems defined on contact manifolds. The motivation for considering contact manifold comes from the fact that they arise naturally in the description of

Equilibrium Thermodynamics (i.e. the description of the thermodynamic properties of matter) [8, 40]. Contact systems (defined by contact vector fields) have been used to formulate reversible and irreversible thermodynamic transformations [40, 57, 35]

Controlled contact systems have recently been proposed in [21, 22] where the contact vector field is augmented with an input map. There have been only few attempts to analyse the interaction of the controlled contact systems with its environment. In [40, 41] a simple example of structure preserving isothermal interaction of two thermodynamic systems is presented in the frame of *closed* contact systems. Some preliminary results on constant interconnection of conservative controlled contact systems [22, 27] where given in [20], and some structural properties, such as necessary conditions for the stability of the linearisation of conservative contact vector fields, where presented in [30]. More recently in [74], the framework of conservative controlled contact systems has been used to propose a control design method. However the closed-loop system is defined as the lift of a controlled system, hence the approach does not encompass control of contact vector fields.

Inspired by the work performed on input-output Hamiltonian systems, the aim of this chapter is to study the conditions under which it is possible to render a controlled contact system again a contact system when applying a state feedback. This is not trivial since the geometric structure of the system may be destroyed due to the state feedback. Hence the first question that arises is: is it possible to apply a state feedback such that the geometric structure of the system is preserved?, i.e., such that the closed-loop system is a contact system with respect to the same contact form as the open-loop system. We shall show that the answer is in general no. We show that the only control that preserves the geometric structure of the contact system is a constant control. This results lead us to study the possibility that the closed-loop system is a contact system with respect to a *new* contact form. We shall show that it is indeed possible to render the closed-loop system a contact system with respect to a new contact form, and moreover we have characterized the conditions for this to be possible. The conditions for structure preserving feedback is formally stated in the form of a matching equation and for strict controlled contact systems we show that, for a particular class of closed-loop contact form and state feedback, the matching equation is reduced to a linear first-order partial differential equation.

The closed-loop contact vector field and contact Hamiltonian function may be related to the closed-loop Hamiltonian vector field and Hamiltonian function resulting from structure preserving feedback of input-output Hamiltonian systems. The main difference in the results is that in control of Hamiltonian systems the geometry is not changed, hence the closed-loop vector field is generated with respect to the same differential form (the symplectic form) as the open-loop vector field; whereas the closed-loop contact vector field is generated with respect to the new contact form. This also introduces, unlike controlled Hamiltonian system, a matching equation in the state feedback and the closed-loop contact form. The relation with the control of input-output Hamiltonian system also motivates the definition of natural outputs for contact systems.

The last part of this chapter is dedicated to study structure preserving feedback of conservative controlled contact systems. This class of contact systems have

the property that they leave a submanifold, called Legendre submanifold, invariant [8, 48]. Hence, to characterize the structure preserving feedback it is necessary to characterize the closed-loop invariant Legendre submanifolds. It is of practical importance to perform this characterization since the generating functions of the open and closed-loop Legendre submanifolds may, for physical systems, be associated with the energy [57, 55, 35, 56]. Hence shaping the closed-loop Legendre submanifold is related to shaping the energy of the system. We show that for conservative controlled contact systems the assignment of closed-loop invariant Legendre submanifolds may be use to parametrize the state feedback.

### 3.1.1 Organization of the chapter

The chapter is organized as follows. In Section 3.2 a short overview of the framework of controlled contact system is presented. In Section 3.3 the question of structure preserving state feedback is addressed and the conditions for achieving it are stated as a general matching equation. Section 3.4 develops the conditions of structure preserving feedback for the case of controlled strict contact systems. It is shown that for a particular class of contact form and state feedback it is possible reduced the general matching equation to a linear first-order PDE and the relation with analogous results for Hamiltonian control system is establish. In Section 3.5 the feedback invariants of controlled contact systems are studied. The results are specialized to irreversible port Hamiltonian systems and used to parametrize the state feedbacks. Finally in Section 3.6 some concluding remarks are given.

### 3.1.2 Main contributions of the chapter

The main contributions of this chapter are the following.

- In Section 3.3 it is proved that only a constant control preserves the open-loop contact structure (Proposition 14), hence a structure preserving feedback necessarily renders the closed-loop system a contact system with respect to a new contact form (Section 3.3, problem 15).

- For strict contact systems the conditions for render the closed-loop system a contact system have been characterized as a matching equation in a modified contact form and a particular class of feedback in Subsection 3.4.2, Proposition 22. Furthermore, the matching equation is a linear first-order PDE and may be solved by using the method of characteristics.

- For conservative controlled contact system the feedback leaving invariant some Legendre submanifolds have been characterized (Subsection 3.5.1, Proposition 30) and it has been suggested to use this invariant condition to define the state feedback. The results have been specialized to irreversible PHS in Subsection 3.5.2, Proposition 31.

## 3.2 Controlled contact systems

Despite that some of the definitions have already been given in the previous chapter but in some canonical coordinates, we shall in the following recall briefly the main definitions and properties of the control contact systems, however in an intrinsic coordinate free notation and the reader is referred to [22, 48, 8] for details. Consider some $2n+1$-dimensional differential manifold $\mathcal{M}$ equipped with a *contact form* denoted by $\theta$.

**Definition 8** *A contact structure on $\mathcal{M}$ is defined by a 1-form $\theta$ of constant class $(2n+1)$ satisfying*

$$\theta \wedge (d\theta)^n \neq 0,$$

*where $\wedge$ denotes the wedge product. The pair $(\mathcal{M}, \theta)$ is then called a* contact manifold*, and $\theta$ a* contact form*.*

According to Darboux's theorem for Pfaffian forms of constant class [48] there exists a set of *canonical coordinates* $(x_0, x, p) \in \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n$ of $\mathcal{M}$ where the contact form $\theta$ is given by

$$\theta = dx_0 - \sum_{i=1}^{n} p_i dx_i$$

where $d$ denotes the exterior derivative. In the following we shall use a particular vector field characteristic of the contact form, called the Reeb vector field.

**Definition 9** *The Reeb vector field $E$ associated with the contact form $\theta$ which is the unique vector field satisfying*

$$i_E\theta = 1 \quad \textit{and} \quad i_E d\theta = 0 \tag{3.1}$$

*where $i_E$ denotes the contraction by the vector field $E$ of differential forms.*

In canonical coordinates the Reeb vector field is expressed as $E = \frac{\partial}{\partial x_0}$. We recall that *contact vector fields* are vector fields which leave the contact distribution invariant.

**Definition 10** *A (smooth) vector field $X$ on the contact manifold $\mathcal{M}$ is a contact vector field with respect to a contact form $\theta$ if and only if there exists a smooth function $\rho \in C^\infty(\mathcal{M})$ such that*

$$L_X\theta = \rho\theta, \tag{3.2}$$

*where $L_X \cdot$ denotes the Lie derivative with respect to the vector field $X$.*

It may be shown that the vector space of contact vector fields and the space of smooth real functions are isomorphic [48] which is stated in the following proposition.

**Proposition 11** [48, pp.318] *The map $\Omega(X) = i_X\theta$ defines an isomorphism from the vector space of contact vector fields in the space of smooth real functions on the contact manifold.*

The function $K = \Omega(X_K)$ is called *contact Hamiltonian* generating the contact vector field denoted by $X_K = \Omega^{-1}(K)$, where $\Omega^{-1}$ is the inverse isomorphism. Finally the function $\rho$ of equation (3.2) is given by $\rho = i_E dK$ where $E$ is the Reeb vector field. A contact system on $\mathcal{M}$ is then defined by $\frac{d}{dt}\tilde{x} = X_K$, $\tilde{x} \in \mathcal{M}$ which, in any set of canonical coordinates, is expressed by the dynamical equation

$$\frac{d}{dt}\begin{bmatrix} x_0 \\ x \\ p \end{bmatrix} = \begin{bmatrix} K \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & -p^\top \\ 0 & 0 & -I_n \\ p & I_n & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial K}{\partial x_0} \\ \frac{\partial K}{\partial x} \\ \frac{\partial K}{\partial p} \end{bmatrix}, \tag{3.3}$$

where $I_n$ denotes the identity matrix of order $n$. The contact structures defines a bilinear product on smooth real functions called *Jacobi bracket* [57, 48, 22] denoted by $\{\cdot,\cdot\}_{\text{Jacobi}}$ and defined on couples of two $C^\infty(\mathcal{M})$ function $Z$ and $G$ as follows

$$\begin{aligned} &\{Z,G\}_{\text{Jacobi}} = \\ &\sum_{k=1}^{n}\left(\frac{\partial Z}{\partial x_k}\frac{\partial G}{\partial p_k} - \frac{\partial G}{\partial x_k}\frac{\partial Z}{\partial p_k}\right) + \left(Z - \sum_{k=1}^{n} p_k \frac{\partial Z}{\partial x_k}\right)\frac{\partial G}{\partial x_0} - \left(G - \sum_{k=1}^{n} p_k \frac{\partial G}{\partial x_k}\right)\frac{\partial Z}{\partial x_0}. \end{aligned} \tag{3.4}$$

Controlled contact systems are defined by contact Hamiltonians which depend not only on the state variables $(x_0, x, p)$ but also on a time dependent input function $u(t) \in L_1^\infty(\mathbb{R})$. In this chapter we shall consider the particular case when the controlled contact system is affine in the input defined according to [21, 22].

**Definition 12** *A controlled contact system affine in the scalar input $u(t) \in L_1^\infty(\mathbb{R})$ is defined by the two functions $K_0 \in C^\infty(\mathcal{M})$, called the* internal contact Hamiltonian *and $K_c \in C^\infty(\mathcal{M})$ called the* interaction (or control) contact Hamiltonian *and the state equation*

$$\frac{d\tilde{x}}{dt} = X_{K_0} + X_{K_c}u, \tag{3.5}$$

*here $X_{K_0}$ and $X_{K_c}$ are the contact vector fields generated by $K_0$ and $K_c$ respectively with respect to the contact form $\theta$.*

## 3.3 State feedback of controlled contact systems

In this chapter we are interested in studying the possibility of applying a state feedback to a controlled contact system such that the closed-system is once again a contact system. In a first attempt we expect to derive the conditions under which the state feedback renders the closed-loop system a contact system with respect to $\theta$, i.e. which class of state feedback $u = \alpha(\tilde{x})$, with $\alpha \in C^\infty(\mathcal{M})$, generates a closed-loop vector field $X$ that is again a contact vector field with respect to the contact form $\theta$. This is the case of controlled Hamiltonian systems [85, 86], where it is possible to define a state feedback such that the closed-loop system is a Hamiltonian system with respect to the same geometric structure as the open-loop system, namely the symplectic structure. In the case of contact systems however

this is not the case. It is actually not possible to define a non-trivial state feedback such that the closed-loop system is a contact system with respect to the canonical contact form $\theta$. This result is given in the following proposition.

**Assumption 13** *The control contact Hamiltonian $K_c \in C^\infty(\mathcal{M})$ vanishes on a submanifold of measure 0 of $\mathcal{M}$.*

**Proposition 14** *Consider the controlled contact system (3.5) and the feedback $u = \alpha(\tilde{x})$ being a smooth function of the state variables. The closed-loop vector field $X$ is a contact vector field with respect to the canonical contact form $\theta$ if and only if $\alpha(\tilde{x}) = \alpha_{cte}$ is constant.*

**Proof.** Recall Cartan's formula: $L_X \cdot = i_X d\cdot + d i_X \cdot$. Then one may compute, using (3.5),

$$\begin{aligned} L_X\theta &= L_{X_{K_0}+\alpha X_{K_c}}\theta \\ &= i_{(X_{K_0}+\alpha X_{K_c})}d\theta + d i_{(X_{K_0}+\alpha X_{K_c})}\theta \\ &= i_{X_{K_0}}d\theta + \alpha i_{X_{K_c}}d\theta + d\left(K_0 + \alpha K_c\right) \\ &= \big(i_{X_{K_0}}d\theta + dK_0\big) + \alpha\big(i_{X_{K_C}}d\theta + dK_c\big) + K_c d\alpha \\ &= L_{X_{K_0}}\theta + \alpha L_{X_{K_c}}\theta + K_c d\alpha \\ &= \left(\rho_0 + \alpha\rho_c\right)\theta + K_c d\alpha \end{aligned} \tag{3.6}$$

where $\rho_0 = i_E dK_0$ and $\rho_c = i_E dK_c$. Hence the vector field $X = X_{K_0} + X_{K_c}\alpha$ is a contact vector field if and only if there exists a function $\phi \in C^\infty(\mathcal{M})$ such that: $K_c d\alpha = \phi\theta$. Using the definition of $\theta$ in local coordinates, $\theta = dx_0 - \sum_{i=1}^n p_i dx_i$, we may write

$$K_c\Big(\tfrac{\partial\alpha}{\partial x^0}dx^0 + \sum_{k=1}^n \tfrac{\partial\alpha}{\partial x^k}dx^k + \sum_{k=1}^n \tfrac{\partial\alpha}{\partial p_k}dp_k\Big) = \phi\Big(dx^0 - \sum_{k=1}^n p_k dx^k\Big),$$

which by the assumption of smoothness of the functions and under the condition that $K_c$ vanishes on a submanifold of measure 0 leads to $\frac{\partial\alpha}{\partial x^k} = -\frac{\partial\alpha}{\partial x^0}p_k$ and $\frac{\partial\alpha}{\partial p_k} = 0$, which implies that $\alpha$ is constant. ■

In summary the only control of an affine controlled contact system which leads to a contact vector field equipped with contact form $\theta$ is the constant control. The resulting contact system is the sum of two contact vector fields with global contact Hamiltonian $K_0 + K_C\alpha_{cte}$. It is interesting to note that this is precisely the case of the interconnection of port-contact systems as defined in [20]. As mentioned before this result differs from the case of feedback control of input-output Hamiltonian systems where the feedbacks leading to a closed-loop Hamiltonian system are characterized as the composition of any function with the control Hamiltonian functions [85, 86]. Since it is not possible to apply a feedback that preserves the canonical contact form it is necessary to explore the possibility of defining a state feedback such that the closed-loop system is a contact system with respect to a *modified* contact structure. This is not completely uncommon in geometric control

theory. For controlled PHS the interconnection and passivity based control (IDA-PBC) method [65, 66, 61] renders the closed-loop system a PHS but with respect to a new geometric structure. Indeed, the PHS is defined with respect to a Poisson bracket [49, 50] and after applying the state feedback the closed-loop system is in general a PHS with respect to a different Poisson bracket. In the following section we will explore the possibility of defining a state feedback such that the closed-loop system is a contact system with respect to a modified contact structure.

## 3.4 State feedback shaping the contact form

Proposition 14 shows that by using non constant state feedback of a controlled contact vector field it is not possible to obtain a contact vector field with respect to *the same contact form*. In this section the feedback conditions under which the closed-loop contact vector field $X$ in (3.5), is again a contact vector field with respect to a *modified contact form* are studied. In the following we shall derive the conditions for the existence of a new contact form $\theta_d$ for which $X$ is a contact vector field. Therefore we shall consider the equivalent condition of the existence of a function $\rho_d \in C^\infty(\mathcal{M})$ such that

$$L_X\theta_d = \rho_d\theta_d. \tag{3.7}$$

Denote $K_d = i_X\theta_d$ the contact Hamiltonian generating $X$ with respect to the contact form $\theta_d$, then $\rho_d = i_{E_d}dK_d$ where $E_d$ denotes the Reeb vector field associated with $\theta_d$. Using the result in (3.6) applied to $\theta_d$, one has

$$\begin{aligned}
L_X\theta_d &= L_{X_{K_0}+\alpha X_{K_c}}\theta_d \\
&= i_{(X_{K_0}+\alpha X_{K_c})}d\theta_d + di_{(X_{K_0}+\alpha X_{K_c})}\theta_d \\
&= (i_{X_{K_0}}d\theta_d) + \alpha(i_{X_{K_c}}d\theta_d) + d(i_{X_{K_0}}\theta_d) + d(\alpha i_{X_{K_c}}\theta_d) \\
&= (i_{X_{K_0}}d\theta_d) + \alpha(i_{X_{K_c}}d\theta_d) + d(i_{X_{K_0}}\theta_d) + \alpha d(i_{X_{K_c}}\theta_d) + (i_{X_{K_c}}\theta_d)d\alpha \\
&= \big[(i_{X_{K_0}}d\theta_d) + d(i_{X_{K_0}}\theta_d)\big] + \alpha\big[(i_{X_{K_C}}d\theta_d) + d(i_{X_{K_c}}\theta_d)\big] + (i_{X_{K_C}}\theta_d)d\alpha \\
&= L_{X_{K_0}}\theta_d + \alpha L_{X_{K_c}}\theta_d + (i_{X_{K_C}}\theta_d)d\alpha
\end{aligned} \tag{3.8}$$

which leads by subtraction with (3.7), to the following problem formulation.

**Problem 15** *Given $X = X_{K_0} + X_{K_c}u$, when does it exist a contact form $\theta_d$, a function $\rho_d \in C^\infty(\mathcal{M})$ and a feedback $u = \alpha \in C^\infty(\mathcal{M})$ in (3.5) such that the following matching equation is satisfied*

$$\rho_d\theta_d = L_{X_{K_0}}\theta_d + \alpha L_{X_{K_c}}\theta_d + (i_{X_{K_C}}\theta_d)d\alpha. \tag{3.9}$$

The matching equation has three unknowns: the state feedback $\alpha$, the new contact form $\theta_d$ and the function $\rho_d$ that is determined by the modified Reeb vector field $E_d$. In the following we proceed to simplify this equation by taking into account some specific aspects of the open and closed-loop contact systems. In this line the following assumption is made.

**Assumption 16** *The controlled contact Hamiltonian and the closed-loop contact Hamiltonian are strict contact Hamiltonians, i.e.,* $\rho_d = \rho_0 = \rho_c = 0$.

This assumption implies that $X$, and respectively $X_{K_0}$ and $X_{K_c}$, leave invariant the contact form itself, $\theta_d$ respectively $\theta$. In canonical coordinates this means that they do not depend on the coordinate $x_0$ associated with the Reeb vector field. This is not a restrictive assumption since for contact systems arising from the modelling of physical systems, the contact Hamiltonian indeed does not depend on the $x_0$ coordinate representing the energy or more generally a thermodynamic potential (see Chapter 2, Section 2.3). Under this assumption the matching equation (3.9) is reduced to a relation on the feedback $\alpha$ and the closed-loop contact form $\theta_d$,

$$L_{X_{K_0}}\theta_d + \alpha L_{X_{K_c}}\theta_d + (i_{X_{K_C}}\theta_d)d\alpha = 0. \tag{3.10}$$

This equation is still very general since $\theta_d$ is any possible contact form. To further specialise the matching equation a specific expression for $\theta_d$, that may be interpreted physically, will be assumed.

### 3.4.1 Matching to the contact form $\theta_d = \theta + dF$

We are interested in deriving a "as much as possible" parametrized matching equation that characterizes the admissible state feedback that renders the system a contact system in closed-loop. Recall that the canonical contact form $\theta$ is related with Gibbs' relation when modelling thermodynamic systems (Chapter 2). Moreover, in that case the $x_0$ coordinate is associated to the energy of the system. This motivates to restrict the closed-loop contact form $\theta_d$ as follows.

**Assumption 17** *The 1-form* $\theta_d$ *is defined as*

$$\theta_d = \theta + dF, \tag{3.11}$$

*with* $F \in C^\infty(\mathcal{M})$ *satisfying* $i_E dF = 0$.

Note that the condition $i_E dF = 0$ is equivalent in canonical coordinates to assume that the function $F$ depends only on $(x, p)$ and not on $x_0$. The closed-loop contact form $\theta_d$ defines actually a contact form.

**Proposition 18** *The 1-form defined by (3.11) is a contact form.*

**Proof.** Recall that $\theta_d$ is a contact form if it is a Pfaffian form of class $2n + 1$, satisfying (see Definition 8),

$$\theta_d \wedge (d\theta_d)^n \neq 0.$$

Note that using $d^2F = 0$ one has

$$\begin{aligned}\theta_d \wedge (d\theta_d)^n &= (\theta + dF) \wedge (d(\theta + dF))^n \\ &= (\theta + dF) \wedge (d\theta)^n\end{aligned}$$

Now proceed by contradiction and assume that $\theta_d \wedge (d\theta_d)^n = 0$. Then, using the fact that $i_E$ is a $\wedge$ antiderivation and the properties (3.1) of the Reeb vector field:

$$\begin{aligned} i_E\left[\theta_d \wedge (d\theta_d)^n\right] &= i_E\left[(\theta + dF) \wedge (d\theta)^n\right] \\ &= i_E(\theta + dF) \wedge (d\theta)^n + (-1)\,(\theta + dF) \wedge i_E\left((d\theta)^n\right) \\ &= (1 + i_E dF) \wedge (d\theta)^n \end{aligned}$$

and $i_E dF = 0$, implies that $(d\theta)^n = 0$ which is contradicting the fact that $\theta$ is of class $2n+1$. ■

**Remark 19** *Note that it has been assumed that $F$ satisfies $i_E dF = 0$. However, from the proof of Proposition 18 it is clear that it is only required that $i_E dF \neq 1$. In this sense the assumption $i_E dF = 0$ is restrictive, but is justified since it has a clear thermodynamic interpretation given as follows.*

The closed-loop contact form (3.11) is given by

$$\begin{aligned} \theta_d = \theta + dF &= \Big(dx_0 - \sum_{i=1}^{n} p_i dx_i\Big) + dF, \\ &= d(x_0 + F) - \sum_{i=1}^{n} p_i dx_i, \\ &= dx_0' - \sum_{i=1}^{n} p_i dx_i. \end{aligned} \tag{3.12}$$

The closed-loop contact form is hence given by canonical contact form $\theta$ changed in the direction of the Reeb vector field (the $x_0$ coordinate). The set of canonical coordinates for $\theta_d$ is now given by $(x_0', x, p)$. Recall that the contact structure appears in the differential-geometric representation of thermodynamic systems [40, 41, 57], where $x_0$ is associated with a thermodynamic potential, such as the energy $U$ or the entropy $S$. Hence physically $\theta_d$ may be related to changing the *energy* of the system. Indeed since $\theta_d$ is defined as the addition to the canonical contact form of an exact form that does not depend on the $x_0$ coordinate, the new canonical coordinate $x_0' = x_0 + F$ defines the "modified energy" of the system (equation 3.12). This interpretation is not too different to the one provided in [40, chap. 6] and [41, chap. 9] for the isothermal interaction of thermodynamic system using contact geometry. In those works it has been shown that through the isothermal interaction of two different thermodynamic systems, each one defined with respect to a different contact structure, the resulting contact structure of the interconnected system is given by the addition of the contact structures with a modified energy coordinate representing the sum of the individual energies. In the case of controlled contact system the interpretation should be performed in terms of the contact Hamiltonians: it is possible to think that the system defined by the internal contact Hamiltonian is interacting with a control system, defined by the controller, through the control vector field. The resulting contact structure $\theta_d$ is then the result of the interaction of system and controller. We may also interpret the closed-loop contact form in

terms of passivity based control (PBC) [89]. In PBC the aim is to add a certain function to the open-loop storage (energy) function such that the resulting closed-loop storage function may be used as Lyapunov function for the controlled system. Hence we may think to give $x_0'$ a similar interpretation. Now, from a geometric point of view, changing the geometry of a system through a state feedback such that the closed-loop system preserves the structure with respect to a new geometric form is not new. For instance in the case of PHS, the IDA-PBC method renders a PHS with respect to a set of new structure matrices and storage function.

Let us express the matching equation (3.10) with $\theta_d$ defined by (3.11) in terms of a matching equation in the function $F$ and the feedback $\alpha$. The Lie derivatives in (3.10) may be developed as

$$L_{X_{K_0}}(\theta + dF) = L_{X_{K_0}}\theta + L_{X_{K_0}}dF = \rho\theta + L_{X_{K_0}}dF$$

with

$$L_{X_{K_0}}dF = i_{X_{K_0}}d(dF) + d(i_{X_{K_0}}dF) = d\left(X_{K_0}(F)\right).$$

Recalling that $\rho_d = \rho_0 = \rho_c = 0$, we have that $L_{X_{K_0}}\theta_d = d\left(X_{K_0}(F)\right)$ and $L_{X_{K_c}}\theta_d = d\left(X_{K_c}(F)\right)$. Furthermore $i_{X_{K_C}}\theta_d = i_{X_{K_C}}(\theta + dF) = K_c + X_{K_C}(F)$. Hence, the matching equation (3.10) becomes

$$d\left(X_{K_0}(F)\right) + \alpha d\left(X_{K_c}(F)\right) + \left[K_c + X_{K_C}(F)\right] d\alpha = 0. \tag{3.13}$$

Since $X = X_{K_0} + X_{K_c}\alpha$, it follows that

$$d(X(F)) = d(X_{K_0}(F)) + \alpha d(X_{K_c}(F)) + X_{K_c}(F)d\alpha.$$

Equation (3.13) may finally be rewritten as the following matching equation in the feedback $\alpha$ and the function $F$

$$d\left(X(F)\right) + K_c d\alpha = 0. \tag{3.14}$$

**Remark 20** *Note that if $d\alpha = 0$ (i.e. $\alpha$ is constant), then (3.13) (or (3.14)) is satisfied if $d\left(X(F)\right) = 0$, or equivalently if $X(F)$ is constant. This in turn is satisfied if $dF \in ann(Span\{X_{K_0}, X_{K_c}\})$, i.e $X(F) = 0$. Two special cases may be identified, namely when $dF = 0$ i.e. $\theta_d = \theta$ (Proposition 14) and when $F$ is an invariant of $X$.*

The matching equation is now characterized in terms of $F$ and $\alpha$. Nevertheless, neither the explicit version (3.13) or the implicit one (3.14) gives us insights on how to solve the matching condition. In order to overcome this obstacle we proceed to decouple the matching equation by choosing a particular class of feedback such that the matching condition becomes a PDE in only one function.

### 3.4.2 Admissible state feedback

In order to solve the matching equation (3.13) we shall consider a particular class of feedback and thereby reduce the problem to a condition on the function $F$. We shall also make the following assumption.

**Assumption 21** *The differential $dK_c$ of the control contact Hamiltonian $K_c \in C^\infty(\mathcal{M})$ vanishes on a submanifold of measure 0 of $\mathcal{M}$.*

Observe that by taking the exterior derivative of (3.14) we get

$$dK_c \wedge d\alpha = 0. \tag{3.15}$$

This leads to consider a candidate feedback function of the interaction contact Hamiltonian function $K_c$

$$\alpha = \Phi' \circ K_c, \tag{3.16}$$

where $\Phi' \in C^\infty(\mathbb{R})$, $\Phi' : \mathbb{R} \to \mathbb{R}$. Note that this control law solves the equation $dK_c \wedge d(\Phi' \circ K_c) = dK_c \wedge (\Phi'' \circ K_c) dK_c = 0$, where $\Phi''(\lambda) = \frac{d}{d\lambda}(\Phi'(\lambda))$. Replacing this control law in (3.13), the equation is reduced to a matching equation in $F$ and $\Phi' \circ K_c$

$$d(X_{K_0}(F)) + (\Phi' \circ K_c) d(X_{K_c}(F)) + (X_{K_c}(F) + K_c)(\Phi'' \circ K_c) dK_c = 0.$$

We would like to derive a simpler version of this equation. Hence we proceed to rewrite it in the form $d(\cdot) = 0$. The previous equation may be written as

$$d\left[X_{K_0}(F) + (\Phi' \circ K_c) X_{K_c}(F)\right] + K_c(\Phi'' \circ K_c) dK_c = 0,$$

and by defining $\Psi(\lambda) = \int_0^\lambda \chi \Phi''(\chi) d\chi$ it may be written as

$$d\left[X_{K_0}(F) + (\Phi' \circ K_c) X_{K_c}(F) + \Psi \circ K_c\right] = 0.$$

It is possible to rewrite this equation in a more convenient manner if $\Psi(\lambda)$ is integrated by parts. In this case the following is obtained

$$d\left[X_{K_0}(F) + (\Phi' \circ K_c) X_{K_c}(F) + K_c(\Phi' \circ K_c) - \Phi \circ K_c\right] = 0,$$

where $\Phi(\lambda) = \int_0^\lambda \Phi'(\chi) d\chi$. This means that there is a constant $c_F \in \mathbb{R}$ such that

$$X_{K_0}(F) + (\Phi' \circ K_c)[K_c + X_{K_c}(F)] - \Phi \circ K_c = c_F. \tag{3.17}$$

The matching condition is hence parametrized by $\Phi \circ K_c$ and $F$. The previous development leads to a characterization of the matching condition in terms of the state feedback and the function $F$, and a characterization of the closed-loop contact Hamiltonian function and vector field in terms of the state feedback, which is presented in the following proposition.

**Proposition 22** *Let $\mathcal{M}$ be a contact manifold with contact form $\theta$ with associated Reeb vector field $E$ and consider the smooth real functions $K_0, K_c, F \in \mathcal{C}^\infty(\mathcal{M})$, such that $i_E K_0 = i_E K_c = i_E F = 0$. Then the closed-loop vector field $X = X_{K_0} + \alpha X_{K_c}$, with $\alpha \in \mathcal{C}^\infty(\mathcal{M})$, is a strict contact vector field with respect to the shaped contact form $\theta_d$ and the shaped contact Hamiltonian $K$, respectively,*

$$\theta_d = \theta + dF \qquad \text{and} \qquad K = K_0 + \Phi \circ K_c + c_F, \tag{3.18}$$

*where $\Phi \in C^\infty(\mathbb{R})$, if and only if*

$$\alpha = \Phi' \circ K_c(x,p),$$

*and the matching equation (3.17) is satisfied. The closed-loop vector field is then denoted by $X = \hat{X}_K$, where $\hat{X}_K$ denotes the contact vector field generated by $K$ with respect to the contact form $\theta_d$.*

**Proof.** By taking the exterior derivative of (3.14) we get $dK_c \wedge d\alpha = 0$ which is a necessary condition for $K_c d\alpha$ to be closed and, by Assumption 21, $d\alpha = \mu dK_c$ for some function $\mu$. However observing that (3.14) implies that $K_c \mu dK_c$ is an *exact* 1-form and using the Assumptions 13 and 21, one obtains that $\mu$ is a function of the interaction contact Hamiltonian function $K_c$. Finally by integration one obtains that the feedback $\alpha$ may be written $\alpha = \varphi \circ K_c$. Now, $\mathbb{R}^{2n+1} \simeq \mathcal{M} \xrightarrow{K_c} \mathbb{R} \xrightarrow{\Phi'} \mathbb{R}$, but $K_c$ fulfils $i_E K_c = 0$ (i.e., it is a strict contact Hamiltonian), hence $\alpha = \Phi' \circ K_c(x,p)$. The fact that $X = X_{K_0} + \alpha X_{Kc}$ is invariant with respect to $\theta_d$ if and only if (3.17) is satisfied follows from the preceding developments. Now, the closed-loop contact Hamiltonian function is given by the contraction of the closed-loop contact Hamiltonian vector field and the closed-loop contact form

$$K = i_X \theta_d.$$

Computing this last expression yields

$$\begin{aligned} K &= i_{X_{K_0}}(\theta + dF) + \alpha i_{X_{K_c}}(\theta + dF), \\ &= K_0 + i_{X_{K_0}} dF + \alpha(K_c + i_{X_{K_c}} dF), \\ &= K_0 + X_{K_0}(F) + \alpha(K_c + X_{K_c}(F)). \end{aligned} \tag{3.19}$$

Replacing the control law in this expression, and since $F(x,p)$ and $\Phi' \circ K_c$ verify (3.17), $K = K_0 + \Phi \circ K_c + c_F$ is obtained. Furthermore, note that since the constant $c_F$ does not change the closed-loop vector field, $K = K_0 + \Phi \circ K_c$ also generates the same contact vector field. Finally, since $X$ is a contact vector field with respect to $\theta_d$ (i.e. $L_X \theta_d = \rho_d \theta_d$), then it is generated by $K$ with respect to the canonical coordinates of the contact form $\theta_d$. Hence, $X$ may be equivalently defined as

$$X = X_{K_0} + \alpha X_{K_c} = \hat{X}_K \tag{3.20}$$

where $\hat{X}_K$ denotes the contact vector field generated by $K$ with respect to the contact form $\theta_d$. ■

**Remark 23** *It is also possible to obtain the expression of the closed-loop contact Hamiltonian by using the representation in coordinates of the closed-loop contact form and vector field. Indeed, the closed-loop contact form is given by*

$$\begin{aligned} \theta_d &= d\left(x_0 + F(x,p)\right) - p^\top dx \\ &= dx_0 - \left(p - \frac{\partial F}{\partial x}\right)^\top dx + \frac{\partial F}{\partial p}^\top dp. \end{aligned} \tag{3.21}$$

*The closed-loop vector field in local coordinates is* $X = X_{K_0} + X_{K_c}\alpha$ *and* $K$ *is given by the contraction of the 1-form* $\theta_d$ *by this vector field. Recalling (3.3),*

$$K = i_X\theta_d = K_0 + \left(\frac{\partial K_0}{\partial x}^\top \frac{\partial F}{\partial p} - \frac{\partial K_0}{\partial p}^\top \frac{\partial F}{\partial x}\right) + \frac{\partial F}{\partial p}^\top p\frac{\partial K_0}{\partial x_0} + \left[K_c + \left(\frac{\partial K_c}{\partial x}^\top \frac{\partial F}{\partial p} - \frac{\partial K_c}{\partial p}^\top \frac{\partial F}{\partial x}\right) + \frac{\partial F}{\partial p}^\top p\frac{\partial K_c}{\partial x_0}\right]\alpha.$$

*Since* $\alpha = \Phi' \circ K_c$ *and* $\frac{\partial K_0}{\partial x_0} = \frac{\partial K_c}{\partial x_0} = 0$ *(and recalling the definition of the symplectic bracket), we have*

$$\begin{aligned} K &= K_0 + (\Phi' \circ K_c)K_c + \{K_0, F\} + (\Phi' \circ K_c)\{K_c, F\}, \\ &= K_0 + \{K_0, F\} + (\Phi' \circ K_c)(K_c + \{K_c, F\}), \\ &= K_0 + X_{K_0}(F) + (\Phi' \circ K_c)[K_c + X_{K_c}(F)]. \end{aligned}$$

*Finally replacing (3.17) in this equation we obtain* $K = K_0 + \Phi \circ K_c + c_F$.

It is possible to interpret Remark 20 in terms of the closed-loop contact Hamiltonian as follows.

**Remark 24** *If* $\alpha$ *is constant, i.e.,* $\alpha = \Phi' \circ K_c = c_k$ *with* $c_k$ *a constant, and since* $\Phi(\gamma) = \int_0^\gamma \Phi'(\chi)d\chi$*, then the closed-loop contact Hamiltonian becomes* $K = K_0 + c_k Kc + c_I$*, where* $c_I$ *is due to an integration constant. Furthermore the matching condition (3.17) becomes*

$$\begin{aligned} \{K_0, F\} + c_k\{K_c, F\} &= c_F, \\ \{K_0 + c_k K_c, F\} &= c_F \end{aligned} \tag{3.22}$$

*Two cases may be identified, namely when* $dF = 0$ *i.e.* $\theta_d = \theta$ *and the closed-loop contact form is not changed with respect to the canonical one; and when* $F$ *is an invariant of the standard Hamiltonian vector fields generated by* $K_0$ *and* $K_c$*, which implies, using the assumption that the contact Hamiltonian functions do not depend on* $x_0$*, that* $F$ *is an invariant of the vector field* $X$.

### 3.4.3 Relation with controlled Hamiltonian systems

Proposition 22 is basically a formal summary of the conditions under which the matching condition (3.13) has been derived. Some aspects that are worth to underline are: it has been assumed that the contact Hamiltonians are strict contact Hamiltonians, i.e., $i_E K_C = 0$, which implies that locally non of them depend on the $x_0$ coordinate and that the assumed state feedback is locally also independent of $x_0$. This justifies Assumption 17 and hence the matching condition is a PDE in the $x$ and $p$ coordinates only. In Proposition 22 the precise expression of the closed-loop contact Hamiltonian is also given. It is equal to the internal contact Hamiltonian plus the composition of the function $\Phi$ and the interaction contact Hamiltonian $K_c$. Furthermore, the feedback is exactly the derivative of the function $\Phi$, $\Phi' = \frac{d}{d\lambda}(\Phi(\lambda))$. This result is similar to the one given by structure preserving

feedback of Hamiltonian systems [85, 86]. The Hamiltonian vector field is defined as

$$X_H + \alpha X_C$$

Where $X_H$ is the vector field generated by the Hamiltonian function $H$ and $X_C$ is the control vector field generated by the control Hamiltonian function $C$. In this case a feedback of the form

$$\alpha = \frac{d}{d\lambda}(P(\lambda)),$$

where $P(C) = P \circ C$ is a smooth function, generates the closed-loop Hamiltonian vector field

$$X_H = X_{H_0 + P \circ C}$$

with closed-loop Hamiltonian function $H = H_0 + P \circ C$. The difference between control of Hamiltonian systems and contact systems is that for the first class of systems the geometry of the system is not changed after feedback. Proposition 14 shows that a state feedback in a contact system necessary changes its contact form, i.e., the geometry of the system is changed in closed-loop. This introduces, unlike in control of Hamiltonian systems, the matching condition (3.17) due to the change in the contact form. It also makes necessary to *distinguish between the vector field generated by the contact form $\theta$ and the closed-loop contact form $\theta_d$*. In Proposition 22 the closed-loop contact vector field is defined with respect to the closed-loop contact form $\theta_d$. Thus it has been denoted by $\hat{X}$, to distinguish it from the open-loop contact vector field $X$ defined with respect to the contact form $\theta$.

### 3.4.4 Input-output contact systems

In [20, 22] $V$-conjugated outputs for conservative contact systems where introduced. These conjugated outputs where defined with respect to an arbitrary differentiable function $V \in \mathcal{C}(\mathcal{M})$ and the interaction contact Hamiltonian function $K_c$. Let us study the expression of these kind of conjugated outputs for the case of strict contact Hamiltonian systems. Consider the differentiable function $V$, then the time derivative of this function along the trajectories of a control affine contact system is given by

$$\frac{dV}{dt} = \{K_0, V\}_{\text{Jacobi}} + p^\top \left( \frac{\partial K_0}{\partial x} - \frac{\partial K_0}{\partial p} \right) \frac{\partial V}{\partial x_0} + \left( \{K_c, V\}_{\text{Jacobi}} + p^\top \left( \frac{\partial K_c}{\partial x} - \frac{\partial K_c}{\partial p} \right) \frac{\partial V}{\partial x_0} \right) u,$$

where (recall equation (3.4)) $\{\cdot, \cdot\}_{\text{Jacobi}}$ denotes the Jacobi bracket [48, 57]. We may also express the previous equation in terms of the usual symplectic bracket

$$\frac{dV}{dt} = \{K_0, V\} + \left( K_0 - p^\top \frac{\partial K_0}{\partial p} \right) \frac{\partial V}{\partial x_0} + \left( \{K_c, V\} + \left( K_c - p^\top \frac{\partial K_c}{\partial p} \right) \frac{\partial V}{\partial x_0} \right) u,$$

The $V$-conjugated outputs is then defined as

$$y_V = \{K_c, V\}_{\text{Jacobi}} + p^\top \left( \frac{\partial K_c}{\partial x} - \frac{\partial K_c}{\partial p} \right) \frac{\partial V}{\partial x_0} = \{K_c, V\} + \left( K_c - p^\top \frac{\partial K_c}{\partial p} \right) \frac{\partial V}{\partial x_0}.$$

The time derivative of $V$ may be written as the balance equation

$$\frac{dV}{dt} = s_V^0 + y_V u,$$

where $s_V^0 = \{K_0, V\} + \left(K_0 - p^\top \frac{\partial K_0}{\partial p}\right) \frac{\partial V}{\partial x_0}$ is the internal source term. This output arises in the study of open-loop conservative contact systems. The conjugated outputs are clearly not uniquely defined, since they depend on the chosen function $V$ and this may be a drawback for the analysis of the system.

The result of Proposition 22 is similar to the one obtained when investigating the feedback equivalence of input-output Hamiltonian systems [85, 86, pp.132-133] with the difference that in this frame the Poisson bracket is the same in open and closed loop whereas for control contact systems the contact form in open loop is different than in closed loop. However in both problems the feedback in defined as the composition of some function with the control Hamiltonian, respectively the control contact Hamiltonian. For input-output Hamiltonian systems the control Hamiltonian defines a natural output. In this section we follow this line and define the natural output of a contact Hamiltonian system in a similar manner.

**Definition 25** *An* (single) input- (single) output contact system *is defined by a affine control contact system of the Definition 12 augmented with the output relation*

$$y = K_c(\tilde{x}). \tag{3.23}$$

One may note immediately that this definition of output also coincides with the more general definition suggested in [11] for control Hamiltonian systems nonlinar in the inputs: $y = \frac{\partial K}{\partial u}(\tilde{x}, u) = K_c(\tilde{x})$ with the definition of the contact Hamiltonian $K = K_0 + uK_c$. One may also note that this output is quite different from $V$-conjugated outputs for conservative contact systems introduced in [22, 20] and defined with respect to an arbitrary smooth function $V \in \mathcal{C}^\infty(\mathcal{M})$ and the interaction contact Hamiltonian function $K_c$. Using the previous definition the state feedback of Proposition 22 may be expressed as an output feedback

$$\alpha = \Phi'(y), \tag{3.24}$$

and the closed-loop contact Hamiltonian is a function of the natural output

$$K = K_0 + \Phi(y) + c_F. \tag{3.25}$$

A question that arises when defining the natural output in this manner is what happens in the case of conservative contact systems arising from the modelling of physical systems. In that case the control contact Hamiltonian vanishes on the Legendre submanifold defining the thermodynamic properties of the system and so does the natural output. From Proposition 14 we know that the only way to preserve the open-loop contact form is using a constant control. Any other state feedback necessarily changes the contact form and hence the invariant Legendre submanifold of the open-loop system is no longer an invariant Legendre submanifold for the closed-loop system. Thus, the particular subspace where $y = K_c = 0$ has no longer a particular meaning for the closed-loop contact system.

### 3.4.5 Feedback equivalence of input-output systems

Having defined input-output contact systems, we may now follow similar questions as for input-output Hamiltonian systems [84], and look for the feedback equivalence of these input-output contact systems. This mean that one looks for a control

$$u\left(t,\,\tilde{x}\right)=\alpha\left(\tilde{x}\right)+v\left(t\right) \tag{3.26}$$

such that the closed-loop system

$$\frac{d\tilde{x}}{dt}=\left(X_{K_0}+X_{K_c}\alpha\left(\tilde{x}\right)\right)+X_{K_c}v \tag{3.27}$$

is again an input-output contact system. From the preceding section we know that the closed-loop drift vector field of (3.27) is a contact vector field when the Proposition 22 is satisfied. In order to have an input-output contact systems remains to check that its input vector field $X_{K_c}$ is also a strict contact vector field with respect to the closed-loop contact form $\theta_d$. This is true if $L_{X_{K_c}}\theta_d=0$ which by

$$\begin{aligned} L_{X_{K_c}}\theta_d &= L_{X_{K_c}}\left(\theta+dF\right) \\ &= L_{X_{K_c}}dF \\ &= dX_{K_c}\left(F\right)=0 \end{aligned}$$

As a consequence, the feedback equivalence of input-output contact systems is summarized in the following proposition.

**Proposition 26** *An input-output contact system defined according to the Definition 25 on some contact manifold $\mathcal{M}$ endowed with the contact form $\theta$ with internal contact Hamiltonian $K_0$ and control Hamiltonian $K_c$ is feedback equivalent using (3.26) to an input-output contact system with respect to the contact form $\theta_d=\theta+dF$ defined in the Assumption 17 if and only if there exists two real numbers $c_1$ and $c_F$ as well as a real function $\Phi\in C^\infty\left(\mathcal{M}\right)$ such that the following system of linear PDE's is satisfied*

$$\begin{aligned} X_{K_c}\left(F\right) &= c_1 \\ X_{K_0}(F)+(\Phi'\circ K_c)[K_c+c_1]-\Phi\circ K_c &= c_F \end{aligned} \tag{3.28}$$

In this section we have characterized the conditions under which it is possible to define a state feedback that generates a closed-loop vector field equipped with a contact form. Using some physically based assumptions the conditions have been reduced to a matching condition in a state feedback and a differentiable function ($\alpha$ and $F$ respectively). We have also defined a class of natural outputs that may be related with Hamiltonian control systems. The interest is now to characterize the possible solutions of the matching equation (3.17). In the following subsection this is addressed from a control perspective.

### 3.4.6 Some remarks on control synthesis

It is clear that the key step in finding a structure preserving feedback for a control contact system is the existence of solutions of (3.17). We now analyse the existence

of solutions of this equation having in mind the objective of control design. In order to simplify the calculus, and without loose of generality, it is assumed that $c_F = 0$. The closed-loop contact Hamiltonian function is given by

$$K = K_0 + \Phi \circ K_c.$$

Consider $K$ as a control design parameter, i.e. $K = K_d$, where $K_d$ is some desired closed-loop contact Hamiltonian function with some prescribed properties. From the previous equation,

$$\Phi \circ K_c = K_d - K_0, \tag{3.29}$$

hence $\Phi \circ K_c$ may be seen as a function that is added to the internal contact Hamiltonian in order to shape it into the desired closed-loop contact Hamiltonian $K_d$. Note that $\Phi \circ K_c$ is the design parameter that shapes the closed-loop contact Hamiltonian $K_d = K_0 + \Phi \circ K_c$. Recall the matching condition (3.17),

$$(X_{K_0} + (\Phi' \circ K_c) X_{K_c})(F) + (\Phi' \circ K_c) K_c - \Phi \circ K_c = 0.$$

Since $K_0$ and $K_c$ are given, and $\Phi \circ K_c$ has been assigned (and hence also $\Phi' \circ K_c$), the previous equation represents a linear first-order PDE in the unknown function $F$. We may express this in the canonical coordinates as

$$\begin{bmatrix} \frac{\partial F}{\partial x} \\ \frac{\partial F}{\partial p} \end{bmatrix}^\top \begin{bmatrix} -\frac{\partial K_0}{\partial p} - (\Phi' \circ K_c)\frac{\partial K_c}{\partial p} \\ \frac{\partial K_0}{\partial x} + (\Phi' \circ K_c)\frac{\partial K_c}{\partial x} \end{bmatrix} + (\Phi' \circ K_c) K_c - \Phi \circ K_c = 0. \tag{3.30}$$

The solutions of this equation represent all possible functions $F$ for a specified $\Phi$. Hence, choosing the desired closed-loop contact Hamiltonian $K_d$, equation (3.29) defines the relation with $\Phi$. Then the matching equation is given by the linear first-order PDE (3.30) and it determines how the closed-loop contact form $\theta_d$ and the Reeb vector field (the coordinate associated to the energy) are shaped.

**Remark 27** *A different approach is to assign the desired contact form $\theta_d$, and hence the desired function $F$, and solve the previous equation in $\Phi$ and $\Phi'$. Since $\Phi' = \frac{d}{d\lambda}(\Phi(\lambda))$, (3.30) may then be rewritten as a linear first-order differential equation in $\Phi$.*

As already mentioned, equation (3.30) is a linear first-order PDE in $F$, hence the solutions of this equation can be computed by using the method of characteristics [1, 23, 59]. In order to illustrate the synthesis a simple illustrative example is presented.

### 3.4.7 Example: the heat exchanger (continued)

Recall from Chapter 2 the heat exchanger but consider for simplicity in this case the input as a controlled heat flux

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \lambda \left( \frac{1}{\frac{\partial U}{\partial x_2}} - \frac{1}{\frac{\partial U}{\partial x_1}} \right) \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial U}{\partial x_1} \\ \frac{\partial U}{\partial x_2} \end{bmatrix} + \frac{1}{\frac{\partial U}{\partial x_2}} \begin{bmatrix} 0 \\ 1 \end{bmatrix} u. \tag{3.31}$$

The IPHS representation is given by

$$\dot{x} = R(x, T(x))J\frac{\partial U}{\partial x}(x) + g(T)u,$$

where $x = [S_1, S_2]$ is the entropy of subsystem 1 and 2, $U(S_1, S_2) = U_1(S_1)+U_2(S_2)$ is the internal energy of the overall system composed of the addition of the internal energies of each subsystem, $u(t)$ the controlled input that corresponds to an external heat source, $\lambda > 0$ denote Fourier's heat conduction coefficient, $\frac{\partial U}{\partial x_i} = T_i(x_i)$, $T(x_i) = T_0 \exp\left(\frac{x_i}{c_i}\right)$, where $T_0$ and $c_i$ are constants, $R(x, T(x)) = \lambda\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$, $J = \left[\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right]$ and $g = \frac{p_2}{T_2}\left[\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right]$. A lift of the heat exchanger may be defined by the contact Hamiltonian $K = K_0 + K_I + K_c u$, with

$$\begin{aligned} K_0(x, p) =& - R(x, p)p^\top J_s T(x), \\ K_c(x, p) =& \frac{p_1}{T_1}\left(1 - \frac{p_2}{T_2}\right), \end{aligned} \tag{3.32}$$

with $R(x, p) = \lambda\left(\frac{p_1 - p_2}{T_1 T_2}\right)$ and $J = \left[\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right]$. The thermodynamic properties of the composed system are simply obtained by considering the Legendre submanifold $\mathcal{L}_U$ generated by the potential $U = U_1 + U_2$,

$$\mathcal{L}_U : \left\{ \begin{array}{ll} x_0 & = U \\ x & = [S_1, S_2]^\top \\ p & = \left[\frac{\partial U}{\partial S_1}, \frac{\partial U}{\partial S_2}\right]^\top = [T_1, T_2]^\top \end{array} \right\}.$$

Hence on $\mathcal{L}_U$ the thermodynamic properties of the system are recovered and the extensive variables may be identified with $x_0$ and $x$, and the intensive variables with $p$. In this section we shall briefly illustrate the Proposition 26 by giving a particular solution to the matching equations (3.17) and (3.28), corresponding to some choice of feedback. It appears that for the solution of the matching equation, it eases the computations and the interpretations of the results, to use another lift of the entropy balance equations (3.31) and modify the internal contact Hamiltonian $K_0$ in (3.32) by adding the following auxiliary contact Hamiltonian

$$K_a = \lambda T_1 \left(\frac{p_1}{T_1} - \frac{p_2}{T_2}\right)^2 + \frac{\lambda_e^2}{2}\frac{p_1^2}{T_1}\left(1 - \frac{p_2}{T_2}\right)^2,$$

and model the heat exchanger with the contact vector field $X_{K_0+K_a} + X_{K_c}u$. This function $K_a$ has been chosen such that it vanishes on $\mathcal{L}_U$ and that $X_{K_a}|_{\mathcal{L}_U} = 0$. As a consequence the restrictions of both contact vector fields $X_{K_0+K_a} + X_{K_c}u$ and $X_{K_0} + X_{K_c}u$ to the Legendre submanifold $\mathcal{L}_U$ are equal and both define admissible lifts of the entropy balance equations of the system.

Choosing $\Phi(\chi) = -\frac{1}{2}\chi^2$, one obtains the control law

$$u(t, \tilde{x}) = \Phi'(K_c)(\tilde{x}) + v(t) = -\lambda_e \frac{p_1}{T_1}\left(1 - \frac{p_2}{T_2}\right) + v(t)$$

A solution of the PDE (3.17) is then given by the function $F = \left(\frac{p_1}{T_1} + \frac{p_2}{T_2}\right)$ which moreover is an invariant of $X_{K_c}$, i.e., $X_{K_c}F = 0$ and satisfies (3.28). According

to the Proposition 26, the closed-loop contact system is an input-output contact system with contact form

$$\theta_d = dx_0' - p^\top dx = d\left(x_0 + \tfrac{p_1}{T_1} + \tfrac{p_2}{T_2}\right) - p^\top dx,$$

and closed-loop contact Hamiltonian

$$K = K_0 + K_a - \tfrac{1}{2}K_c^2 + vK_c.$$

It is necessary to establish some control design criteria to define a meaningful state feedback. For this purpose it is of interest to study the feedback invariants of controlled contact systems. Indeed, the Legendre submanifold of contact systems modelling thermodynamic systems represents the energy of those systems. Hence it makes sense to study the properties of the Legendre submanifold of the closed-loop contact systems to choose the state feedback and parametrize the matching equation. We devote the next section to study this aspect.

## 3.5 On closed-loop invariant Legendre submanifolds

We shall develop the results of the previous section by considering under which condition the obtained contact system in closed-loop is also a *conservative* contact system. Indeed then the closed-loop system may again be restricted to some invariant Legendre submanifold and the control reduced to a state feedback in the $x$ coordinates only. Therefore the feedback should be chosen such that closed-loop system is defined by a contact vector field generated by a contact Hamiltonian satisfying an invariance condition. As mentioned in Chapter 2, a *conservative controlled contact system* is a control contact system which leaves invariant some Legendre submanifold. If the Legendre submanifold is defined by Gibbs' relation representing the thermodynamic properties of a physical system, then the conservative contact contact systems are the representations of open irreversible thermodynamic systems in the complete Thermodynamic Phase Space [40, 41, 57, 55, 56, 22, 27]. We recall the definition of a conservative contact system (Definition 4, Section 2.3 of Chapter 2).

**Definition 28 ([22])** *A* conservative control contact system *with respect to the Legendre submanifold $\mathcal{L}$ is defined as a control contact system with the contact Hamiltonians satisfying the invariance condition*

$$K_0\big|_{\mathcal{L}} = 0, \quad K_c\big|_{\mathcal{L}} = 0, \tag{3.33}$$

*where $\cdot|_{\mathcal{L}}$ denotes the restriction to $\mathcal{L}$.*

**Remark 29** *Recall that a Legendre submanifold is defined with respect to a particular contact form $\theta$: it is actually defined by the equation $\theta = 0$ [8, 48]. Hence it should be noticed that a Legendre submanifold for the open-loop system is not necessary a Legendre submanifold for the closed-loop system ,since the contact form is necessary changed after applying a state feedback (Proposition 14).*

Recall that the closed-loop contact Hamiltonian is a function of the sum of the internal contact Hamiltonian $K_0$ and the composed function $\Phi \circ K_c$. We shall now check the invariance condition of a Legendre submanifold which is satisfied if the restriction of $K$ vanishes. The type of Legendre submanifolds that are worth to be studied are the ones that are different from the Legendre submanifolds $\mathcal{L}$ of the canonical contact structure. Indeed, from Remark 29 if $\mathcal{L}$ is an invariant Legendre submanifold with respect to $\theta$ and $\theta_d$ then $F(x,p) = 0$ i.e. the contact form is not changed in closed-loop. This in turn implies a constant feedback. The kind of submanifold of interest are the ones different from $\mathcal{L}$. This interest have a physical motivation. The Legendre submanifold is related with the energy of the system, for instance for a thermodynamic system $\mathcal{L}_U$ is generated by the internal energy $U$. Thus shaping the energy of the system is related to shaping the invariant Legendre submanifold. We shall denote the shaped Legendre submanifold with respect to $\theta_d$ by $\mathcal{L}_d$ and we expect it to be related with the stability properties of the closed-loop contact vector field.

### 3.5.1 Invariance on shaped Legendre submanifolds

The invariance of the closed-loop contact vector field on $\mathcal{L}_d$ is of interest since we may use this condition as a control design objective. For instance, it might be easier to analyse stability of the closed-loop system on a different Legendre submanifold. Before continuing let us recall from Proposition 22 that the closed-loop contact Hamiltonian is given by (3.18)

$$K = K_0 + \Phi \circ K_c + c_F$$

In the following we will assume that $\mathcal{L}_d$ is a Legendre submanifold associated to the contact form $\theta_d$, i.e., $\mathcal{L}_d$ is defined by the equation $\theta_d = 0$. The following propositions characterizes the conditions for $\mathcal{L}_d$ to be an invariant of the closed-loop vector field $X$.

**Proposition 30** *The closed-loop contact vector field $X$ leaves $\mathcal{L}_d$ invariant if and only if*

$$K_0\big|_{\mathcal{L}_d} + \Phi \circ K_c\big|_{\mathcal{L}_d} = -c_F. \tag{3.34}$$

**Proof.** From (3.19)

$$K\big|_{\mathcal{L}_d} = K_0\big|_{\mathcal{L}_d} + \Phi \circ K_c\big|_{\mathcal{L}_d} + c_F,$$

that proves the result. ■

For the particular case when $c_F = 0$ equation (3.34) reduces to

$$K_0\big|_{\mathcal{L}_d} + \Phi \circ K_c\big|_{\mathcal{L}_d} = 0.$$

Proposition 30 may be used to find a function $\Phi$ such that the contact vector field leaves $\mathcal{L}_d$ invariant. Once $\Phi$ is found we can obtain the state feedback by derivation of $\Phi$. Finally we need to check that the matching condition (3.30) is verified, i.e., that it exists a closed-loop contact form $\theta_d$ for the closed vector field associated to the solution of Proposition 30. If this contact form exists then it will be such that

$\theta_d = 0$ on $\mathcal{L}$ since it has been derived using the invariance condition. Indeed in the canonical coordinates of the open-loop contact form $\theta$ the closed-loop contact form is written as

$$\theta_d = d(x_0 + F) - \sum_{i=1}^{n} p_i dx_i.$$

But all the derivations have been performed using the canonical coordinates associated to the closed-loop contact form

$$\theta_d = dx_0' - \sum_{i=1}^{n} p_i dx_i,$$

where the new canonical coordinate $x_0'$ is given by $x_0 + F$ in the old canonical coordinates. Hence it is not necessary to know the expression of $F$ to define the invariant Legendre submanifold and the control law. It is only necessary to solve the matching equation to guarantee the existence of $\theta_d$. This approach will be further developed in the subsequent sections.

### 3.5.2 Invariance on Legendre submanifolds of lifted IPHS

As previously discussed it is desirable to parametrize the matching equation. A design criteria to select the function $\Phi$ and thereby the state feedback $\alpha = \Phi'$ is necessary. Once these functions have been chosen it is possible to use (3.30) to verify the existence of a closed-loop contact form $\theta_d$ for the closed-loop vector field. In this section we will further develop on the conditions under which a controlled conservative contact system defined as the lift of a IPHS (Chapter 2 Section 2.3) subject to a structure preserving state feedback leaves invariant a desired Legendre submanifold. Our interest is to generate a Legendre submanifold that it is related with some desired performance property, as for instance a reference temperature. We will call the generating function of the Legendre submanifold $U_d$ and the Legendre submanifold $\mathcal{L}_{U_d}$.

It is of interest that the closed-loop contact system leaves invariant the Legendre submanifold given by a desired function $U_d(x)$. In the new canonical coordinates this Legendre submanifold is expressed as

$$\mathcal{L}_{U_d} : \left\{ x_0^d = U_d(x), \quad x = x, \quad p = \frac{\partial U_d}{\partial x}(x) \right\}. \tag{3.35}$$

Proposition 30 characterizes the conditions under which the closed-loop contact Hamiltonian vanishes on $\mathcal{L}_{U_d}$. Recall the lift of IPHS to the TPS (equation (2.17)),

$$\begin{aligned} K_0 + K_c &= \left( \frac{\partial U}{\partial x} - p \right)^\top \left( R\left(x, \tfrac{\partial U}{\partial x}\right) J \frac{\partial U}{\partial x}(x) + W\left(x, \tfrac{\partial U}{\partial x}\right) + g\left(x, \tfrac{\partial U}{\partial x}\right) u \right), \\ &= - p^\top R\left(x, \tfrac{\partial U}{\partial x}\right) J \frac{\partial U}{\partial x}(x) + \left( \frac{\partial U}{\partial x} - p \right)^\top \left( W\left(x, \tfrac{\partial U}{\partial x}\right) + g\left(x, \tfrac{\partial U}{\partial x}\right) u \right), \end{aligned}$$

The Legendre submanifold left invariant by the contact system is

$$\mathcal{L}_U = \left\{ x_0 = U(x), x = x, p = \frac{\partial U}{\partial x}(x) \right\}.$$

Note that on $\mathcal{L}_U$ the vector field $X$ is precisely the dynamic of the lifted thermodynamic system. The previously defined contact Hamiltonian is composed of the sum of the internal contact Hamiltonian $K_0 = -p^\top RJ\frac{\partial U}{\partial x}$ and the interaction contact Hamiltonian

$$K_c = \left(\frac{\partial U}{\partial x} - p\right)^\top (W + gu)\,.$$

We are studying the single input affine case hence we divide the interaction contact Hamiltonian in the purely control and interaction part. Since our input is $u$ we can define

$$K_I = \left(\frac{\partial U}{\partial x} - p\right)^\top W \quad \text{and} \quad K_c = \left(\frac{\partial U}{\partial x} - p\right)^\top g,$$

where we have explicitly separated the interaction contact Hamiltonian in the control part $K_c$ and the interaction part $K_I$. We may then formulate the following proposition for lifted IPHS as follows.

**Proposition 31** *The closed-loop contact vector field $X$, defined by the lift of a IPHS, leaves $\mathcal{L}_{U_d}$ invariant if and only if*

$$-R\left(x, \tfrac{\partial U_d}{\partial x}\right)\frac{\partial U_d}{\partial x}^\top J\frac{\partial U}{\partial x} + \left(\frac{\partial U}{\partial x} - \frac{\partial U_d}{\partial x}\right)^\top W\left(x, \tfrac{\partial U_d}{\partial x}\right) + \Phi \circ K_c\big|_{\mathcal{L}_{U_d}} = -c_F. \quad (3.36)$$

**Proof.** The proof follows by noting that the developments of the chapter are also true for the contact Hamiltonian system

$$X_K = X_{\bar{K}_0} + X_{K_c}u,$$

with $\bar{K}_0 = K_0 + K_I$. Then equation (3.34) of Proposition 30 becomes

$$K_0\big|_{\mathcal{L}_{U_d}} + K_I\big|_{\mathcal{L}_{U_d}} + \Phi \circ K_c\big|_{\mathcal{L}_{U_d}} = -c_F, \quad (3.37)$$

and by replacing the contact Hamiltonians corresponding to the lift of a IPHS the result is proved. ■

In order to design a feedback law that leaves $\mathcal{L}_{U_d}$ invariant, (3.36) should be evaluated on the restriction defined by $p = \frac{\partial U_d}{\partial x}(x)$ and solved for $\Phi \circ K_c$. Equation (3.36) is parametrized by the contact Hamiltonian function and the desired Legendre submanifold. Furthermore, the control contact Hamiltonian $K_c$ defines the argument of $\Phi \circ K_c$. This is of particular interest since the specific form of $K_c$ will determine the possible feedbacks. In the following example we illustrate on the heat exchanger the design of a state feedback that leaves a submanifold defining a desired hyper-plane invariant.

### 3.5.3 Example: the heat exchanger (continued)

Recall from Chapter 2 the heat exchanger

$$\begin{bmatrix}\dot{S}_1\\ \dot{S}_2\end{bmatrix} = \lambda\left(\frac{1}{\frac{\partial U}{\partial S_2}} - \frac{1}{\frac{\partial U}{\partial S_1}}\right)\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}\begin{bmatrix}\frac{\partial U}{\partial S_1}\\ \frac{\partial U}{\partial S_2}\end{bmatrix} + \lambda_e\begin{bmatrix}0\\ \frac{1}{\frac{\partial U}{\partial S_2}} - \frac{1}{u}\end{bmatrix}u,$$

and its representation as IPHS

$$\dot{x} = R(x, T(x))J\frac{\partial U}{\partial x}(x) + W + g(T)u$$

where $x = [S_1, S_2]$ is the entropy of subsystem 1 and 2, $U(S_1, S_2) = U_1(S_1) + U_2(S_2)$ is the internal energy of the overall system composed of the addition of the internal energies of each subsystem, $u(t)$ the controlled input that corresponds to an external heat source, $\lambda > 0, \lambda_e > 0$ denote Fourier's heat conduction coefficients, $\frac{\partial U}{\partial x_i} = T_i(x_i)$, $T(x_i) = T_0 \exp\left(\frac{x_i}{c_i}\right)$, where $T_0$ and $c_i$ are constants, $R(x, T(x)) = \lambda\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$, $J = \left[\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right]$, $W = -\lambda_e \left[\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right]$ and $g = \frac{\lambda_e}{T_2}\left[\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right]$. The lift of the heat exchanger may be defined by the contact Hamiltonian (Chapter 2 Subsection 2.3.2) $K = K_0 + K_I + K_c u$, with

$$K_0 = -Rp^\top J_s T, \quad K_I = \left(\frac{\partial U}{\partial x} - p\right)^\top W, \quad K_c = \left(\frac{\partial U}{\partial x} - p\right)^\top g, \tag{3.38}$$

where

$$R(x, p) = \lambda\left(\frac{p_1 - p_2}{T_1 T_2}\right), \quad g(x) = \frac{\lambda_e}{T_2}\begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{3.39}$$

The thermodynamic properties of the composed system are simply obtained by considering the Legendre submanifold $\mathcal{L}_U$ generated by the potential $U = U_1 + U_2$,

$$\mathcal{L}_U : \left\{ \begin{array}{ll} x_0 & = U \\ x & = [S_1, S_2]^\top \\ p & = \left[\frac{\partial U}{\partial S_1}, \frac{\partial U}{\partial S_2}\right]^\top = [T_1, T_2]^\top \end{array} \right\}.$$

Hence on $\mathcal{L}_U$ the thermodynamic properties of the system are recovered and the extensive variables may be identified with $x_0$ and $x$, and the intensive variables with $p$.

We shall first illustrate that it is not straightforward to construct the feedback control such that the closed-loop contact Hamiltonian is well defined. Indeed the regularity of the open-loop contact Hamiltonian does in general not guarantee the regularity of the closed-loop contact Hamiltonian.

Let us design a control such that the closed-loop contact Hamiltonian associated to the heat exchanger leaves invariant a desired Legendre submanifold. Assume that the desired Legendre submanifold is a plane generated by the function

$$U_d(x_1, x_2) = (x_1 + x_2)\, T^*,$$

where $T^*$ is a desired temperature. The desired Legendre submanifold is given by

$$\mathcal{L}_{U_d} : \left\{ \begin{array}{ll} x_0^d & = U_d(x) \\ x & = x \\ p & = \frac{\partial U_d}{\partial x}(x) = \begin{bmatrix} T^* & T^* \end{bmatrix}^\top \end{array} \right\}. \tag{3.40}$$

We may directly use (3.36) to verify Proposition 31. Replacing the previously defined internal, interaction and control contact Hamiltonians in (3.36) and restricting it to $\mathcal{L}_{U_d}$ we obtain

$$-\lambda_e(T_2 - T^*) + \Phi \circ K_c\big|_{\mathcal{L}_{U_d}} = 0,$$

where we have used the fact that for the chosen lift, (3.38), (3.39), $R(x,T^*)=0$ and thus $K_0|_{\mathcal{L}_U}=0$. This implies that $\Phi\circ K_c\big|_{\mathcal{L}_{U_d}}=\lambda_e(T_2-T^*)$. In order to design $\Phi$ it is necessary to study $K_c$:

$$K_c(x,p)=\lambda_e\frac{T_2-P_2}{T_2}=\lambda_e\left(1-\frac{P_2}{T_2}\right)$$
$$K_c(x,p):\mathbb{R}^{2n}\to\mathbb{R}$$

Furthermore, the restriction of $K_c$ to $\mathcal{L}_{U_d}$ is given by $K_c(x,T^*)=\lambda_e\frac{T_2-T^*}{T_2}$. $\Phi$ is an arbitrary function, hence we may define

$$\Phi\circ K_c(x,p)=-T^*\lambda_e\left(\frac{K_c}{K_c-\lambda_e}\right)=\lambda_e\left(T_2-p_2\right)\frac{T^*}{p_2}. \tag{3.41}$$

On the restriction to $\mathcal{L}_{U_d}$ we have $\Phi\circ K_c\big|_{\mathcal{L}_{U_d}}=\lambda_e(T_2-T^*)$. Despite that Proposition 30 is satisfied with this solution the closed-loop contact Hamiltonian is not well defined on the whole TPS. There is a singularity at $p_2=0$ where the closed-loop contact Hamiltonian is not defined, hence $\Phi$ given by (3.41) is not a valid solution for the feedback synthesis.

In order to overcome the obstacle of non-regularity of the closed-loop contact Hamiltonian we may redefine $K_c$ and $K_I$. Indeed since $K_0|_{\mathcal{L}_U}=0$ the particular form of $\Phi$ is determined by the particular form of $K_c$ and $K_I$. A possible choice of $K_c$ and $K_I$ for which $\Phi$ is well defined is

$$K_I(x,p)=\left(\tfrac{\partial U}{\partial x}-p\right)^\top W(x,p),$$
$$K_c(x,p)=\begin{bmatrix}1-e^{\lambda_e\left(\frac{p_1}{T_1}-1\right)} & 1-e^{\lambda_e\left(\frac{p_2}{T_2}-1\right)}\end{bmatrix}g,$$

where

$$W(x,p)=-\lambda_e\frac{p_2}{T_2}\begin{bmatrix}0\\1\end{bmatrix},\quad\text{and}\quad g=\begin{bmatrix}0\\1\end{bmatrix}$$

Let us now show that this choice allows to define a regular $\Phi$. First note that either $K_I$ or $K_c$ depend on $x_0$, hence the associated contact vector fields are strict contact vector fields. Once again, equation (3.36) may be used to verify Proposition 30. Replacing the previously redefined contact Hamiltonians in (3.36) and restricting it to $\mathcal{L}_{U_d}$ we obtain

$$-\lambda_e(T_2-T^*)\frac{T^*}{T_2}+\Phi\circ K_c\big|_{\mathcal{L}_{U_d}}=0,$$

since $K_0|_{\mathcal{L}_U}=0$. This implies that on the restriction defined by $\mathcal{L}_{U_d}$

$$\Phi\circ K_c\big|_{\mathcal{L}_{U_d}}=\lambda_e(T_2-T^*)\frac{T^*}{T_2}.$$

In order to find a function $\Phi$ that satisfies the previous equation it is necessary to study the new control contact Hamiltonian $K_c$ and its restriction to the desired Legendre submanifold. The control contact Hamiltonian is defined as the function

$$K_c(x,p)=1-e^{\lambda_e\left(\frac{p_2}{T_2}-1\right)}=1-e^{\lambda_e\left(\frac{p_2-T_2}{T_2}\right)},$$
$$K_c(x,p):\mathbb{R}^{2n}\to]-\infty,1[\subset\mathbb{R}.$$

The restriction of $K_c$ to $\mathcal{L}_{U_d}$ is given by $K_c(x, T^*) = 1 - e^{\lambda_e\left(\frac{T^*-T_2}{T_2}\right)}$. Since 1 is not in the image of $K_c$ we may perform the following operations on $K_c$:

$$\ln(1 - K_c) = \ln\left(e^{\lambda_e\left(\frac{p_2-T_2}{T_2}\right)}\right) = \lambda_e \frac{p_2 - T_2}{T_2}.$$

We may then define $\Phi$ as a function of $K_c$ as

$$\Phi \circ K_c(x, p) = \Phi(x, p) = -T^* \ln(1 - K_c) = \lambda_e(T_2 - p_2)\frac{T^*}{T_2}.$$

Furthermore, on the restriction on $\mathcal{L}_{U_d}$ we have

$$\Phi \circ K_c\big|_{\mathcal{L}_d} = \Phi(x, T^*) = \lambda_e(T_2 - T^*)\frac{T^*}{T_2}, \tag{3.42}$$

hence Proposition 30 is satisfied and $\mathcal{L}_{U_d}$ is an invariant Legendre submanifold of the closed-loop contact vector field. The state feedback is simply obtained by derivation of $\Phi$. Recall that the state feedback $\alpha = \Phi'$ and $\Phi$ are related through $\Phi(\gamma) = \int_0^\gamma \Phi'(\chi)d\chi$. Thus

$$\Phi'(\gamma) = \frac{d\Phi}{d\gamma}(\gamma).$$

From this relation we obtain

$$\alpha = \Phi' \circ K_c(x, p) = \frac{T^*}{1 - K_c(x, p)} = T^* e^{-\lambda_e\left(\frac{p_2}{T_2}-1\right)}.$$

Hence the previous state feedback renders the desired Legendre submanifold invariant. Furthermore, since $\mathcal{L}_{U_d}$ is an invariant Legendre submanifold, on the restriction to $\mathcal{L}_{U_d}$ it is possible to define the state feedback as a function of $n$ variables only. Hence, on $\mathcal{L}_{U_d}$, the control law $\alpha$ is given by the restriction of $\Phi'$ to $\mathcal{L}_{U_d}$

$$\alpha\left(x, \frac{\partial U_d}{\partial x}(x)\right) = \alpha(x, T^*) = \Phi'(K_c(x, T^*)) = T^* e^{-\lambda_e\left(\frac{T^*}{T_2}-1\right)}.$$

The stability properties of the closed-loop contact system are not studied in this chapter, but it is straightforward to verify that the proposed state feedback stabilizes the closed-loop system at the desired temperature $T^*$.

The matching equation is given by the linear first-order PDE in the function $F$, (3.30). This linear first-order PDE may be solved by using the method of characteristics [1, 23, 59]. Hence the contact form $\theta_d = \theta + dF$ exists. ■

## 3.6 Conclusion

Structure preserving state feedbacks of controlled contact systems have been studied. It has been proved that the only feedback that preserves the canonical contact form $\theta$ is the constant feedback (Proposition 14). Hence, the closed-loop system may be render a contact system only with respect to a *new* contact form. The

conditions for the existence of a new contact structure and a state feedback have been derived. Furthermore, for strict contact systems these conditions have been developed assuming a specific closed-loop differential form. The closed-loop differential form, denoted $\theta_d$, has been assumed as the sum of the open-loop contact form and the exterior derivative of a function $F$ that fulfils the condition that it does not depend on the coordinate associated to the Reeb vector field, i.e., $i_E F = 0$. The closed-loop contact form is then defined by the expression: $\theta_d = \theta + dF$. It has been shown (Proposition 18) that $\theta_d$ is a contact form and that locally only the coordinate associated to Reeb vector field, i.e. $x_0$ is changed. Furthermore for thermodynamic systems this coordinate may be associated to the energy, hence the control may be interpreted as changing the energy of the system. Using the assumption of a strict contact Hamiltonian system and the specific closed-loop contact form the closed-loop contact Hamiltonian system has been characterized for a class of state feedbacks in terms of a matching equation (Proposition 22). For the particular class of state feedbacks the expressions for the closed-loop contact vector field and contact Hamiltonian have also been given.

The relation with controlled input-output Hamiltonian system has been addressed. It has been shown that the expression of the closed-loop contact Hamiltonian function has the same form as the expression of the closed-loop Hamiltonian function. The difference is that in the case of controlled Hamiltonian system the differential form associated to the system is not changed, hence the geometry is conserved. This implies for instance that the closed-loop vector field is generated by the closed-loop contact Hamiltonian function but with respect to a different differential form, whereas the closed-loop Hamiltonian vector field is generated with respect to the same differential form as the open-loop Hamiltonian vector field. The relation with input-output Hamiltonian systems has also motivated the definition of a natural output (Definition 25) for controlled contact systems which is simply the control contact Hamiltonian. The state feedback may then be interpreted as an output feedback with respect to this natural output.

The chapter concludes with the study of invariant Legendre submanifolds for the closed-loop contact vector field. Since the closed-loop contact vector field is defined by a different contact form than the canonical contact form, the open-loop invariant Legendre submanifolds are not necessary invariant Legendre submanifolds of the closed-loop contact vector field. It is of special interest to study the Legendre submanifold that leaves invariant the closed-loop vector field since the Legendre submanifold may be associated with the energy of the system. Hence the closed-loop invariant Legendre submanifold may be related with a closed-loop energy function. The condition for the existence of invariant Legendre submanifolds for the closed-loop contact system has been given and specialized for the case of lifted irreversible PHS (Propositions 30 and 31). This condition has then been used as design criteria to select the state feedback and apply Proposition 22 to derive the closed-loop contact form.

# Chapter 4

# Stability and control of strict contact systems

## 4.1 Introduction

In the previous chapter the conditions for structure preserving feedback of contact vector fields, affine in the inputs, have been given. For strict contact vector fields the matching conditions have further been developed and for a particular class of contact form and state feedback these conditions have been characterized. It has also been suggested to design a feedback such that the closed-loop contact vector field leaves a desired Legendre submanifold invariant.

The similarities with structure preserving feedback of input-output Hamiltonian systems [85, 86] have also been addressed. The stability properties however differs considerably from the ones of input-output Hamiltonian systems. For Hamiltonian systems the storage function is a natural Lyapunov function candidate and the state feedback is chosen such that the equilibrium point is changed. For contact system on other hand it is not natural to consider the contact Hamiltonian function as a possible Lyapunov function candidate. Moreover, the contact systems of main interest are defined by the lift of some physical system to the TPS. For that class of contact systems the contact Hamiltonian function is more likely associated with a kind of virtual power [22], not energy as the Hamiltonian function of Hamiltonian system.

In [30] a local study of the stability on Legendre submanifolds has been performed in local coordinates using linearisation techniques. It has been shown that the zeros situated on a Legendre submanifold corresponds to saddle points of the contact vector field and sufficient conditions for local stability on a Legendre submanifold have been given using linearisation. For lifted dynamic system the stability on the Legendre submanifold have been characterized in terms of the dynamic system. Furthermore it has been shown that for the lift of physical systems the stability may be characterized in terms of the thermodynamic properties of the systems.

In this chapter we analyse the equilibrium and stability properties of contact

vector fields starting from geometric arguments. The existence of zeros of contact vector fields has been shortly mentioned in [20, pp.43], commenting on the results on decomposition of contact vector fields presented in [48]. From a geometric point of view the existence of zeros implies that the vertical and horizontal component of the contact vector field have to vanish independently at the zero. The vertical component vanishes if and only if the contact Hamiltonian function vanishes at the zero. This by itself imposes a strong condition for the existence of zeros on the contact Hamiltonian function. Furthermore, it also defines a manifold which contains all zeros. The conditions for the existence of zeros are completed with the requirement for the horizontal component to vanish. For strict contact vector fields the condition for the horizontal component to vanish is reduced to the exterior derivative of the contact Hamiltonian being zero. In canonical coordinates these conditions corresponds to the ones presented in [30] for the existence of zeros of contact vector fields.

The local stability of the contact vector field is analysed first on the complete TPS. It is shown that for strict contact vector fields it is in general not possible to achieve global stability. The reason is that the Jacobian of strict contact vector fields has either $n$ unstable eigenvalues or $2n+1$ eigenvalues on the imaginary axis. For the purpose of stabilization in closed-loop, this suggest to study the partial stability on some $n$ dimensional subspace rather than the global stability of the contact vector field. More precisely we show that $2n$ eigenvalues are symmetric with respect to the imaginary axis and that they may be characterized by a symplectic Hamiltonian subsystem. It its well known that a pair of invariant submanifolds for Hamiltonian vector fields are given by a stable and unstable Lagrangian submanifold [89]. This may permit to define a stable invariant Legendre submanifold for the closed loop contact system generated by the same function that defines the Lagrangian submanifold for the Hamiltonian subsystem.

Since global stability is in general not possible (and not of interest for lifts of dynamic systems) we study the partial stability of the contact vector field on a Legendre submanifold. This means that on the restriction of the contact vector field to a Legendre submanifold we expect the restricted system to be asymptotically stable. Note that this kind of partial stability is included in the problems of stability to the components of a vector $y$ (briefly, $y$-stability problems) of an equilibrium position $x^\top = (y^\top, z^\top)$ of ordinary differential equations [95, 4]. Hence, it may be studied by using generalizations of Lyapunov's direct method [95]. However, the partial stability that we are interested in is given by a geometric property of the system an is hence better encompassed in the framework of partial stability of part of the state variables with respect to a given subspace. [52, 13].

To characterize the stability of strict contact vector fields on a Legendre submanifold we restrict the system to the submanifold of interest and apply Lyapunov's direct method on the restriction. This is possible since the Legendre submanifold is left invariant by the contact vector field and the trajectories remains in the submanifold. The stability conditions are then parametrized by the open-loop contact Hamiltonians, the feedback law and the closed-loop invariant Legendre submanifold. For conservative contact systems defined by the lift of a dynamic system we have been more specific and a Lyapunov function candidate has been proposed. The

conditions for stability have been parametrized by the dynamic system, the control law and the Legendre submanifold.

Finally the framework of conservative contact system is used to reinterpret the control by matching of vector fields. By lifting an open-loop vector field and a target vector field the matching of vector fields is interpreted as the matching of contact Hamiltonian functions. The matching condition can then be solved on the extended TPS and the stability, in the sense of Lyapunov, be viewed as a partial stability problem parametrized by a Legendre submanifold. A control design method is proposed and it is interesting to remark that the well known interconnection and damping assignment passivity based control approach (IDA-PBC) [65, 66] may be interpreted within its frame.

### 4.1.1 Organization of the chapter

The chapter is organized as follows. Section 4.2 presents some important properties of contact vector fields that permit to interpret the zeros geometrically. In section 4.3 the zeros and the stability properties of contact vector field are analysed in canonical coordinates. Some remarks on local stability of strict contact systems and the relation with the stability of Hamiltonian systems are also presented. In subsection 4.3.4 we give sufficient conditions for partial stability on an invariant Legendre submanifold and specialise these conditions for conservative contact systems. Section 4.4 presents a control design method that uses the framework of contact system to derive and interpret the stability conditions. Finally some closing remarks are presented in section 4.5.

### 4.1.2 Main contributions of the chapter

The main contributions of the chapter are the following.

- It is shown that the linearisation of strict contact vector fields possesses one eigenvalue at zero and $2n$ eigenvalues symmetric with respect to the imaginary axis (Proposition 39). Hence, since the linearised contact vector field posses in general $n$ unstable eigenvalues, it is in general unstable.

- The partial stability on a Legendre submanifold is characterized using Lyapunov's direct method. The Lyapunov function candidate may be constructed using $2n$ states variables (Proposition 43) or with respect to $n$ energy or co-energy variables (Corollaries 44 and 45).

- For controlled conservative contact system defined by the lift of a dynamic system the stability conditions on an invariant Legendre submanifold have been parametrized by the vector field of the dynamic system, the feedback law and the dynamic system (Proposition 46).

- The framework of conservative contact systems has been used to propose a control design method that consists of the matching of contact Hamiltonian functions defined by the lift of vector fields. This permits to solve a matching

equation on an extended space, relaxing some conditions, to match the open-loop and target vector fields. The stability condition is then parametrized by the Legendre submanifold with respect to which the lift has been performed (Proposition 48). Some interesting aspects of this method is that IDA-PBC and the control design using co-energy variables may be characterized within the framework (Corollaries 49 and 50).

## 4.2 Contact vector fields, their invariants and dynamical properties

In this section we perform an abstract analysis of the dynamical properties of contact vector fields. This permits to have a more geometric insight on the stability analysis developed in canonical coordinates in Section 4.3.

### 4.2.1 Decomposition of vector fields and one-forms of a contact manifold

The results recalled in this section are all taken from [48, chap.5]. Consider a contact manifold $\mathcal{M}$ of dimension $2n+1$ with contact form $\theta$ with Reeb vector field $E$.

We recall the decomposition of the tangent bundle and of vector fields.

**Proposition 32 ([48])** *The tangent bundle $T\mathcal{M}$ may be decomposed into*

$$T\mathcal{M} = \ker d\theta \oplus \ker \theta \tag{4.1}$$

*where* $\ker d\theta$*, called* vertical bundle*, is of rank* 1 *and is generated by the Reeb vector field and* $\ker \omega\theta$*, called* horizontal bundle*, is of rank* $2n$*. Every vector field $X$ on $\mathcal{M}$ may be decomposed in a unique way into*

$$X = \underbrace{(i_X\theta)\, E}_{\in \ker d\theta} + \underbrace{(X - (i_X\theta)\, E)}_{=\mathcal{H}(X)\in \ker\theta = \mathcal{C}} \tag{4.2}$$

*where $(i_X\theta)\, E$ is horizontal and $(X - (i_X\theta)\, E)$ is horizontal and is denoted by $\mathcal{H}(X)$.*

By duality one may decompose the cotangent bundle and Pfaffian forms as is formulated in the following proposition.

**Proposition 33 ([48])** *The cotangent bundle $T^*\mathcal{M}$ may be decomposed into*

$$T^*\mathcal{M} = \mathcal{E} \oplus \mathcal{F}$$

*where $\mathcal{E}$ is the vector sub-bundle of rank* 1 *generated by the the contact form $\theta$ (i.e. $\mathcal{E}$ defines the contact structure) and $\mathcal{F} = Ann(\ker d\theta)$ is the annihilator of* $\ker d\theta$*, the vector sub-bundle of rank* $2n$ *of the* semi-basic 1-forms*, that is the 1-forms $\phi$ satisfying*

$$i_E\phi = 0.$$

*Every Pfaffian form $\gamma$ on $\mathcal{M}$ may be decomposed in a unique way into*

$$\gamma = \underbrace{(i_E\gamma)\,\theta}_{\in\mathcal{E}} + \underbrace{(\gamma - (i_E\gamma)\,\theta)}_{\in\mathcal{F}}$$

*where $(\gamma - (i_E\gamma)\,\theta)$ is semi-basic.*

These decomposition allow to define an isomorphism between horizontal vector fields and semi-basic Pfaffian forms (corresponding, loosely speaking, to the $\{\cdot,\cdot\}$ "Poisson-like tensor" appearing in the expression of contact vector fields (3.3).

**Proposition 34 ([48])** *The mapping*

$$\begin{array}{rcl} \theta^\flat : \mathfrak{X}(\mathcal{M}) & \to & \Lambda(\mathcal{M}) \\ X & \mapsto & i_X d\theta \end{array}$$

*carries any vector field into a semi-basic form. Furthermore the restriction of $\theta^\flat\big|_{\mathcal{C}}$ to the vector space $\mathcal{C}$ of horizontal vector fields is an isomorphism onto the space $\mathcal{F}$ of semi-basic 1-forms. And its inverse is denoted by $\theta^\sharp : \mathcal{F} \to \mathcal{C}$.*

### 4.2.2 Reminder on some properties of contact vector fields

Using the definitions recalled in the preceding subsection, and according to the theorem 13.3 in [48, p. 319], the isomorphism $\Omega$ between contact vector fields $X_K \in \mathcal{M}$ and differentiable functions $K \in \mathcal{M}'$, defined by the contact form $\theta$, is expressed by

$$K = \Omega(X_K) = i_{X_K}\theta$$

and its inverse is

$$\Omega^{-1}(K) = X_K = K\,E + \theta^\sharp\,(dK - (i_E dK)\,\theta) \tag{4.3}$$

where $K\,E$ is the vertical and $\theta^\sharp\,(dK - (i_E dK)\,\theta)$ is the horizontal components of the contact vector field. Note that if the contact Hamiltonian $K$ is is a first integral of the Reeb vector field (that is, its differential $dK$ is semi-basic, i.e. satisfies $i_E dK = 0$), then

$$X_K = K\,E + \theta^\sharp\,(dK)$$

and leaves invariant the contact form and is called *strict contact vector field* (it is an *infinitesimal automorphism of the Pfaffian structure*).

Recall [48, pp.319-320] that the isomorphism $\Omega$ is also a Lie algebra isomorphism when considering the *Jacobi bracket* $[Z,\,G]_\theta$ of two differentiable functions $Z$ and $G$ , defined by

$$\begin{array}{rcl} [Z,\,G]_\theta & = & \Omega\left(\left[\Omega^{-1}(Z)\,,\,\Omega^{-1}(G)\right]\right) \\ & = & \Omega\left([X_Z,\,X_G]\right) \\ & = & i_{X_Z}dG - G\,i_E dZ \\ & = & -i_{X_G}dZ + Z\,i_E dG \\ & = & -i_{X_Z}i_{X_G}d\theta + Z\,i_E dG - G\,i_E dZ \end{array} \tag{4.4}$$

One may also note (according to the Remark 13.6 [48, p. 320]) that if two functions $Z$ and $G$ are first integrals of the Reeb vector field, then their Jacobi bracket is the pull-back of the symplectic bracket of functions $Z_P$ and $G_P$ defined on the quotient manifold $P$

$$[Z,\, G]_\theta = d\theta\,(X_Z,\, X_G) = \pi^*\,\{Z_P,\, G_P\}$$

which amounts to express in an intrinsic way the fact that in canonical coordinates, one see that the Jacobi bracket of functions that are first integrals of the Reeb vector field reduces to a symplectic bracket.

### 4.2.3 Equilibria of a contact vector fields and invariant submanifolds

As a preliminary remark (see [20, p.43]), note that from the skew symmetry of the Jacobi bracket (4.4), that $[K,\, K]_\theta = 0$ and one deduces

$$\begin{aligned} L_{X_K} K &= i_{X_K} dK \\ &= K\, i_E dK \end{aligned}$$

which implies that :

1. if $K$ is an invariant of the Reeb vector field ($i_E dK = 0$ on $\mathcal{M}$), it is also an invariant of the contact vector field $X_K$ that it generates: $L_{X_K} K = 0$. This implies that if $K^{-1}\,(r)\,,\ r \in \mathbb{R}$ defines a differentiable submanifold (of co-rank 1) then the latter is invariant by the vector field $X_K$.
2. if $K$ satisfies $i_E dK \neq 0$ on $\mathcal{M}$, then only the submanifold defined by $K^{-1}\,(0)$, if it exists, is invariant by the vector field $X_K$.

Now let us look for equilibria of the dynamical system defined by a contact vector field, in other words zeros of the contact vector field, that is $\tilde{x}^* \in \mathcal{M}$ such that $X_K\,(\widetilde{x}^*) = 0$. Such a zero is, according to the decomposition of a contact vector field into its vertical and horizontal components in (4.3), given by

$$K\,(\tilde{x}^*) = 0 \quad \text{and} \quad \theta^\sharp\,(dK - (i_E dK)\,\theta)\big|_{\tilde{x}^*} = 0. \tag{4.5}$$

It is noted in [48, p.322] that the second condition implies: $dK\,(\tilde{x}^*) \wedge \theta\,(\tilde{x}^*) = 0$. In the case when $dK$ is semi-basic the preceding equation is reduced to

$$K\,(\tilde{x}^*) = 0 \quad \text{and} \quad \theta^\sharp\,(dK)\big|_{\tilde{x}^*} = 0 \tag{4.6}$$

The following proposition characterizes the manifold containing the zeros of the contact vector field.

**Proposition 35** *Assume that there exists a zero, denoted by $\widetilde{x}^*$, of the contact vector field $X_K$. Assume that $S$ is a differentiable manifold of constant dimension $2n$, invariant by $X_K$ and defined as*

$$S = K^{-1}\,(0)\,.$$

*Then the set of zeros is*

$$\widetilde{x}^* = \left\{\widetilde{x} \in S |\ \theta^\sharp\,(dK - (i_E dK)\,\theta)\big|_S = 0.\right\} \tag{4.7}$$

**Corollary 36** *Assume that there exists a zero, denoted by $\widetilde{x}^*$, of the strict contact vector field $X_K$, i.e., $dK$ is semi-basic. Then the set of zeros is*

$$\widetilde{x}^* = \left\{ \widetilde{x} \in S |\ \theta^\sharp \left( dK \right) \big|_S = 0 \right\} \tag{4.8}$$

**Proof.** Assuming that there exists a zero of the vector field implies that the set

$$S = K^{-1}\left(0\right)$$

is not empty. Furthermore all zeros of the contact vector field belong to $S$. The restriction of $X_K$ to $S$ is horizontal: $X_K|_S = \theta^\sharp \left( dK - \left( i_E dK \right) \theta \right) \big|_S$. If $dK$ is semi-basic, then the restriction of $X_K$ to $S$ is the restriction of the horizontal vector field: $X_K|_S = \theta^\sharp \left( dK \right) \big|_S$. ■

From this discussion we see that if $dK$ is semi-basic it does not make sense to look for stability on the complete $2n+1$ dimensional space, since the zeros are characterized by $dK|_S = 0$ that defines the zeros on the $2n$ dimensional horizontal space. Thus, for the case of strict contact vector fields (i.e., their contact Hamiltonian function do not depend on $x_0$) the stability conditions are stated in terms of a partial stability problem on the submanifold $S$. In the following section we shall interpret these results in terms of canonical coordinates.

## 4.3 Stability analysis of contact vector fields in canonical coordinates

In this section the stability of contact system is addressed using canonical coordinates. First we study the local stability of the contact vector field by using linearisation techniques [46]. These results are extensions of the results of local stability of conservative contact system presented in [30]. We then address the global stability of the open-loop controlled contact system by using Lyapunov's second method [46].

### 4.3.1 Local stability and equilibrium points

In order to analyse the equilibrium points and the dynamic behaviour of the contact vector field around the equilibrium points we use the following results presented in [30].

**Proposition 37 ([30])** *Consider a contact manifold $(\mathcal{M}, \theta)$ and a contact vector field $X_K$. $X_K$ is generated by the contact Hamiltonian function $K(x_0, x, p)$ given in the canonical coordinates $(x_0, x, p)$. Let us consider a state $(x_0^*, x^*, p^*) \in (\mathcal{M}, \theta)$. Then $(x_0^*, x^*, p^*) \in \{(x_0, x, p) | X_K(x_0, x, p) = 0\}$ if and only if the following condi-*

*tions are fulfilled:*

$$\begin{aligned}
&\left.\frac{\partial K}{\partial p}\right|_{(x_0^*,x^*,p^*)} = 0,\\
&K(x_0^*,x^*,p^*) = 0,\\
&\left.\frac{\partial K}{\partial x}\right|_{(x_0^*,x^*,p^*)} = -p^* \left.\frac{\partial K}{\partial x_0}\right|_{(x_0^*,x^*,p^*)}.
\end{aligned}$$

This proposition is the local version of Proposition 35 expressed in the canonical coordinates. For the case of strict contact vector fields (i.e., $dK$ is semi-basic) we have the following corollary.

**Corollary 38 ([30])** *Consider a contact manifold $(\mathcal{M},\theta)$ and a contact vector field $X_K$ generated by the contact Hamiltonian function $K(x_0,x,p)$ given in the canonical coordinates $(x_0,x,p)$. Assume that $K(x_0,x,p)$ does not depend on $x_0$. Let us consider a state $(x_0^*,x^*,p^*)\in(\mathcal{M},\theta)$. Then $(x_0^*,x^*,p^*)\in\{(x_0,x,p)|X_K(x_0,x,p)=0\}$ if and only if $(x_0^*,x^*,p^*)$ is a critical point and a zero of $K(x_0,x,p)$.*

This corollary is the local version of Corollary 36 expressed in the canonical coordinates. To check if the equilibrium points are locally stable it suffices to compute the Jacobian matrix of the contact vector field and verify that all its eigenvalues are strictly negative when evaluated at the equilibrium points. The Jacobian of the contact vector field (3.3) is given by

$$\frac{\partial X_K}{\partial(x_0,x,p)}(x_0^*,x^*,p^*) = DX_K =$$
$$\left[\begin{array}{ccc}
\frac{\partial^\top K}{\partial x_0} - p^\top\left(\frac{\partial^2 K}{\partial p\partial x_0}\right)^\top & \frac{\partial^\top K}{\partial x} - p^\top\left(\frac{\partial^2 K}{\partial p\partial x}\right)^\top & -p^\top\left(\frac{\partial^2 K}{\partial p^2}\right)^\top\\
-\left(\frac{\partial^2 K}{\partial p\partial x_0}\right)^\top & -\left(\frac{\partial^2 K}{\partial p\partial x}\right)^\top & -\left(\frac{\partial^2 K}{\partial p^2}\right)^\top\\
p\left(\frac{\partial^2 K}{\partial x_0^2}\right)^\top + \left(\frac{\partial^2 K}{\partial x\partial x_0}\right)^\top & p\left(\frac{\partial^2 K}{\partial x_0\partial x}\right)^\top + \left(\frac{\partial^2 K}{\partial x^2}\right)^\top & \frac{\partial^\top K}{\partial x_0} I_n + p\left(\frac{\partial^2 K}{\partial x_0\partial p}\right)^\top + \left(\frac{\partial^2 K}{\partial x\partial p}\right)^\top
\end{array}\right]_{(x_0^*,x^*,p^*)}$$

From a first inspection of the linearisation it seems not possible to obtain important information regarding the local behaviour of the vector field. However, if the contact Hamiltonian function is not a function of $x_0$ the following proposition follows.

**Proposition 39** *Consider a contact manifold $(\mathcal{M},\theta)$ and a contact vector field $X_K$ generated by the contact Hamiltonian function $K(x_0,x,p)$ given in the canonical coordinates $(x_0,x,p)$. Assume that $K(x_0,x,p)$ does not depend on $x_0$. Let us consider an equilibrium state $(x_0^*,x^*,p^*)\in(\mathcal{M},\theta)$ of $X_K$. Then zero is eigenvalue of $DX_K$ and the remaining $2n$ eigenvalues are symmetrical with respect to the imaginary axis.*

**Proof.** If $K(x_0, x, p)$ does not depend on $x_0$ the Jacobian is given by the following expression

$$DX_K = \begin{bmatrix} 0 & -p^{*\top}\frac{\partial^2 K}{\partial x \partial p} & -p^{*\top}\frac{\partial^2 K}{\partial p^2} \\ 0 & -\frac{\partial^2 K}{\partial x \partial p} & -\frac{\partial^2 K}{\partial p^2} \\ 0 & \frac{\partial^2 K}{\partial x^2} & \left(\frac{\partial^2 K}{\partial x \partial p}\right)^\top \end{bmatrix}_{(x_0^*, x^*, p^*)} = \begin{bmatrix} 0 & -p^{*\top}A & -p^{*\top}B \\ 0 & -A & -B \\ 0 & C & A^\top \end{bmatrix} \tag{4.9}$$

with $A = \frac{\partial^2 K}{\partial x \partial p}(x_0^*, x^*, p^*)$, $B = B^\top = \frac{\partial^2 K}{\partial p^2}(x_0^*, x^*, p^*)$, $C = C^\top = \frac{\partial^2 K}{\partial x^2}(x_0^*, x^*, p^*)$. $\frac{\partial K}{\partial x}(x_0^*, x^*, p^*) = 0$ has been used from Corollary 38. The characteristic polynomial of $DX_K$ is given by $\det(DX_K - \lambda I)$, where $\det(\cdot)$ denotes the determinant. $\det(DX_K - \lambda I)$ may be evaluated by using cofactor expansion with respect to the first column and the properties of the determinant of block matrices [51]. The characteristic polynomial is given by

$$\begin{aligned} \det(DX_K - \lambda I) &= -\lambda \det\left(\begin{bmatrix} -(A - \lambda I) & -B \\ C & (A - \lambda I)^\top \end{bmatrix}\right), \\ &= \lambda \det(A - \lambda I) \det\left((A + \lambda I) - B(A - \lambda I)^{-1} C\right), \\ &= \lambda \det(A + \lambda I) \det\left((A - \lambda I) - C(A + \lambda I)^{-1} B\right), \end{aligned} \tag{4.10}$$

where it has been assumed that the inverse matrices $(A - \lambda I)^{-1}$ and $(A + \lambda I)^{-1}$ exist. It follows from the previous equation that $\lambda = 0$ is always solution and that the remaining $2n$ eigenvalues are symmetrical with respect to the imaginary axis. ■

The expression of $DX_K$ (equation (4.9)) shows that the column corresponding to $x_0$ is zero. Hence the remaining $2n$ eigenvalues are only function of the $x, p$-coordinates. This is expected from Corollary 36. It can be clearly observed that the strict contact vector field behaves as a cascade system since $x_0$ does not influence the remaining coordinates. This is also true for the non-linear contact vector field since $\frac{\partial K}{\partial x_0} = 0$. Let us analyse the local stability properties of the controlled systems proposed in chapter 3.

### 4.3.2 Local stability of the structure preserving feedback law

In this section the local and partial stability of closed-loop contact field subject to the class of structure preserving state feedback defined in chapter 3 is analysed. Before proceeding it is convenient to recall some key aspects of the development of chapter 3. The most important is that in closed-loop the canonical coordinates are changed. Recall from Proposition 22, section 3.4, chapter 3, that under the assumption that the contact Hamiltonians do not depend on the $x_0$ coordinate a candidate closed-loop contact form is given by

$$\theta_d = \theta + dF,$$

with $F(x, p)$ a function on $(x, p)$ only. In the canonical coordinates this is expressed as

$$\theta_d = \theta + dF = d(x_0 + F) - \sum_{i=1}^{n} p_i dx_i.$$

Hence the closed-loop contact form may be defined with respect to the new canonical coordinates

$$(x_0', x, p) = (x_0 + F, x, p).$$

For this closed-loop contact form the control law

$$\alpha(x_0, x, p) = \Phi' \circ K_c(x_0, x, p),$$

with $\Phi'$ a smooth function of $K_c(x_0, x, p)$, renders the closed-loop system a contact system with respect to the new contact form $\theta_d$. With respect to this new contact form the closed-loop contact vector field is generated by the closed-loop contact Hamiltonian

$$K = K_0 + \Phi \circ Kc, \tag{4.11}$$

where $\Phi'(\lambda) = \frac{\partial}{\partial \lambda}(\Phi(\lambda))$ (see Proposition 22, section 3.4, chapter 3). The closed-loop contact vector field may thus be analysed as the contact vector field generated by $K = K_0 + \Phi \circ Kc$ with respect to the new contact form $\theta_d$ with canonical coordinates $(x_0', x, p)$.

The closed-loop contact Hamiltonian does not depend on $x_0'$, hence Corollary 38 may be applied to characterize the closed-loop equilibrium points. We have the following conditions

$$\left.\frac{\partial K}{\partial p}\right|_{(x_0'^*, x^*, p^*)} = \left(\frac{\partial K_0}{\partial p} + \frac{\partial K_c}{\partial p}\frac{\partial \Phi}{\partial K_c}\right)_{(x_0'^*, x^*, p^*)} = 0, \tag{4.12}$$

$$K(x_0'^*, x^*, p^*) = K_0(x_0'^*, x^*, p^*) + \Phi \circ K_c(x_0'^*, x^*, p^*) = 0, \tag{4.13}$$

$$\left.\frac{\partial K}{\partial x}\right|_{(x_0'^*, x^*, p^*)} = \left(\frac{\partial K_0}{\partial x} + \frac{\partial K_c}{\partial x}\frac{\partial \Phi}{\partial K_c}\right)_{(x_0'^*, x^*, p^*)}. \tag{4.14}$$

Since $\left.\frac{\partial \Phi}{\partial K_c}\right|_{(x_0'^*, x^*, p^*)} = \Phi'(x_0'^*, x^*, p^*) = u^*(x^*, p^*)$, where $u^*(x^*, p^*)$ corresponds to the equilibrium input value for $(x^*, p^*)$, conditions (4.12) and (4.14) may be rewritten as

$$\left.\frac{\partial K}{\partial p}\right|_{(x_0'^*, x^*, p^*)} = \left(\frac{\partial K_0}{\partial p} + \frac{\partial K_c}{\partial p}u^*\right)_{(x_0'^*, x^*, p^*)} = 0, \tag{4.15}$$

$$\left.\frac{\partial K}{\partial x}\right|_{(x_0'^*, x^*, p^*)} = \left(\frac{\partial K_0}{\partial x} + \frac{\partial K_c}{\partial x}u^*\right)_{(x_0'^*, x^*, p^*)} = 0. \tag{4.16}$$

Since the closed-loop contact Hamiltonian does not depend on $x_0'$ Proposition 39 may be used to analyse local stability. The Jacobian $DX_K$ is given by

$$DX_K = \begin{bmatrix} 0 & -{p^*}^\top A_K & -{p^*}^\top B_K \\ 0 & -A_K & -B_K \\ 0 & C_K & A_K^\top \end{bmatrix} \tag{4.17}$$

with $A_K = \left(\frac{\partial^2 K}{\partial x \partial p} + \frac{\partial^2 K_c}{\partial x \partial p}\Phi'\right)_{(x_0'^*, x^*, p^*)}$, $B = B^\top = \left(\frac{\partial^2 K}{\partial p^2} + \frac{\partial^2 K_c}{\partial p^2}\Phi'\right)_{(x_0'^*, x^*, p^*)}$ and $C = C^\top = \left(\frac{\partial^2 K}{\partial x^2} + \frac{\partial^2 K_c}{\partial x^2}\Phi'\right)_{(x_0'^*, x^*, p^*)}$. $\frac{\partial K}{\partial x}(x_0'^*, x^*, p^*) = \frac{\partial K}{\partial p}(x_0'^*, x^*, p^*) = 0$ have been used from equations (4.15) and (4.16) to derive (4.17).

### 4.3.3 Relation with Hamiltonian system

The linearization of the strict contact vector field $DX_K$ may be split into several block matrices. More precisely, the lower right corner is composed by the square matrix

$$\begin{bmatrix} -A & -B \\ C & A^\top \end{bmatrix} \tag{4.18}$$

that corresponds to the linearisation of a Hamiltonian system [89]. To be more precise about this subject we recall some results on Hamiltonian systems.

Consider the cotangent bundle $T^*M$, of some $n$-dimensional manifold $M$, with symplectic form $\omega = \sum_{i=1}^{n} dp_i \wedge dx_i$. Let $H : T^*M \to \mathbb{R}$ be a smooth function, called Hamiltonian function. Then the Hamiltonian vector field $\mathfrak{X}_H$ on $T^*M$ corresponding to $H$ is defined by setting $\omega(\mathfrak{X}_H, Z) = -dH(Z)$ for every vector field $Z$ on $T^*M$. In canonical coordinates $(x, p)$ for $T^*M$ the Hamiltonian equations

$$\dot{x} = \frac{\partial H}{\partial p}(x,p), \quad \dot{p} = -\frac{\partial H}{\partial x}(x,p)$$

are obtained. The linearization of $\mathfrak{X}_H$ at $(x^*, p^*)$ is given by

$$D\mathfrak{X}_H = \mathcal{H} = \begin{bmatrix} \frac{\partial^2 H}{\partial x \partial p} & \frac{\partial^2 H}{\partial p^2} \\ -\frac{\partial^2 H}{\partial x^2} & \frac{\partial^2 H}{\partial p \partial x} \end{bmatrix}(x^*, p^*) = \begin{bmatrix} A_H & B_H \\ -C_H & -A_H^\top \end{bmatrix}$$

The matrix $\mathcal{H}$ is a Hamiltonian matrix since $\mathcal{H}^\top J + J\mathcal{H} = 0$, with $J$ the matrix $J = \left(\begin{smallmatrix} 0 & -I \\ I & 0 \end{smallmatrix}\right)$. The equilibrium point $(x^*, p^*)$ is called hyperbolic if $DX_K$ does not have purely imaginary eigenvalues. By the fact that $D\mathfrak{X}_H$ is Hamiltonian it follows that the eigenvalues of $D\mathfrak{X}_H$ are symmetrical with respect to the imaginary axis and that there exist a stable and an unstable stable $n$ dimensional invariant subspace [88, 89] for the Hamiltonian vector field.

**Proposition 40 ([88])** *Suppose $(x^*, p^*)$ is a hyperbolic equilibrium for $\mathfrak{X}_H$. Then there exists a unique maximal submanifold $N^- \subset T^*M$ through $(x^*, p^*)$, called the stable invariant submanifold, satisfying the following:*

1. *$N^-$ is invariant for $\mathfrak{X}_H$,*
2. *$\mathfrak{X}_H$ restricted to $N^-$ is globally asymptotically stable (with regard to $(x^*, p^*)$),*
3. *$N^-$ is tangent at $(x^*, p^*)$ to the stable eigenspace of $D\mathfrak{X}_H$.*

*Analogously, there exists a unique maximal submanifold $N^+ \subset T^*M$ through $(x^*, p^*)$, called the unstable invariant submanifold, satisfying the following:*

1. *$N^+$ is invariant for $\mathfrak{X}_H$,*
2. *$-\mathfrak{X}_H$ restricted to $N^+$ is globally asymptotically stable (with regard to $(x^*, p^*)$),*
3. *$N^+$ is tangent at $(x^*, p^*)$ to the unstable eigenspace of $D\mathfrak{X}_H$.*

**Proposition 41 ([87])** *Suppose $(x^*, p^*)$ is hyperbolic equilibrium of $\mathfrak{X}_H$. Then the stable and unstable invariant manifolds $N^-$ and $N^+$ are Lagrangian submanifolds.*

Propositions 40 and 41 suggest to use the "Hamiltonian like" part of the vector field to perform the control design. It would be convenient to characterize the stable Lagrangian submanifold of the Hamiltonian system defined by the $x, p$ coordinates of the contact vector field

$$\begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial K}{\partial x} \\ \frac{\partial K}{\partial p} \end{bmatrix}. \tag{4.19}$$

This Lagrangian submanifold may then be used to define an invariant Legendre submanifold for the contact system. Indeed since $N^-$ is of dimension $n$ it defines the following Legendre submanifold

$$\mathcal{L}_{N^-} = \left\{ x_0 = N^-(x) \quad x = x \quad p = \frac{\partial N^-}{\partial x}(x) \right\}.$$

We have not further developed this relation between the Lagrangian submanifold of the Hamiltonian part and Legendre submanifolds of the contact system, but it seems promising to consider this aspect in future work.

The previous results justify to study the stability of the contact vector field on the restriction to a (stable) invariant Legendre submanifold of the contact system as it has been performed in [30]. In [30] the conditions for local stability on a Legendre submanifold have been given for contact vector fields generated by a contact Hamiltonian function that depends or does not depend on $x_0$. We will only mention the particular case when the canonical coordinates of a Legendre submanifold $\mathcal{L}$ fulfils the relation

$$\mathcal{L} = \left\{ x_0 = U(x) \quad x = x \quad p = \frac{\partial U}{\partial x}(x) \right\}. \tag{4.20}$$

with $U(x)$ the generating function of $\mathcal{L}$. Then the local stability of the contact vector field on the restriction to $\mathcal{L}$ is simply determined by the location on the complex plane of the eigenvalues of the matrix

$$-\left( A + B \frac{\partial^2 U}{\partial x^2}(x_0^*, x^*, p^*) \right).$$

For conservative contact systems it follows from Proposition 37 that the equilibrium points are located on $\mathcal{L}$. Hence, as it has already been mentioned in [30], for lifted physical systems the equilibrium points of the contact vector field on the restriction to $\mathcal{L}$ coincides with the equilibrium points of the physical system.

Let us now analyse the stability of the closed-loop contact vector field on the restriction to an invariant Legendre submanifold of $\theta_d$. On the new canonical coordinate a class of invariant Legendre submanifold $\mathcal{L}_d$ fulfils the relation

$$\mathcal{L}_d = \left\{ x_0' = U_d(x) \quad x = x \quad p = \frac{\partial U_d}{\partial x}(x) \right\}. \tag{4.21}$$

with $U_d(x)$ the generating function of $\mathcal{L}_d$. The local stability of the closed-loop contact vector field on the restriction to $\mathcal{L}_d$ is simply determined by the location on the complex plane of the eigenvalues of the matrix [30]

$$-\left( A_K + B_K \frac{\partial^2 U_d}{\partial x^2}(x^*) \right).$$

### 4.3.4 Partial stability on a Legendre submanifold

In this subsection the conditions for the stability on the restriction to a Legendre submanifold $\mathcal{L}$ are developed. Let us first define the what we mean by partial stability on a Legendre submanifold.

**Definition 42** *Consider a contact manifold $(\mathcal{M}, \theta_d)$ and a set of canonical coordinates $(x'_0, x, p)$, a contact vector field $X = X_{K_0} + X_{K_c}\Phi'$, with strict contact Hamiltonian $K(x,p) = K_0(x,p) + \Phi \circ K_c(x,p)$, and a Legendre submanifold $\mathcal{L} \subset \mathcal{M}$ solution to the Pfaffian equation $\theta_d = 0$. Then, given an initial state $(x'_0(0), x(0), p(0)) \in \mathcal{L}$, the equilibrium state $(x'^*_0, x^*, p^*) \in \mathcal{L}$ of $X$ is partially asymptotically stable if there exists a constant $\delta > 0$ such that, if $\|(x'_0(0), x(0), p(0)) - (x'^*_0, x^*, p^*)\| < \delta$ then*

$$\lim_{t\to\infty} \|(x'_0(0), x(0), p(0)) - (x'^*_0, x^*, p^*)\| = 0$$

The previous definition just implies that a contact vector field is partially asymptotically stable, or shortly partially stable, if for any initial state on an invariant Legendre submanifold $\mathcal{L}$, the trajectories remain on $\mathcal{L}$ and converges to the equilibrium state $(x'^*_0, x^*, p^*) \in \mathcal{L}$. Lyapunov's direct method [46] may be used to establish the conditions for stability on an invariant Legendre submanifold. The Lyapunov function candidate should be constructed on the $n$ dimensional space where $\mathcal{L}$ is defined. On $\mathcal{L}$, it is only necessary to use $n$ variables to express the remaining $n+1$. Hence the Lyapunov function candidate may be defined in three different ways:

- $V(x,p) :\in \mathbb{R}^n \times \mathbb{R}^n \subset \mathcal{M} \to \mathbb{R}$, such that restricted to $\mathcal{L}$ it is a Lyapunov function,
- $V(x) :\in \mathbb{R}^n \subset \mathcal{M} \to \mathbb{R}$, such that if $p(x) = p|_{\mathcal{L}}$ it is a Lyapunov function, and
- $V(p) :\in \mathbb{R}^n \subset \mathcal{M} \to \mathbb{R}$, such that if $x(p) = x|_{\mathcal{L}}$ it is a Lyapunov function,

The following proposition and corollaries characterizes each one of the previous situations for the controlled contact system defined in chapter 3.

**Proposition 43** *Consider a contact manifold $(\mathcal{M}, \theta_d)$ and a set of canonical coordinates $(x'_0, x, p)$, a contact vector field $X = X_{K_0} + X_{K_c}\Phi'$, with strict contact Hamiltonian $K(x,p) = K_0(x,p) + \Phi \circ K_c(x,p)$, a Legendre submanifold $\mathcal{L} \subset \mathcal{M}$ solution to the Pfaffian equation $\theta_d = 0$, an initial state $(x'_0(0), x(0), p(0)) \in \mathcal{L}$ and the equilibrium state $(x'^*_0, x^*, p^*) \in \mathcal{L}$ of $X$. Let $V(x,p) : \mathcal{M} \to \mathbb{R}$ be a continuously differentiable function on $\mathcal{M}$ such that*

$$\begin{aligned} V(x^*, p^*) = 0 \quad \text{and} \quad V(x,p)|_{\mathcal{L}} > 0 \text{ in } \{\mathcal{L} - (x^*_0, x^*, p^*)\}, \\ \frac{dV}{dt} = \{K_0, V\}|_{\mathcal{L}} + \{K_c, V\}|_{\mathcal{L}}\Phi' \circ K_c|_{\mathcal{L}} < 0, \\ \forall (x_0, x, p)|_{\mathcal{L}} \in \{\mathcal{L} - (x^*_0, x^*, p^*)\}. \end{aligned}$$

*Then $(x_0, x, p) = (x^*_0, x^*, p^*)$ is asymptotically stable on $\mathcal{L}$.*

The following corollaries follows directly from the previous proposition.

**Corollary 44** *Let $V(x) : \mathcal{M} \to \mathbb{R}$ be a continuously differentiable function on $\mathcal{M}$ such that*

$$\begin{aligned} V(x^*) = 0 \quad \text{and} \quad V(x)|_{\mathcal{L}} > 0 \text{ in } \{\mathcal{L} - (x_0^*, x^*, p^*)\}, \\ \frac{dV}{dt} = -\left.\frac{\partial K_0}{\partial p}\frac{\partial V}{\partial x}\right|_{\mathcal{L}} - \left.\frac{\partial K_c}{\partial p}\frac{\partial V}{\partial x}\right|_{\mathcal{L}} \Phi' \circ K_c|_{\mathcal{L}} < 0, \\ \forall (x_0, x, p)|_{\mathcal{L}} \in \{\mathcal{L} - (x_0^*, x^*, p^*)\}. \end{aligned}$$

*Then $(x_0, x, p) = (x_0^*, x^*, p^*)$ is asymptotically stable on $\mathcal{L}$.*

**Corollary 45** *Let $V(p) : \mathcal{M} \to \mathbb{R}$ be a continuously differentiable function on $\mathcal{M}$ such that*

$$\begin{aligned} V(p^*) = 0 \quad \text{and} \quad V(p)|_{\mathcal{L}} > 0 \text{ in } \{\mathcal{L} - (x_0^*, x^*, p^*)\}, \\ \frac{dV}{dt} = \left.\frac{\partial K_0}{\partial x}\frac{\partial V}{\partial p}\right|_{\mathcal{L}} + \left.\frac{\partial K_c}{\partial x}\frac{\partial V}{\partial p}\right|_{\mathcal{L}} \Phi' \circ K_c|_{\mathcal{L}} < 0, \\ \forall (x_0, x, p)|_{\mathcal{L}} \in \{\mathcal{L} - (x_0^*, x^*, p^*)\}. \end{aligned}$$

*Then $(x_0, x, p) = (x_0^*, x^*, p^*)$ is asymptotically stable on $\mathcal{L}$.*

**Proof.** On the restriction to $\mathcal{L}$ the contact vector field leaves $\mathcal{L}$ invariant an only $n$ independent variables are required to characterize the dynamic of the system. Since $V(x,p)|_{\mathcal{L}} > 0$, $V$ qualifies as Lyapunov function candidate no matter the partition defining the Legendre submanifold (see theorem in [8, pp.367] for a local characterization of Legendre submanifolds). The derivative with respect to time of $V$ is given by

$$\frac{dV}{dt} = \{K, V\} = \{K_0 + \Phi \circ K_c, V\} = \{K_0, V\} + \{K_c, V\}\Phi' \tag{4.22}$$

since $\frac{\partial K}{\partial x_0'} = \frac{\partial K_c}{\partial x_0'} = 0$ and $\frac{\partial \Phi}{\partial K_c} = \Phi'$. Since $(x_0'(0), x(0), p(0)) \in \mathcal{L}$ and $\mathcal{L}$ is invariant the trajectories remain in $\mathcal{L}$. Thus if $\frac{dV}{dt}\big|_{\mathcal{L}} < 0$ for all $\{\mathcal{L} - (x_0^*, x^*, p^*)\}$ and $V(x^*, p^*) = 0$ the system is asymptotically stable on $\mathcal{L}$.

Corollaries 44 and 45 are proved by computing the Poisson brackets in (4.22) and replacing $\frac{\partial V}{\partial p} = 0$ and $\frac{\partial V}{\partial x} = 0$ respectively. ■

In the chapter 3 it has been shown that structure preserving feedback of a conservative contact systems leads to a closed-loop contact system with respect to a new contact form $\theta_d$. This implies that the open-loop invariant Legendre submanifold is not longer left invariant by the closed-loop contact vector field. The closed-loop contact vector field may however leave a *different* Legendre submanifold invariant. It is of interest is to characterize the stability of the closed-loop contact vector field on this invariant Legendre submanifold. This is analysed in the following subsection.

### 4.3.5 A class of Lyapunov functions for conservative contact systems

Let us consider the lift of the controlled dynamic system

$$\dot{x} = f(x) + g(x)u(t) \tag{4.23}$$

to the TPS as an affine controlled conservative contact system equipped with contact form $\theta$, with contact vector field

$$X = X_K + X_{K_c} u(t), \tag{4.24}$$

with contact Hamiltonian functions

$$K_0 = \left(\frac{\partial U}{\partial x}(x) - p\right)^\top f(x,p), \quad K_c = \left(\frac{\partial U}{\partial x}(x) - p\right)^\top g(x,p), \tag{4.25}$$

respectively. The contact Hamiltonian vector field leaves invariant the Legendre submanifold $\mathcal{L}_U$ defined in (4.20). Let us assume that the structure preserving feedback proposed in chapter 3 is applied to the system. The closed-loop system is then given by

$$X = X_K + X_{K_c}\Phi' = \hat{X}_K \tag{4.26}$$

equipped with contact form $\theta_d$ and with closed-loop contact Hamiltonian

$$K = K_0 + \Phi \circ K_c. \tag{4.27}$$

We are interested in study the stability on an invariant Legendre submanifold of $\hat{X}_K$. Let us denoted this Legendre submanifold by $\mathcal{L}_d$. We define the function

$$V(x,p) = \left(\frac{\partial U}{\partial x}(x) - p^*\right)^\top \left(\frac{\partial U}{\partial x}(x) - p^*\right) \tag{4.28}$$

We may use this function, that may be interpreted as a measure of distance to $\mathcal{L}_U$, as Lyapunov function candidate on $\mathcal{L}_d$.

**Proposition 46** *The closed-loop contact vector field $\hat{X}_K$ is partially stable on $\mathcal{L}_d$ and converges asymptotically to the point $p^* \subset \mathcal{L}_d$ if*

$$\left.\frac{\partial f}{\partial x}\right|_{\mathcal{L}_d} + \left.\frac{\partial f}{\partial p}\right|_{\mathcal{L}_d} \frac{\partial^2 U}{\partial x^2} + \left(\left.\frac{\partial g}{\partial x}\right|_{\mathcal{L}_d} + \left.\frac{\partial g}{\partial p}\right|_{\mathcal{L}_d} \frac{\partial^2 U}{\partial x^2}\right)\Phi'|_{\mathcal{L}_d} > 0. \tag{4.29}$$

**Proof.** The time derivative of (4.28) along $X = \hat{X}_K$ is given by

$$\begin{aligned}
\frac{dV}{dt} =& -\left(\frac{\partial K_0}{\partial x} + \frac{\partial K_c}{\partial x}\Phi'\right)\left(\frac{\partial U}{\partial x} - p^*\right) - \left(\frac{\partial K_0}{\partial p} + \frac{\partial K_c}{\partial p}\Phi'\right)\frac{\partial^2 U}{\partial x^2}\left(\frac{\partial U}{\partial x} - p^*\right), \\
=& -\left[\frac{\partial^2 U}{\partial x^2}\left(f + g\Phi'\right) + \left(\frac{\partial f}{\partial x} + \frac{\partial g}{\partial x}\Phi'\right)^\top \left(\frac{\partial U}{\partial x} - p^*\right)\right]\left(\frac{\partial U}{\partial x} - p^*\right) \\
& -\left[-(f + g\Phi') + \left(\frac{\partial f}{\partial p} + \frac{\partial g}{\partial p}\Phi'\right)^\top \left(\frac{\partial U}{\partial x} - p^*\right)\right]\frac{\partial^2 U}{\partial x^2}\left(\frac{\partial U}{\partial x} - p^*\right), \\
=& -\left(\frac{\partial U}{\partial x} - p^*\right)^\top \left[\frac{\partial f}{\partial x} + \frac{\partial f}{\partial p}\frac{\partial^2 U}{\partial x^2} + \left(\frac{\partial g}{\partial x} + \frac{\partial g}{\partial p}\frac{\partial^2 U}{\partial x^2}\right)\Phi'\right]\left(\frac{\partial U}{\partial x} - p^*\right).
\end{aligned}$$

By Proposition 43, $V$ defines a Lyapunov function candidate for the closed-loop system on the restriction to $\mathcal{L}_d$. Hence if condition (4.29) is satisfied then $X|_{\mathcal{L}_d} = \hat{X}_K|_{\mathcal{L}_d}$ is partially asymptotically stable. ■

It it is interesting to note that the stability condition is a "Jacobian" like condition on the $x$ and $p$ coordinates. If the the open-loop contact Hamiltonian functions are such that $f$ and $g$ do not depend on $p$, then the stability condition is simply given by

$$\left.\frac{\partial f}{\partial x}\right|_{\mathcal{L}_d} + \left.\frac{\partial g}{\partial x}\right|_{\mathcal{L}_d} \Phi'|_{\mathcal{L}_d} > 0.$$

These are the Jacobians of $f$ and $g$ in the original state variables ($x$ variables). Proposition 46 may be used to investigate the stability of a lifted dynamical system on an invariant Legendre submanifold of the closed-loop contact system.

In the following section we use the lift of dynamic systems to propose a control synthesis methodology for dynamic systems. Unlike the results presented until now the method does not aim to characterize a control for the lifted system, but for the dynamic system defining the lift. In this sense the approach may be understood as the interpretation of the stability conditions of controlled dynamic systems on a Legendre submanifold defining the thermodynamic properties of the system.

## 4.4 Using conservative contact system formalism for Lyapunov based control

In this section the framework of conservative contact system is used to interpret the control of dynamic systems by matching vector fields. Unlike the results of the previous sections the aim here is not to define a state feedback for the contact vector field, but for the dynamic system defining a lift on the TPS. The contact framework and the definition of invariant Legendre submanifolds is hence instrumental to characterize and physically interpret the stability conditions of a closed-loop dynamic system.

Recently in [37, 38] contact forms and Legendre transformations have been used to analyse interconnection of thermodynamic systems. It has been suggested to use the prolongation of a vector field defined on a Legendre submanifold to define a vector field, which is not a contact vector field, on the complete TPS. These results may be compared with the ones obtained in this section since the contact framework is instrumentally used to derive some matching equation and stability conditions for closed-loop dynamic systems. The contact vector field in this case is obtained by lifting a controlled dynamic system, hence it is indeed a contact vector field generated by a conservative contact Hamiltonian. The invariant Legendre submanifold is then used to characterize the conditions for partial stability of the contact vector field. This is of interest for thermodynamic systems since the control design may be performed using extensive and intensive variables as if they where independent variables. It is interesting to remark that the well known interconnection and damping assignment passivity based control approach (IDA-PBC) [65, 66] may be interpreted within its framework.

### 4.4.1 Interpreting the matching of vector fields

In this section we shall introduce the method by showing that the assignment of a closed-loop vector field amounts to equating closed-loop and desired contact Hamiltonian by lift into some contact manifold. Therefore let us first define a lift of a nonlinear system into an extended space endowed with a contact structure. Consider a nonlinear control system described by the state equation

$$\dot{x} = f(x) + g(x)u(t), \tag{4.30}$$

For the control design we shall consider the lift of the control system (4.30) to the control contact vector system (on the TPS) generated by the contact Hamiltonian

$$K(x,p) = \left(\frac{\partial U}{\partial x}(x) - p\right)^{\top} (f(x) + g(x)u(t)) \,. \tag{4.31}$$

The contact Hamiltonian (4.31) is affine in the input, hence may be written as

$$K(x_0,x,p) = K_0(x_0,x,p) + K_c(x_0,x,p)u(t) \tag{4.32}$$

Consider now the control objective is to achieve a desired closed-loop system $\dot{x} = f_d(x)$ by state feedback. In this section we suggest to solve this problem in the TPS, by using the function $\alpha(x_0,x,p)$, to match the following closed-loop contact Hamiltonian function

$$K(x_0,x,p) + K_c(x_0,x,p)\alpha(x_0,x,p) = K_d(x_0,x,p). \tag{4.33}$$

**Remark 47** *This is different than considering the control contact vector field generated by (4.32) and matching it by feedback to the vector field generated by $K_d$. Indeed it has been showed (Proposition 14, section 3.3, chapter 3) that*

$$\Omega^{-1}\left(K_0(x_0,x,p) + K_c(x_0,x,p)\alpha(x_0,x,p)\right) = \\ \Omega^{-1}\left(K_0(x_0,x,p)\right) + \alpha(x_0,x,p)\Omega\left(K_c(x_0,x,p)\right)$$

*if and only if $\alpha(x_0,x,p)$ is a constant function.*

Using the same lift of the desired closed-loop vector field $f_d$, one defines the target contact Hamiltonian $K_d$:

$$K_d(x,p) = \left(\frac{\partial U}{\partial x}(x) - p\right)^{\top} f_d(x). \tag{4.34}$$

Using the fact that the contact Hamiltonian are all linear in $p$, it is evident that equating the contact Hamiltonians (4.31) and (4.34) on the whole TPS is equivalent to equating the contact vector fields. One obtains the control law $u = \alpha(x)$,

$$\alpha(x) = g^{\dagger}(x)(f_d(x) - f(x))$$

where $g^\dagger(x) \in \mathbb{R}^m \times \mathbb{R}^n$ is the pseudo inverse of $g(x)$, with the condition that

$$g^\perp(x)(f_d(x) - f(x)) = 0, \tag{4.35}$$

where $g^\perp(x) = I_n - g(x)g^\dagger(x)$ is a left hand full rank annihilator of $g(x)$. The previous condition is a trivial matching condition when a controlled vector field is made equal to a desired one.

Using the lift (4.31), matching contact Hamiltonians is equivalent to matching vector fields. However, using other lifts, it is possible to define both vector fields in terms of all the coordinates of the TPS as $n$ dimensional vector fields $f(x_0, x, p)$ and $f_d(x_0, x, p)$ respectively *parametrized* by $p$ and $x_0$. Hence by lift of the system in the extended space the matching condition may be stated as

$$g^\perp(x_0, x, p)(f_d(x_0, x, p) - f(x_0, x, p)) = 0. \tag{4.36}$$

This equation should be solved over the whole TPS, hence the matching condition is with respect to $2n+1$ independent variables instead of $n$. However when restricted to the Legendre submanifold $\mathcal{L}_U$, all the functions become function of $x$ only; this might also be seen as a sort of feedback (defined by the restriction on the Legendre submanifold) on the parametrized vector fields.

### 4.4.2 Stability of the closed-loop system

The stability of the closed-system should be addressed considering that the control design has been developed in the $2n+1$ dimensional TPS, but the initial condition and the time evolution of the closed-loop system are in a $n$ dimensional manifold given by the restriction of the contact vector field to a Legendre submanifold. Moreover, we know from the discussion of the preceding sections that stability of strict contact vector fields is only meaningful on the restriction to a Legendre submanifold. Hence, the stabilization can be stated as a problem of partial stability on the Legendre submanifold of interest. Even though the stability analysis follows the same reasoning as the stabilization of conservative contact system on some Legendre submanifold presented in subsection 4.3.5, it differs since in this case the interest is to stabilise the closed-loop system on the same Legendre submanifold as with respect the the lift has been defined. The stability conditions follows then from Proposition 43. Let us consider a differentiable function $V(x,p) : \mathcal{M} \to \mathbb{R}$. Its time derivative along the trajectories of the closed-loop system is given by

$$\frac{dV}{dt} = \{K_d, V\} = \frac{\partial V}{\partial p}^\top \frac{\partial K_d}{\partial x} - \frac{\partial V}{\partial x}^\top \frac{\partial K_d}{\partial p}. \tag{4.37}$$

Now, consider the lift of a desired parametrized $n$ dimensional vector field $f_d(x,p)$ in the TPS, $K_d = \left(\frac{\partial U}{\partial x}(x) - p\right)^\top f_d(x,p)$, equation (4.37) becomes

$$\frac{dV}{dt} = \frac{\partial V}{\partial p}^\top \left[\frac{\partial^2 U}{\partial x^2}^\top f_d + \frac{\partial f_d}{\partial x}^\top \left(\frac{\partial U}{\partial x} - p\right)\right] - \frac{\partial V}{\partial x}^\top \left[-f_d + \frac{\partial f_d}{\partial p}^\top \left(\frac{\partial U}{\partial x} - p\right)\right].$$

On $\mathcal{L}_U$ this equation reduces to

$$\frac{dV}{dt}(x,p)\bigg|_{p=\frac{\partial U}{\partial x}} = \left(\frac{\partial^2 U}{\partial x^2}(x)\frac{\partial V}{\partial p}(x,p) + \frac{\partial V}{\partial x}(x,p)\right)^\top f_d(x,p)\bigg|_{p=\frac{\partial U}{\partial x}}. \tag{4.38}$$

The control design method is stated as follows.

**Proposition 48** *Consider a dynamic system*

$$\dot{x} = f\left(x, \tfrac{\partial U}{\partial x}(x)\right) + g\left(x, \tfrac{\partial U}{\partial x}(x)\right) u(t) \tag{4.39}$$

*and the conservative contact Hamiltonian defined as the lift of a parametrized vector field $f(x,p) + g(x,p)u(t)$,*

$$K(x,p) = \left(\frac{\partial U}{\partial x}(x) - p\right)^\top (f(x,p) + g(x,p)u(t)) \tag{4.40}$$

*such that the restriction of the vector field generated by (4.40) on $\mathcal{L}_U$ generates (4.39). Consider the target dynamic*

$$\dot{x} = f_d(x) \tag{4.41}$$

*and the conservative contact Hamiltonian defined as the lift of a parametrized vector field $f_d(x,p)$,*

$$K_d(x,p) = \left(\frac{\partial U}{\partial x}(x) - p\right)^\top f_d(x,p) \tag{4.42}$$

*such that the restriction of the vector field generated by (4.42) on $\mathcal{L}_U$ generates (4.41) and verifies the PDE*

$$g^\perp(x,p)\left(f_d(x,p) - f(x,p)\right) = 0. \tag{4.43}$$

*Consider an equilibrium state $(x_0^*, x^*, p^*) \in \mathcal{L}_U \subset \mathcal{M}$ of $X_{K_d}$. Let $V(x,p) : \mathcal{M} \to \mathbb{R}$ be a continuously differentiable function on $\mathcal{M}$ such that $V(x^*,p^*) = 0$ and $V(x,p)|_{\mathcal{L}_U} > 0$ in $\{\mathcal{L}_U - (x_0^*, x^*, p^*)\}$, $\frac{dV}{dt}|_{\mathcal{L}_U} = \{K_d, V\}|_{\mathcal{L}_U} < 0$ for all $(x_0, x, p)|_{\mathcal{L}_U} \in \{\mathcal{L}_U - (x_0^*, x^*, p^*)\}$. Then the feedback law*

$$\alpha(x,p) = g^\dagger(x,p)\left(f_d(x,p) - f(x,p)\right)\big|_{p=\frac{\partial U}{\partial x}} \tag{4.44}$$

*stabilises asymptotically the point $(x_0, x, p) = (x_0^*, x^*, p^*)$ on $\mathcal{L}_U$.*

**Proof.** From the expression of the contact vector field in canonical coordinates (3.3) the dynamic of the $x$-coordinate generated on the TPS by the contact Hamiltonian (4.40) is

$$\dot{x} = f(x,p) + g(x,p)u(t) - \left[\frac{\partial}{\partial p}\left(f(x,p) + g(x,p)u(t)\right)\right]^\top \left(\frac{\partial U}{\partial x}(x) - p\right),$$

restricted to $\mathcal{L}_U$ (4.39) is obtained and same observation applies for the closed-loop contact Hamiltonian. Equation (4.43) and (4.44) follow directly from Proposition 11 and equation (4.33). Since $K$ does not depend on $x_0$, $K(x^*,p^*) = 0$, $p^* = \frac{\partial U}{\partial x}(x^*)$, $(x^*,p^*) \in \mathcal{L}_U$ and is also an equilibrium of (4.39). Finally, since $\left(x(0), p(0) = \frac{\partial U}{\partial x}(0)\right) \in \mathcal{L}_U$, by Proposition 43 $V(x,p)\big|_{p=\frac{\partial U}{\partial x}}$ qualifies as Lyapunov function for (4.41). ■

### 4.4.3 Control of PHS and IPHS

Following the preceding construction the lift of the PHS into the TPS is defined by the contact Hamiltonian:

$$K(x,p) = \left(\frac{\partial U}{\partial x} - p\right)^{\top} \left(J(x)\frac{\partial U}{\partial x}(x) + g(x)u(t)\right) = \\ - p^{\top} J(x)\frac{\partial U}{\partial x}(x) + \left(\frac{\partial U}{\partial x}(x) - p\right)^{\top} g(x)u(t), \quad (4.45)$$

with $K_0(x,p) = -p^{\top} J(x)\frac{\partial U}{\partial x}(x)$ and $K_c(x,p) = \left(\frac{\partial U}{\partial x}(x) - p\right)^{\top} g(x)$. Note that with this choice of lift, if the Hamiltonian $U$ has the dimension of energy, the contact Hamiltonian $K$ has the dimension of power and may be interpreted as the virtual work in variational calculus in Mechanics [21].

Consider that the closed-loop objective is to modify the Hamiltonian function. The target PHS is then given by

$$f_d(x) = J(x)\frac{\partial U_d}{\partial x}(x). \quad (4.46)$$

In this case the only term modified is the Hamiltonian function: $U_d(x) = U(x) + U_a(x)$ where $U_a(x)$ is the added Hamiltonian function and the control law $u = \alpha$ is given by

$$\alpha(x) = g^{\dagger}(x)J(x)\frac{\partial U_a}{\partial x}(x).$$

where the added potential $U_a$ should satisfy the matching condition (4.35), the PDE

$$g^{\perp}(x)J(x)\frac{\partial U_a}{\partial x}(x) = 0, \quad (4.47)$$

which is a particular case the IDA-PBC method [66, 61].

The lift of an IPHS on the TPS may be performed as discussed in chapter 2. If the objective is to modify the Hamiltonian, keeping invariant the structure matrix, the following target vector field is considered

$$f_d(x) = R\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right) J\frac{\partial U_d}{\partial x}(x).$$

The lift of $f_d(x)$ renders the following matching condition

$$g^{\perp}\left(x, \tfrac{\partial U}{\partial x}(x)\right) R\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right) J\frac{\partial U_a}{\partial x}(x) = 0. \quad (4.48)$$

The lift of the open-loop system can also be done considering a parametrized vector field that on $\mathcal{L}_U$ is equal to $f\left(x, \frac{\partial U}{\partial x}(x)\right)$

$$f(x,p) = R\left(x,p\right) J\frac{\partial U}{\partial x}(x) + g\left(x,p\right) u(t) \\ f(x,p)\big|_{p=\frac{\partial U}{\partial x}} = f\left(x, \tfrac{\partial U}{\partial x}(x)\right).$$

The matching condition is then parametrized by $p$ and given by

$$g^{\perp}(x,p)R\left(x,p\right)J\frac{\partial U_a}{\partial x}(x)=0. \tag{4.49}$$

In equation (4.49) the structure matrix and input map are parametrized by the co-state variable $p$. Thus if $U(x)$ is a nonlinear function of the states and (implicitly) the co-states, it will in general be easier to solve the matching equation on the TPS (where $p$ and $x$ are independent variables) than over the restriction on $\mathcal{L}_U$ where $p=\frac{\partial U}{\partial x}$. On $\mathcal{L}_U$ the matching condition is given by (4.48). The target vector may of course have a different form. In particular a target vector field

$$f_d(x)=R_d\left(x,\tfrac{\partial U_d}{\partial x},\tfrac{\partial S_d}{\partial x}\right)J_d\frac{\partial U_d}{\partial x}(x).$$

modifies both the energy and the structure as a function of the desired energy. In the sequel we will consider a more general definition of the target vector field given by

$$f_d(x,p)=M\left(x,p\right)\frac{\partial U_d}{\partial x}(x,p),$$

where $M\in\mathbb{R}^n\times\mathbb{R}^n$ is a control design matrix. Equation (4.38) then becomes

$$\left.\frac{dV}{dt}(x,p)\right|_{p=\frac{\partial U}{\partial x}}=\left(\frac{\partial^2 U}{\partial x^2}(x)\frac{\partial V}{\partial p}(x,p)+\frac{\partial V}{\partial x}(x,p)\right)^{\top}M(x,p)\left.\frac{\partial U_d}{\partial x}(x,p)\right|_{p=\frac{\partial U}{\partial x}}.$$

If additionally $U_d(x,p)=V(x,p)$, the previous equation may be rewritten as

$$\left.\frac{dU_d}{dt}(x,p)\right|_{p=\frac{\partial U}{\partial x}}= \left(\frac{\partial^2 U}{\partial x^2}(x)\frac{\partial U_d}{\partial p}(x,p)+\frac{\partial U_d}{\partial x}(x,p)\right)^{\top}M(x,p)\left.\frac{\partial U_d}{\partial x}(x,p)\right|_{p=\frac{\partial U}{\partial x}}, \tag{4.50}$$

and Proposition 48 may be restated in terms of $U_d(x,p)$ replacing (4.38) by (4.50). The relation with the usual IDA-PBC can be made by considering the target dynamic defined as: $f_d(x)=M(x)\frac{\partial U_d}{\partial x}(x)$, i.e. depending only in $x$. Then applying Proposition 48 leads to the following corollary.

**Corollary 49** *If the open-loop control contact Hamiltonian is chosen as the lift of a vector field depending only on the x-coordinate, $f(x)$ and $g(x)$, the target dynamic chosen as a dissipative PHS, $f_d(x)=M(x)\frac{\partial U_d}{\partial x}(x)$, $M(x)=J(x)-R(x)$, where $R(x)=R(x)^{\top}>0$, and $V$ as the desired Hamiltonian, $V=U_d(x)$ then (4.50) reduces to $\dot{U}_d(x)=-\frac{\partial U_d}{\partial x}^{\top}(x)R(x)\frac{\partial U_d}{\partial x}(x)<0$, and the matching condition to*

$$g^{\perp}(x)\left(M(x)\frac{\partial U_d}{\partial x}(x)-f(x)\right)=0.$$

Hence the IDA-PBC design procedure is obtained. In a similar manner the open-loop contact Hamiltonian may be immersed in the TPS as the parametrized vector field $f_d(x,p) = M(x,p)\frac{\partial U_d}{\partial p}$. In this case the target dynamic is given by the gradient of $U_d(x,p)$ with respect to the co-energy variables $p$. This leads to consider the following corollary.

**Corollary 50** *If the open-loop drift vector field and input map are immersed in the TPS as parametrized vector fields $f(x,p)$ and $g(x,p)$ respectively, the target system chosen as the parametrized vector field $f_d(x,p) = M(x,p)\frac{\partial U_d}{\partial p}(p)$ and $V(x,p) = U_d(p)$. Then equation (4.38) is given by*

$$\frac{dU_d}{dt}(x,p)\Big|_{p=\frac{\partial U}{\partial x}} = \frac{\partial U_d}{\partial p}^{\top}(p)\frac{\partial^2 U}{\partial x^2}^{\top} M(x,p)\frac{\partial U_d}{\partial p}(p)\Big|_{p=\frac{\partial U}{\partial x}}, \tag{4.51}$$

*and the matching condition is*

$$g^{\perp}(x,p)\left(M(x,p)\frac{\partial U_d}{\partial p}(p) - f(x,p)\right) = 0.$$

*The stability is ensured provided that $\frac{\partial^2 U}{\partial x^2}^{\top} M\left(x, \frac{\partial U}{\partial x}\right) < 0$.*

In Corollary 50 the matching and the stability condition are given in terms of the co-states ($p$ coordinates) and the generating function of the Legendre submanifold. In the case of thermodynamic systems the invariant Legendre submanifold is defined by the thermodynamic properties of the system. Corollary 49 and 50 show that the design procedure can be stated in terms of the state variables $x$ of the original vector field $f(x)$, in terms of the co-state variables $p$ or as a combination of both (note the relation with Proposition 43) and Corollaries 44 and 45). Corollary 50 also shows that using the co-state variables $p$ in the control design the Hessian of the generating function of the Legendre submamifold, $\frac{\partial^2 U}{\partial x^2}$, has to be taken into account to assure the stability of the system. This allows to take for instance the intensive variables of a thermodynamic system as independent variables to solve the matching equation (4.43), and take into account the relation with the extensive variable through matrix $\frac{\partial^2 U}{\partial x^2}$ (defined by the thermodynamic properties) to assure stability.

### 4.4.4 Example: the heat exchanger

Consider two simple thermodynamic systems, indexed by 1 and 2 (for instance two ideal gases), which may interact only through a heat flow through a conducting wall. The dynamic of this system is described by the following IPHS

$$\begin{bmatrix}\dot{S}_1\\ \dot{S}_2\end{bmatrix} = \lambda\left(\frac{1}{\frac{\partial U}{\partial S_2}} - \frac{1}{\frac{\partial U}{\partial S_1}}\right)\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}\begin{bmatrix}\frac{\partial U}{\partial S_1}\\ \frac{\partial U}{\partial S_2}\end{bmatrix} + \begin{bmatrix}0\\ u\end{bmatrix} = f(x,u)$$

where $x = [S_1, S_2]$ is the entropy of subsystem 1 and 2, $U(S_1,S_2) = U_1(S_1)+U_2(S_2)$ is the internal energy of the overall system composed of the addition of the internal

energies of each subsystem, $u(t)$ the controlled input that corresponds to an entropy flow, and $\lambda > 0$ denotes Fourier's heat conduction coefficient. Remark that $\frac{\partial U}{\partial S_i} = T_i(S_i)$ and $g^\perp = [1, 0]$ is an annihilator for the input map. The temperature is modelled as an exponential function of the entropy $T_i(S_i) = T_0 e^{\frac{S_i}{C_{vi}}}$ [14], where the constants $T_0$, $C_{v1}$ and $C_{v2}$ are respectively a reference temperature and the calorific capacitance of subsystem 1 and 2. This system has been widely studied from a modelling perspective using the contact Hamiltonian framework in [22]. There are infinite possibilities to immerse this system in the TPS [30], however to illustrate the use of the co-state variables $p$ in the control design the lift is performed as

$$K(x,p) = \left(\frac{\partial U}{\partial x} - p\right)^\top f(p,u) = \left(\begin{bmatrix}\frac{\partial U}{\partial x_1}\\ \frac{\partial U}{\partial x_2}\end{bmatrix} - \begin{bmatrix}p_1\\ p_2\end{bmatrix}\right)^\top \left[\lambda\left(\frac{1}{p_2} - \frac{1}{p_1}\right)\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}\begin{bmatrix}p_1\\ p_2\end{bmatrix} + \begin{bmatrix}0\\ u\end{bmatrix}\right].$$

By choosing the target dynamic as the parametrized vector field

$$f_d(x,p) = \underbrace{\begin{bmatrix}m_{11} & m_{12}\\ m_{21} & m_{22}\end{bmatrix}}_{M}\begin{bmatrix}\frac{\partial U_d}{\partial p_1}\\ \frac{\partial U_d}{\partial p_2}\end{bmatrix},$$

with $m_{ij}$, $i, j \in \{1, 2\}$ to be determined, and immerse it in the TPS with respect to $\mathcal{L}_U$, the matching condition is

$$m_{11}\frac{\partial U_d}{\partial p_1} + m_{12}\frac{\partial U_d}{\partial p_2} + \lambda\mathcal{R}(p)p_2 = 0 \tag{4.52}$$

where $\mathcal{R}(p) = \frac{p_1 - p_2}{p_1 p_2}$. If $U_d$ is chosen as a quadratic function dependent only on the $p$-coordinate, $U_d(p) = \sum_{i=1}^{2}\frac{1}{2}(p_i - p_i^*)^2$, the previous equation becomes

$$m_{11}(p_1 - p_1^*) + m_{12}(p_2 - p_2^*) + \lambda\mathcal{R}(p)p_2 = 0.$$

By selecting $m_{11} = -\frac{\lambda}{p_1}$ and $m_{12} = \frac{\lambda}{p_1}$ and noting that in equilibrium $p_1^* = p_2^*$ the matching condition is solved. In order to achieve stability (4.51) must be negative, implying that $\frac{\partial^2 U}{\partial x^2}^\top M(x,p)\big|_{p=\frac{\partial U}{\partial x}} < 0$. The matrix $\frac{\partial^2 U}{\partial x^2}$ is defined by the thermodynamic properties of the system and in this case given by

$$\frac{\partial^2 U}{\partial x^2} = \begin{bmatrix}\frac{T_1(x_1)}{C_{v1}} & 0\\ 0 & \frac{T_2(x_2)}{C_{v2}}\end{bmatrix}.$$

Selecting $m_{21} = -m_{12}\frac{C_{v2}}{C_{v1}}\frac{p_1}{p_2}$ and $m_{22}(x,p)$ as a positive definite smooth function

$$\frac{\partial^2 U}{\partial x^2}^\top M(x,p)\big|_{p=\frac{\partial U}{\partial x}} = -\lambda\begin{bmatrix}\frac{1}{C_{v1}} & -\frac{1}{C_{v1}}\\ \frac{1}{C_{v1}} & \frac{T_2(x_2)}{C_{v2}}m_{22}\end{bmatrix} < 0. \tag{4.53}$$

Finally the feedback law is given by (4.44) and by Corollary 50 the closed-loop system is stable and given by the IPHS

$$\begin{bmatrix}\dot{S}\\ \dot{S}\end{bmatrix} = -\begin{bmatrix}\frac{1}{T_1(S_1)} & -\frac{1}{T_1(S_1)}\\ \frac{C_{v2}}{C_{v1}T_2(S_2)} & m_{22}\end{bmatrix}\begin{bmatrix}T_1(S_1) - T_1^*\\ T_2(S_2) - T_2^*\end{bmatrix}.$$

Despite that the system model is on the dynamic of the extensive variables $x$, the control design has been made entirely in the intensive variables $p$, recovering the relation $p = \frac{\partial U}{\partial x}(x)$ only in (4.53) (hence $p$ may be viewed as a state feedback) simplifying the solution of (4.52). The same control law could have been obtained by using IDA-PBC, however in that case the Lyapunov function is not quadratic, but an exponential-quadratic function due to the exponential relation between temperature and entropy, and hence the matching equation is more involved.

## 4.5 Conclusion

The local and partial stability properties of controlled contact systems have been addressed and characterized for strict contact vector fields. A local analysis based on linearisation techniques shows that the Jacobian matrix evaluated at an equilibrium point possesses one eigenvalue at zero, associated with the $x_0$ coordinate, and $2n$ symmetric eigenvalues with respect to the imaginary axis, associated with the $x, p$ coordinates (Proposition 39). Hence, in general there are always $n$ unstable eigenvalues and global stability is not possible. This suggest to look for partially stable submanifolds. In the structure of the Jacobian matrix we find that the block matrix associated to the $x, p$ coordinates may be identified with the linearisation of a Hamiltonian vector field. It is well known that a set of invariant submanifold for a Hamiltonian vector field is composed of a stable and unstable Lagrangian submanifold. This suggest to study the *partial* stability of the contact vector field on the subspace characterized by the stable Lagrangian submanifold. Furthermore, the stable Lagrangian submanifold defines a Legendre submanifold for the contact vector field.

Since strict contact vector fields may only be partially stable on some subspace, Lyapunov's direct method has been used to characterize the conditions for stability on an invariant Legendre submanifold. On the Legendre submanifold the contact vector field may be expressed using only $n$ independent variables, hence the Lyapunov function should be defined with respect to $n$ variables that are independent on the Legendre submanifold. This means that the Lyapunov function may be function of $x$,$p$ or a combination of $x$ and $p$ (Proposition 43, Corollaries 44 and 45).

For conservative contact systems defined by the lift of a vector field we have been more specific. A class of Lyapunov function that may be interpreted as the distance of the open-loop Legendre submanifold to a point of the closed-loop Legendre submanifold has been proposed. The condition for stability is parametrized by the Jacobian of the *lifted* closed-loop vector field restricted to the closed-loop invariant Legendre submanifold (Proposition 46).

Finally the framework of conservative contact systems has been used to interpret the matching condition of vector fields and the stability properties of controlled dynamic systems. This has been done by matching the contact Hamiltonian function generated by the lift of an open-loop controlled vector field with a desired contact Hamiltonian function defined by the lift of a target vector field. The lifts have been performed with respect to the same Legendre submanifold hence the control design reduces to a relaxed matching condition and a characterization of the stability

conditions in terms of the Legendre submanifold that defines the lift (Proposition 48). Furthermore IDA-PBC may be interpreted within this approach (Corollary 49).

# Chapter 5

# Conclusion

## 5.1 General conclusion

This Thesis has proposed a modelling and control approach for thermodynamic processes using the framework of port Hamiltonian (PHS) and contact systems.

In Chapter 2 a class dynamic system has been defined and called irreversible PHS (Definition 1). This class of dynamic system is an extension of PHS since it shares some key features: It is defined by a structure matrix that maps the interconnection (internal structure network) of the system and a Hamiltonian function that for physical system corresponds to the total energy of the system. Additionally IPHS includes as a necessary condition for its definition the existence of an entropy like function, that is expressed through a non-linear relation of states and co-states. It has been shown that the IPHS encompasses a large set of thermodynamic systems, including heat exchangers and continuous stirred tank reactors (CSTR) (Proposition 5). For thermodynamic processes the irreversible entropy production is expressed by positive definite function and by a Poisson bracket defined by the structure matrix of the system evaluated on the entropy and the energy.

The IPHS has been used to define a class of conservative contact systems. The regularity of the lift has been discussed and a constructive method to perform the lift has been suggested. The proposed modelling approach has been illustrated with details on the CSTR. IPHS and contact Hamiltonian representations for the model of the CSTR have been proposed (Propositions 5, 6 and 7) and physical interpretations of the systems have been provided.

In Chapter 3 structure preserving state feedback of controlled contact systems has been studied. It has been shown that the only feedback that preserves the canonical contact form is the constant feedback (Proposition 14). Hence, the closed-loop system may be render a contact system only with respect to a new contact form. The conditions for the existence of a new contact structure and a state feedback have been derived. Furthermore, for strict contact systems these conditions have been developed assuming a specific closed-loop contact form (Proposition 18). For strict contact systems the closed-loop contact system has been characterized for a class of state feedback in terms of a matching equation (Proposition 22). The

expressions for the closed-loop contact vector field and contact Hamiltonian have also been given.

Structure preserving feedback of contact system may be related with structure preserving feedback of input-output Hamiltonian systems. It has been shown that the expression of the closed-loop contact Hamiltonian function has the same form as the expression of the closed-loop Hamiltonian function. The difference between the structure preserving feedback of these systems is that for the closed-loop contact system the geometry is changed since the closed-loop contact form is different to the open-loop contact form. On other for Hamiltonian system the closed-loop system is still equipped with a symplectic form. The relation with input-output Hamiltonian systems has motivated the definition of a natural output (Definition 25) for controlled contact systems.

It has been shown that the study of closed-loop invariant Legendre submanifolds is of special interest since the closed-loop contact system is defined with respect to a different contact form than the canonical contact form. Hence the open-loop invariant Legendre submanifolds are no longer invariant Legendre submanifolds for the closed-loop contact vector field. The conditions for the existence of invariant Legendre submanifolds for the closed-loop contact system have been given and specialized for the case of lifted IPHS (Propositions 30 and 31). The closed-loop invariant Legendre submanifold has then been used to parametrize the state feedback and closed-loop contact form.

In Chapter 4 the local and partial stability properties of controlled contact systems have been addressed. For strict contact vector fields a local analysis shows that the linearised system possesses one eigenvalue in the imaginary axis, associated with the $x_0$ coordinate, and $2n$ symmetric eigenvalues with respect to the imaginary axis, associated with the $x, p$ coordinates (Proposition 39). Hence, in general there are always $n$ unstable eigenvalues and global stability is not possible. This suggest to look for partially stable subspaces and justifies from a stability point of view the study of closed-loop invariant Legendre submanifolds (Propositions 30 and 31). Actually, embedded in the structure we find a Hamiltonian vector field, thus the stable and unstable subspaces may be related with Lagrangian submanifolds of the embedded Hamiltonian system. Furthermore, the stable Lagrangian submanifold may be use to define an invariant Legendre submanifold for the contact vector field.

Lyapunov's direct method has been used to characterize the conditions for partial stability of strict contact vector fields. This has been performed by analysing the stability conditions of the vector field on an invariant Legendre submanifold (Proposition 43, Corollaries 44 and 45). For conservative contact systems defined by the lift o a $n$ dimensional dynamic system a class of Lyapunov function that may be interpreted as the distance of the open-loop Legendre submanifold to a point of the closed-loop Legendre submanifold has been proposed. The condition for stability on the closed-loop Legendre submanifold is parametrized by the Jacobian of the lifted closed-loop vector field restricted to the closed-loop invariant Legendre submanifold (Proposition 46).

In Chapter 4 an approach that uses the framework of conservative contact systems to synthesis control laws on a Legendre submanifold has been proposed. The approach does not involve structure preserving feedback of contact system, but

rather uses the contact Hamiltonian framework to interpret the stability conditions. The methodology consists in comparing the lifts of an open-loop vector field with the lift of a controlled vector field subject to a state feedback (Proposition 48). An interesting remark is that IDA-PBC may be interpreted within this approach (Proposition 49).

## 5.2 Future research

The results of this Thesis are only a grain of sand for the understanding of controlled contact systems. They are also the opening of many interesting research problems. Among the most important is the study of the system dynamic properties of contact systems, like local, global and partial stability. In this line the characterisation of the dynamic properties by embedding the contact systems into symplectic Hamiltonian systems with homogeneous Hamiltonian function [48] seems interesting. Another aspect that remains to be studied, that is of great importance for control purposes, is the study of the system theoretic properties of general (non conservative) contact control systems (controllability, observability, etc.,). It is also of practical interest to extend the developed results to the multi-input case. In that case we expect some integrability conditions to pop up in the matching equations. In the same line we are interested in applying the control design to practical examples, like the CSTR with multiple equilibria and other irreversible thermodynamic control systems.

Another aspect of this work that seems interesting to further develop is the use of IPHS for control purposes. The particular structure of IPHS and its clear thermodynamic interpretation should indeed be of practical use for the synthesis of passivity based controllers for irreversible thermodynamic processes.

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