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AN EXTENSION OF HAMILTONIAN SYSTEMS TO THE THERMODYNAMIC PHASE SPACE: TOWARDS A GEOMETRY OF NONREVERSIBLE PROCESSES

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It is shown that the intrinsic geometry associated with equilibrium thermodynamics, namely the contact geometry, provides also a suitable framework in order to deal with irreversible thermodynamical processes. Therefore we introduce a class of dynamical systems on contact manifolds, called *conservative contact systems*, defined as contact vector fields generated by some contact Hamiltonian function satisfying a compatibility condition with some Legendre submanifold of the contact manifold. Considering physical systems' modeling, the Legendre submanifold corresponds to the definition of the thermodynamical properties of the system and the contact Hamiltonian function corresponds to the definition of some irreversible processes taking place in the system. Open thermodynamical systems may also be modeled by augmenting the conservative contact systems with some input and output variables (in the sense of automatic control) and so-called input vector fields and lead to the definition of *port contact systems*. Finally complex systems consisting of coupled simple thermodynamical or mechanical systems may be represented by the *composition* of such port contact systems through algebraic relations called interconnection structure. Two examples illustrate this composition of contact systems: a gas under a piston submitted to some external force and the conduction of heat between two media with external thermostat.

Keywords: irreversible thermodynamics, contact structure, Hamiltonian systems.

1. Introduction

Hamiltonian systems are defined by two objects: firstly their geometric structure (symplectic or pseudo-Poisson bracket and Dirac structure) which amounts to define some skew-symmetric tensor fields on the state space, and secondly a generating

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function, called Hamiltonian function. This geometric structure characterizes fundamental properties of physical systems stemming from variational formulations, the existence of symmetries or constraints [1, 20, 6, 9, 3], or the topological interconnection structure of circuits [25] and mechanisms [23]. For physical systems, the Hamiltonian function is given by the total energy of the system. Hamiltonian systems are well suited for the formulation of *reversible* physical systems where the dissipation is neglected, as it is often the case in mechanics or electromagnetism [3, 18]. Hamiltonian systems have also been extended to model *open physical systems*, i.e. systems exchanging energy with their environment, in the context of control by introducing input-output and port Hamiltonian systems [4, 36, 39, 38, 7, 40, 21].

In the case when dissipation is taken into account, Hamiltonian systems have been extended by considering tensor fields which are no more skew-symmetric, defining a so-called Leibniz bracket [33, 7]. However, in this case, the Hamiltonian function is no more invariant, and the dissipative Hamiltonian system does not represent the conservation of energy. It may be observed that the Hamiltonian function corresponds more precisely to the free energy of the system, in the sense of thermodynamics, and that the dissipative Hamiltonian system corresponds to models of physical systems in thermal equilibrium. The *simultaneous* expression of irreversibility and conservation of energy is obtained by taking into account the properties of matter defined in terms of its internal energy [5, 8]. The irreversibility appears in the form of entropy source terms coupling the energy dissipation in any physical domain with entropy creation. Precisely these entropy creation terms are the obstacle which prevent to cast the entropy balance equation into the Hamiltonian frame as may be illustrated on the very elementary example of heat conduction [10].

In order to overcome this contradiction, we shall use an alternative geometric structure, the contact structure [3, 20], which may be associated with thermodynamic systems. Indeed, the description of the properties of matter leads to an enormous variety of complex constitutive laws, elaborated in the frame of reversible thermodynamics [35]. The geometric structure of thermodynamics has been elaborated in terms of contact geometry, endowing the Thermodynamic Phase Space (denoted TPS) with a contact structure [13, 14, 5, 17, 26–28]. Reversible thermodynamic transformations have been expressed as contact vector fields generated by some function related to state functions associated with the thermodynamic properties of the system [31, 29, 30]. Finally, some contact vector fields associated with irreversible thermodynamic transformations for systems near equilibrium have been proposed in [16].

In this paper we shall propose a class of dynamic systems defined by contact vector fields that may be seen as the lift of Hamiltonian systems on the TPS as well as an extension of these systems that allow to cope with irreversible thermodynamic processes. The first aim is to show precisely the extension of Hamiltonian systems needed to express simultaneously the irreversibility associated with dissipative phenomena and the conservation of energy. The second aim is to define a class of irreversible open systems which may be associated with systems arising from irreversible thermodynamics.

In Section 1 we shall recall the basic concepts of contact geometry in the context of reversible thermodynamics. In Section 2, we shall lift Hamiltonian systems, possibly dissipative, onto the TPS and define an associated contact vector field. In Section 3 these contact vector fields are generalized to a class of systems called *conservative contact systems* defined for isolated as well as open systems.

2. Contact structures for reversible thermodynamics

The first geometric formulation of thermodynamics has been given by Gibbs [13, 14] and has then been developed by Carathéodory [5], Hermann [17], leading later to formalization by Mrugała and coworkers [26, 27, 31]. In this section we shall briefly recall in which sense the contact geometry is associated with the Thermodynamic Phase Space (TPS) and reversible thermodynamics, following closely [26, 31]. Along this section we shall also recall some fundamental objects of contact geometry used in this paper, and refer the reader to [20, 1, 3] for their detailed presentation.

2.1. Thermodynamic Phase Space and contact structure

The contact structure emerges in relation with the description of the thermodynamic properties of matter. Indeed, these thermodynamic properties are defined by $n+1$ extensive variables (such as internal energy, volume, number of moles of chemical species, entropy) and by the so-called *fundamental equation* defining the internal energy as a function U of the remaining n extensive variables[1] [13, 14]. The fundamental equation defines a n-dimensional submanifold of $\mathbb{R}^{n+1}$ denoted by $\mathcal{N}$ in the sequel and characterizing the thermodynamic properties of some system in the space of extensive variables. However, in practice, the thermodynamic properties are defined using n additional variables, the *intensive variables* (such as pressure, chemical potential and temperature) which may be directly related with measurements. The Thermodynamic Phase Space is the space of first jets over $\mathcal{N}$, and the submanifold defining the thermodynamic properties is the 1-jet of U. As a consequence the Thermodynamic Phase Space associated with the differentiable manifold $\mathcal{N}$ of extensive variables, may be identified with the manifold $\mathbb{R} \times T^*\mathcal{N}$ [20]. This construction actually endows the TPS with a contact structure which is briefly recalled below.

Let now $\mathcal{M}$ denote a $(2n+1)$-dimensional, connected, differentiable smooth manifold.

DEFINITION 1 [20]. A *contact structure* on $\mathcal{M}$ is determined by a 1-form θ of constant class $(2n+1)$. The pair $(\mathcal{M}, \theta)$ is then called a *contact manifold*, and θ a *contact form*.[2]

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[1] A variable is qualified as *extensive* when it characterizes the thermodynamical state of the system and its total value is given by the sum of its constituting parts. In this paper we shall define the extensive variables as being the basis variables on which the fundamental equation is defined.

[2] For clarity, as we only consider *trivial* contact structure, we do not make a distinction between contact and *strictly* contact structures as in [20].

Consider some differentiable manifold $\mathcal{N}$. Define its associated space of 1-jets of functions on $\mathcal{N}$, denoted by $\mathcal{T}$ and called in the sequel Thermodynamic Phase Space associated with $\mathcal{N}$. It may be shown [20] that this space of 1-jets is identifiable with

$$\mathcal{T} \cong \mathbb{R} \times T^*\mathcal{N}, \tag{1}$$

and is endowed with a trivial contact structure defined by θ. According to Darboux theorem [15], the contact form is globally given by

$$\theta = dx^0 - \sum_{i=1}^{n} p_i dx^i, \tag{2}$$

in the canonical coordinates $(x^0, x^1, \dots, x^n, p_1, \dots, p_n)$.

EXAMPLE 1. For a simple thermodynamic system, the Thermodynamic Phase Space is defined in the following canonical coordinates: x^0 denotes the energy U, and the pairs (x^i, p_i) denote the pairs of conjugated extensive variables (the entropy $x^1 = S$, the volume $x^2 = V$, and the number of mole $x^3 = N$) and intensive variables (the temperature $p_1 = T$, minus the pressure $p_2 = -P$, and the chemical potential $p_3 = \mu$). In this case, the contact form is the Gibbs form

$$\theta = dU - TdS + PdV - \mu dN. \tag{3}$$

2.2. Thermodynamic properties and Legendre submanifolds

Actually the thermodynamic properties expressed in the TPS may also be defined as the submanifold where Gibbs' form vanishes, that is points where the Gibbs relation is satisfied [17, 3, 26]. This corresponds to the definition of a canonical submanifold of a contact structure, called Legendre submanifold (playing an analogous role as Lagrangian submanifolds for symplectic structures).

DEFINITION 2 [20]. A *Legendre submanifold* of a $(2n + 1)$-dimensional contact manifold $(\mathcal{M}, \theta)$ is an n-dimensional integral submanifold $\mathcal{L} \subset \mathcal{M}$ of θ.

Legendre submanifolds may be defined locally by some generating functions as follows.

THEOREM 1 [2]. *For a given set of canonical coordinates and any partition $I \cup J$ of the set of indices $\{1, \dots, n\}$ and for any differentiable function $F(x^i, p_J)$ of n variables, $i \in I$, $j \in J$, the formulae*

$$x^0 = F - p_J \frac{\partial F}{\partial p_J}, \qquad x^J = -\frac{\partial F}{\partial p_J}, \qquad p_I = \frac{\partial F}{\partial x^I} \tag{4}$$

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

This corresponds to the practical definition of the thermodynamic properties of thermodynamic systems where the generating functions are called *thermodynamic potentials*, such as the enthalpy or the free energy.

EXAMPLE 2. Consider the properties of an ideal gas which is usually defined by the so-called state equation. One way to express its thermodynamic properties in the TPS endowed with the contact form

$$\theta_G := dG + SdT - VdP - \mu_i dN^i \tag{5}$$

is to use as coordinates the temperature T, the pressure P and the number of moles N. In this case the generating function is the Gibbs free energy G:

$$G(T, P, N) = \frac{5}{2} NRT(1 - \ln(T/T_0)) - NT(s_0 - R\ln(P/P_0)), \tag{6}$$

where R is the ideal gas constant and P_0, T_0, s_0 are some references. The variables are given by $x'^0 = G$, $x' = (T, P, N)$ and $p' = (-S, V, \mu)$. The associated Legendre submanifold is then

$$\begin{cases} x'^0 = G(T, P, N) = U'(T, P, N), \\ p'_1 = -S(T, P, N) = \dfrac{\partial G}{\partial T} = Ns_0 + \dfrac{5}{2} NR\ln(T/T_0) - RN\ln(P/P_0), \\ p'_2 = V(T, P, N) = \dfrac{\partial G}{\partial P} = NRT/P, \\ p'_3 = \mu(T, P, N) = \dfrac{\partial G}{\partial N} = \dfrac{5}{2} RT - TS/N. \end{cases}$$

Notice that the coordinate x'^0 corresponds to the internal energy expressed in the independent coordinates (T, P, N) and that the third equation corresponds to the state equation $PV = NRT$ of an ideal gas.

However, one may choose as well as coordinates of the Legendre submanifold, the extensive variables: the entropy S, the volume V and the number of moles N via the Legendre transform $(x'^0, x', p') \mapsto (x^0, x, p)$ given by $x^0 = U$, $x = (S, V, N)$, $p = (T, -P, \mu)$. In this case the generating function is the internal energy

$$U(S, V, N) = G - P\frac{\partial G}{\partial P} - T\frac{\partial G}{\partial T} = \frac{3}{2} NRT_0 \exp[\gamma(S, V, N)] \tag{7}$$

obtained by the Legendre transform of G, and where the second equation of the previous Legendre submanifold provides

$$\gamma(S, V, N) = \big(S - Ns_0 + RN\ln(NRT_0) - RN\ln(VP_0)\big)/\big(\tfrac{3}{2}RN\big). \tag{8}$$

The contact form is then given by (3), and the Legendre submanifold describing the properties of the gas is now expressed by

$$\begin{cases} x^0 = U(S, V, N) = \dfrac{3}{2} N R T_0 \exp[\gamma(S, V, N)], \\ p_1 = T(S, V, N) = \dfrac{\partial U}{\partial S} = T_0 \exp[\gamma(S, V, N)], \\ p_2 = P(S, V, N) = \dfrac{\partial U}{\partial V} = N R T_0 \exp[\gamma(S, V, N)]/V, \\ p_3 = \mu(S, V, N) = \dfrac{\partial U}{\partial N} = \left(\frac{5}{2} R - S/N\right) T_0 \exp[\gamma(S, V, N)] \end{cases} \tag{9}$$

2.3. Contact vector fields and reversible transformations

Finally we shall recall the expressions of transformations of thermodynamic systems, which have the main property to leave invariant Legendre submanifolds defining thermodynamic properties. This is represented in the geometric language by contact transformations. We recall the definition of a particular class of vector fields, called *contact vector fields*, which preserves the contact structure, as well as the definition of the *Jacobi bracket* on the space of smooth functions on the TPS [1, 3, 20]. We then give illustrations of reversible transformations which have been treated in detail in [29, 30].

PROPOSITION 1 [20]. *A vector field X on $(\mathcal{M}, \theta)$ is a* contact vector field *if and only if there exists a differentiable real-valued function ρ on $\mathcal{M}$ such that*

$$\mathcal{L}(X)\,\theta = \rho\,\theta, \tag{10}$$

where $\mathcal{L}(X)\cdot$ denotes the Lie derivative with respect to the vector field X. If $\rho = 0$ then X is called an infinitesimal automorphism of the contact structure.

Analogously to the case of Hamiltonian vector fields, one may associate a generating function to any contact vector field. Actually there exists an isomorphism Φ between contact vector fields and differentiable function on $\mathcal{M}$, which associates a contact vector field X to a function called *contact Hamiltonian.*

PROPOSITION 2. *The map*

$$\Phi(X) = i(X)\theta, \tag{11}$$

where $i(X)\cdot$ denotes the contraction of a form by the vector field X, defines an isomorphism from the vector space of contact vector fields in the space of smooth real functions on $\mathcal{M}$. The function $f = \Phi(X)$ is called contact Hamiltonian *associated with the vector field X denoted by*

$$X_f = \Phi^{-1}(f), \tag{12}$$

where Φ^{-1} is the inverse isomorphism.

The contact vector field X_f may be expressed in canonical coordinates in terms of the generating function f as follows,

$$X_f = \left(f - \sum_{k=1}^{n} p_k \frac{\partial f}{\partial p_k}\right)\frac{\partial}{\partial x^0} + \frac{\partial f}{\partial x^0}\left(\sum_{k=1}^{n} p_k \frac{\partial}{\partial p_k}\right) + \sum_{k=1}^{n}\left(\frac{\partial f}{\partial x^k}\frac{\partial}{\partial p_k} - \frac{\partial f}{\partial p_k}\frac{\partial}{\partial x^k}\right). \quad (13)$$

It is worth noting that the set of contact vector fields forms a Lie subalgebra of the Lie algebra of vector fields on $\mathcal{M}$ [20].

PROPOSITION 3 ([20], p. 20). *The isomorphism* Φ *defined in Proposition* 2 *defines on differentiable functions on* $\mathcal{M}$, *the following Lie bracket called* Jacobi bracket,

$$\{f, g\} = i([X_f, X_g])\theta. \quad (14)$$

Its expression in canonical coordinates is given by

$$\{f, g\} = \sum_{k=1}^{n}\left(\frac{\partial f}{\partial x^k}\frac{\partial g}{\partial p_k} - \frac{\partial g}{\partial x^k}\frac{\partial f}{\partial p_k}\right) + \left(f - \sum_{k=1}^{n} p_k \frac{\partial f}{\partial p_k}\right)\frac{\partial g}{\partial x^0} - \left(g - \sum_{k=1}^{n} p_k \frac{\partial g}{\partial p_k}\right)\frac{\partial f}{\partial x^0}. \quad (15)$$

Let us consider an example of such contact vector fields in the context of thermodynamics given by Mrugała [30] and associated with *reversible transformations* of thermodynamic systems.

EXAMPLE 3 [30]. Consider a thermodynamic system defined by the Legendre submanifold $\mathcal{L}_\Phi$ generated, in canonical coordinates, by a thermodynamic potential $\Phi(x^i, p_j)$, for $i \in I$, $j \in J$, $I \cup J = \{1, \ldots, n\}$, as the internal energy U, the enthalpy H, etc. Examples of invariant transformations, in the sense that the trajectories starting on $\mathcal{L}_\Phi$ stay on it, are given by the contact vector fields X_f with contact Hamiltonians such as

$$f = x^0 - \Phi + p_j \frac{\partial \Phi}{\partial p_j}, \qquad f = PV - NRT. \quad (16)$$

In thermodynamics, these correspond to basic reversible transformations. It is interesting to note that in the first case of these reversible transformations, the contact Hamiltonian is entirely defined by the generating function (a partial Legendre transform) of the Legendre submanifold defining the thermodynamic properties.

An important property of the reversible transformations is that they leave invariant the Legendre submanifold associated with its thermodynamical properties. This may be checked by using the following result [31, 30].

THEOREM 2. [31] *Let* $(\mathcal{M}, \theta)$ *be a contact manifold and denote by* $\mathcal{L}$ *a Legendre submanifold. Then* X_f *is tangent to* $\mathcal{L}$ *if and only if* f *is identically zero on* $\mathcal{L}$.

Notice that by definition, contact Hamiltonians defining reversible transformations, such as (16), satisfy the invariance condition of Theorem 2. In the sequel this invariance condition will play a fundamental role in the definition of extensions of these vector fields.

3. Lift of Hamiltonian dynamics to the Thermodynamic Phase Space

In this section, as a preliminary step towards the definition of contact systems *including phenomenological laws,* we shall consider the lift of reversible port Hamiltonian systems as well as of dissipative Hamiltonian systems.

In the first part we shall consider port Hamiltonian systems [22, 39, 38] and their lift to the TPS associated with their state space $\mathcal{N}^3$ defined in Eq. (1) [11]. In this way we shall define a first class of contact systems generated by *internal* contact Hamiltonian associated with the drift Hamiltonian vector field, and by *interaction* contact Hamiltonians associated with input vector fields. In the second part, we shall lift a dissipative Hamiltonian system [7, 33] to some extended TPS [12]. This space is obtained by considering two additional variables, namely the entropy and the temperature of some external thermostat. For this class of systems we shall define a contact vector field generated by a contact Hamiltonian which generates the entropy creation associated with energy dissipation.

3.1. Lift of port Hamiltonian systems

Let us first recall briefly the definition of a port Hamiltonian system [22, 39] defined on a pseudo-Poisson manifold $\mathcal{N}$. Consider an n-dimensional differential manifold $\mathcal{N}$ endowed with a pseudo-Poisson bracket $\{.,.\}_{\text{gen}}$ (i.e. Jacobi's identities are not necessarily satisfied). Denote by Λ its associated pseudo-Poisson tensor, and by $\Lambda^\#$ the vector bundle map $\Lambda^\# : T^*\mathcal{N} \to T\mathcal{N}$ satisfying $\Lambda(\alpha,\beta) = \langle \alpha, \Lambda^\#(\beta)\rangle$, $\forall(\alpha,\beta) \in T^*\mathcal{N} \times T^*\mathcal{N}$. A *port Hamiltonian system* [22, 39] is defined by a Hamiltonian function $H_0(x) \in C^\infty(\mathcal{N})$, an input vector $u(t) = (u_1,\dots,u_m)(t)^T \in \mathbb{R}^m$ function of t, m input vector fields $g_1,\dots,g_m$ on $\mathcal{N}$, and the equations

$$\begin{cases} \dot{x} = \Lambda^\#(\mathrm{d}_x H_0(x)) + \sum_{i=1}^m u_i(t)\, g_i(x), \\ y^j = \mathcal{L}(g_j) H_0(x), \end{cases} \tag{17}$$

where $y = (y^1,\dots,y^m)$ is called the *port output* variable (or *port conjugated output*), and $\mathcal{L}(\cdot)$ denotes the Lie derivative. Port Hamiltonian systems are extensions of Hamiltonian systems which allow to model reversible physical systems which are *open* in the sense that they undergo some exchange of energy with their environment [22, 39]. They appear naturally in the modeling of driven mechanical systems [40] or electrical circuits [24, 39]. Interpreting the Hamiltonian function H_0 as the total energy of a physical system, it appears that the energy is not conserved but satisfies the following *power balance equation,*

$$\frac{dH_0}{dt} = \sum_{i=1}^m u_i\, y^i, \tag{18}$$

[3]Notice that we will still denote by $\mathcal{N}$ the state space, although its components are no longer usually called extensive variables but *energy* variables. However, energy (resp. co-energy) variables play analogous fundamental role in the Hamiltonian framework as extensive (resp. intensive) variables in thermodynamics.

where the product of the port-conjugated input and output variables is the flow of energy into the system through its boundary.

Despite the fact that port Hamiltonian systems represent reversible physical systems, one may still have a thermodynamic perspective on them, and define some analogue of the TPS. Indeed, consider as space of extensive variables the manifold $\mathbb{R}\times\mathcal{N} \ni (x^0, x)$, and the fundamental equation $x^0 = H_0(x)$. The Hamiltonian function H_0 (or, in the same way, its graph) defines some analogue of the thermodynamic properties for a reversible system in the space of extensive variables $\mathbb{R}\times\mathcal{N} \ni (x^0, x)$. Using (1), one may associate with the base manifold $\mathcal{N}$, the $(2n+1)$-dimensional TPS

$$\mathbb{R} \times T^*\mathcal{N} \ni x' = (x^0, x, p), \tag{19}$$

endowed with the canonical contact form (2). The 1-jet of the function H_0 may be identified with the Legendre submanifold generated by $H_0(x)$ of the TPS $\mathbb{R} \times T^*\mathcal{N}$, and characterizes an analogue of thermodynamic properties for the port Hamiltonian system[4]. The lift of the port Hamiltonian system (17) on the TPS $\mathbb{R} \times T^*\mathcal{N}$ may be defined as the following control contact system. Its construction is completely analogous to the control Hamiltonian systems defined on symplectic manifolds [4, 36]. Consider the *internal contact Hamiltonian*[5]

$$K_0 = -\Lambda(p, d_x H_0), \tag{20}$$

and the *interaction contact Hamiltonians*

$$K_j = u_j(t).i(g_j)(d_x H_0 - p). \tag{21}$$

The lift of the port Hamiltonian system (17) on the Thermodynamical Phase Space $\mathbb{R} \times T^*\mathcal{N}$ is then defined as the *control contact system*

$$\frac{dx'}{dt} = X_{K_0} + \sum_{j=1}^{m} X_{K_j} =: X(x', u). \tag{22}$$

Notice firstly that, by construction, the two contact Hamiltonians (20) and (21) satisfy the invariance condition of Theorem 2 with respect to the Legendre submanifold $\mathcal{L}_{H_0}$ generated by the Hamiltonian $H_0(x)$. Hence they generate contact vector fields that leave invariant $\mathcal{L}_{H_0}$, and so does their linear combination $X(x', u)$. By construction the *restriction* to the Legendre submanifold $\mathcal{L}_{H_0}$ of the conservative system generated by these contact Hamiltonians, projected on the x-coordinates, gives the dynamic equation of (17) [11][6]. Secondly, it is interesting to note that the Legendre submanifold is generated by the internal Hamiltonian H_0 of the port

[4]This Legendre submanifold is the analogue for the contact manifold $\mathbb{R}\times T^*\mathcal{N}$ of the Lagrangian submanifold generated by $H_0(x)$ in the cotangent bundle $T^*\mathcal{N}$.

[5]Note that this internal contact Hamiltonian $K_0 = \mathcal{L}(\Lambda^{\#}(d_x H_0(x)))(p)$ is precisely the Hamiltonian function of the lift of the vector field $\Lambda^{\#}(d_x H_0(x))$ on the cotangent space $T^*\mathcal{N}$.

[6]Moreover its projection on the conjugated p-coordinates is related to its adjoint variational system. And it has been shown that the invariance condition of the Legendre submanifold $\mathcal{L}_{H_0}$ may be related to the power balance equation (18) [11].

Hamiltonian system which has the *dimension of energy* for models of physical systems, and that *the contact Hamiltonians have the dimension of power*. The internal contact Hamiltonian (20) is defined by the pseudo-Poisson tensor, and the interaction Hamiltonians (21) are defined by the input vector fields; they may be interpreted as some *virtual power* associated with the interconnection structure of the physical system giving rise to the dynamics [24, 39].

3.2. Lift of Hamiltonian systems with dissipation

We consider now the case of an autonomous *dissipative* Hamiltonian system [7] and its lift to the TPS.

Set $\mathcal{N}$ as an n-dimensional differentiable manifold endowed with a pseudo-Poisson tensor denoted by Λ, and a symmetric positive 2-contravariant tensor denoted by Δ. The tensor $B = \Lambda - \Delta$ endows the manifold $\mathcal{N}$ with a Leibniz structure [33], and defines the vector bundle maps $B_R^\sharp : T^*\mathcal{N} \to T\mathcal{N}$ satisfying

$$B(\alpha, \beta) = \langle \alpha, B_R^\sharp(\beta) \rangle, \qquad \forall\, (\alpha, \beta) \in T^*\mathcal{N} \times T^*\mathcal{N}. \tag{23}$$

A *dissipative Hamiltonian system* [33] with energy function H_0 is then defined by the differential equation

$$\dot{x} = B_R^\sharp(d_x H_0(x)). \tag{24}$$

The Hamiltonian function H_0 is not an invariant of such systems and its time variation is

$$\frac{dH_0}{dt} = -\Delta(d_x H_0(x),\, d_x H_0(x)). \tag{25}$$

Interpreting the Hamiltonian function as the energy of a physical system, this is the *power balance equation* expressing the loss of energy induced by some dissipative phenomenon.

In the sequel we shall lift this dissipative Hamiltonian system to a contact system in such a way to express simultaneously the first principle of thermodynamics (conservation of the total energy of the system) and the second principle (positive entropy creation). Therefore, in the first step, we shall define an augmented state space using a thermodynamic perspective. Indeed, the power balance equation (24) may also be interpreted as the conversion of the energy (expressed by the Hamiltonian $H_0(x)$) into some heat flow. This heat flow is accumulated in the form of the internal energy which, for instance, may be the energy of some thermostat to which the system is coupled. This internal energy may be defined by

$$U(S) = T_0\, S \tag{26}$$

where $T_0 \in \mathbb{R}_+^*$ is the constant temperature delivered by the thermostat, and $S \in \mathbb{R}$ is its state, its entropy[7]. With the system composed of the dissipative Hamiltonian

[7]This thermostat corresponds to some simple thermodynamic system with constant temperature $T = \frac{\partial U}{\partial T} = T_0$, with finite entropy but infinite heat capacitance. The total energy of the system coupled to the thermostat becomes $H_e(x, S) = H_0(x) + T_0\, S$, and its Legendre transform with respect to S is then H_0 which may now be interpreted as the *free* energy of the whole system.

system coupled with the thermostat, one may associate the space of extensive variables, an $(n+2)$-dimensional manifold $\mathbb{R} \times \mathcal{N}_e \ni (x^0, x, S)$ with $\mathcal{N}_e = \mathcal{N} \times \mathbb{R}$ denoting the extended base space of the coupled system. The coupled system may be endowed with some thermodynamic properties defined by the fundamental equation $x^0 = H_e(x, S)$ where H_e denotes the *total* energy of the coupled system,

$$H_e(x, S) := H_0(x) + U(S) = H_0(x) + T_0 S. \tag{27}$$

Using (1), one may associate with the base manifold $\mathcal{N}_e$, the *extended* TPS

$$\mathcal{T}_e := \mathbb{R} \times T^*\mathcal{N}_e \ni (x^0, x, S, p, p_S), \tag{28}$$

where the intensive variable p_S conjugated to S corresponds to the temperature of the thermostat. This extended TPS is endowed with the contact form θ_e defined in canonical coordinates by

$$\theta_e := dx^0 - \sum_{i=1}^{n} p_i \, dx^i - p_S dS. \tag{29}$$

The function $H_e(x, S)$ defined in (27) generates the Legendre submanifold

$$\mathcal{L}_{H_e} = \left\{ x^0 = H_e(x, S), x, S, p = \frac{\partial H_e}{\partial x} = \frac{\partial H_0}{\partial x}, p_S = \frac{\partial H_e}{\partial S} = T_0 \right\}. \tag{30}$$

This Legendre submanifold is simply the product of the Legendre submanifold generated by H_0 on the TPS $\mathbb{R} \times T^*\mathcal{N}$ of the reversible pseudo-Hamiltonian system (with $\Delta = 0$) according to Section 3.1 and the trivial manifold $\{(S, T) = (S, T_0), S \in \mathbb{R}\} \subset \mathbb{R}^2$ corresponding to the definition of the thermostat.

In the second step we shall define a contact vector field on the TPS (28) that is a lift of the dissipative Hamiltonian system in the following sense: it expresses conservation of the total energy H_e and the entropy balance equation associated with the dissipated energy (25). Therefore consider the contact Hamiltonian

$$K_e := -B(p, d_x H_0(x)) - \frac{p_S}{T_0} \Delta(d_x H_0(x), d_x H_0(x)). \tag{31}$$

It consists of the sum of two terms. The first term is bilinear in the intensive variables p and in the differential $d_x H_0$ and depends on the Leibniz tensor B. It is defined in a very similar way as for the contact Hamiltonian (20) associated with reversible Hamiltonian systems where the pseudo-Poisson tensor Λ is replaced by the Leibniz tensor B. The second term is deduced from the invariance condition (Theorem 2), and is defined solely by the symmetric bracket Δ associated with the dissipation. It may be noted that this term *is no more linear in the differential* $d_x H_0$. This is a distinguishing feature of irreversible processes: the nonlinearity allows to take into account the entropy creation due to irreversibility.

By construction, this contact Hamiltonian K_e vanishes on the Legendre submanifold $\mathcal{L}_{H_e}$ and hence the contact vector field generated by K_e leaves it invariant.

Its restriction to $\mathcal{L}_{H_e}$, projected to the extensive variables (x, S) is

$$\begin{cases} \dot{x} = B_R^\sharp(d_x H_0(x)), \\ \dot{S} = \frac{1}{T_0}\Delta(d_x H_0(x), d_x H_0(x)) =: \sigma. \end{cases} \tag{32}$$

The first equation is simply the definition of the dissipative Hamiltonian system (24). The second equation gives the variation of the entropy S of the thermostat and corresponds to the entropy balance equation with σ being the entropy creation due to the dissipation. The heat flow $T_0\sigma$ into the thermostat is precisely the flow of energy dissipated in the physical domain with state variables $x \in \mathcal{N}$.

Furthermore the generating function H_e defining thermodynamic properties of the augmented system is now conserved,

$$\frac{dH_e}{dt} = B(d_x H_0(x), d_x H_0(x)) + \frac{T_0}{T_0}\Delta(d_x H_0(x), d_x H_0(x)) = 0. \tag{33}$$

Hence the contact vector field X_{K_e} expresses *simultaneously* the irreversibility in terms of entropy creation, and energy conservation.

REMARK 1. It is important to note that the previous construction may be easily adapted to the case where one assumes some nontrivial thermodynamic properties (i.e. not assuming that the system is isothermal and in equilibrium with a thermostat) defined by some other Legendre submanifold $\mathcal{L}$ of the extended TPS. The second nonlinear term of the contact Hamiltonian K_e defined in (31) has then to be modified in order to ensure the invariance condition $K_e|_{\mathcal{L}} = 0$ (cf. Theorem 2).

REMARK 2. In [16], pp. 311–317, Grmela presents a comparable construction of a contact vector field associated with dissipative Hamiltonian systems. The system represents a physical system in thermal equilibrium at the constant temperature T_0. The dynamics in the extensive variables $x \in \mathcal{N} = \mathbb{R}^n$ near the equilibrium is given by the dissipative Hamiltonian system

$$\dot{x} = (T_0 J - D)\frac{\partial \phi}{\partial x}, \tag{34}$$

where J is a skew-symmetric matrix, D a positive definite matrix and $\phi(x)$ is a potential function defining the thermodynamic properties. This system is lifted to the TPS $\mathbb{R} \times T^*\mathcal{N} \cong \mathbb{R}^{2n+1} \ni (x^0, x, p)$ as a contact vector field with contact Hamiltonian

$$\Psi(x, p) = +\frac{1}{2}p^t D p - \frac{1}{2}\frac{\partial \phi}{\partial x} D \frac{\partial \phi}{\partial x} - T_0 p^t J \frac{\partial \phi}{\partial x}. \tag{35}$$

It may be noted that the contact Hamiltonian satisfies the invariance condition of Theorem 2 and hence leaves invariant the Legendre submanifold generated by ϕ. However, the difference with respect to the construction that we have proposed above is that the temperature appears as a constant parameter, and that the pair of entropy and temperature variables do not appear in the definition of the state space.

As a consequence the entropy balance equation is not expressed and the potential ϕ is not an invariant of the dynamics

$$\frac{d\phi}{dt} = -\frac{\partial \phi}{\partial x} D \frac{\partial \phi}{\partial x}. \tag{36}$$

4. Conservative control contact systems

In this section we shall propose a general definition of contact systems representing both the invariance of the thermodynamic properties of a system (defined by Gibbs relations) and the fluxes due to thermodynamical nonequilibrium conditions. In a first part we shall consider isolated systems whose dynamics is generated solely from some internal nonequilibrium conditions. In a second part, we shall extend these systems to open systems for which part of the dynamics is generated by some nonequilibrium conditions of the system with its environment. The third part concludes with the definition of pairs of conjugated variables, called port variables, enabling the expression of such interactions with the environment and related to a global power balance equation.

4.1. Isolated systems

In this paragraph we shall define a class of systems which generalize the lifted dissipative systems presented in Section 3.2. This class of systems expresses the two fundamental features of irreversible thermodynamics: the dynamics leaves invariant thermodynamic properties, and the dynamics is defined by some fluxes generated by some phenomenological laws associated with the thermodynamic nonequilibrium.

DEFINITION 3. A *conservative contact system* is defined as a set $(\mathcal{M}, \theta, \mathcal{L}, K_0)$, where $(\mathcal{M}, \theta)$ is a contact manifold, $\mathcal{L}$ a Legendre submanifold and K_0 a contact Hamiltonian satisfying the invariance condition (i.e. K_0 is identically zero on $\mathcal{L}$). The dynamics is then given by the differential equation $\dot{x}' = X_{K_0}$.

A conservative contact system is simply a dynamical system defined on a contact manifold by a contact vector field which furthermore satisfies the invariance condition of Theorem 2 with respect to some Legendre submanifold. In terms of modeling of physical systems, the Legendre submanifold defines the thermodynamic properties of a physical system. This might be the state equations of an ideal gas presented in an Example 1, or the (free) energy of a reversible Hamiltonian system as presented in Section 3.1. The contact Hamiltonians generating the vector field corresponds to dynamical phenomena due to nonequilibrium conditions. We have seen two examples of such contact Hamiltonian for reversible Hamiltonian systems (the nonequilibrium condition consists in this case in the interdomain coupling represented by the Poisson tensor), and dissipative Hamiltonian systems in Section 3. However, contact Hamiltonians may be quite general functions allowing to cope with a great variety of phenomenological laws, near thermodynamical equilibrium or not.

We shall conclude with two simple examples: a gas in a cylinder undergoing some nonadiabatic transformation, and the heat conduction between two gases.

EXAMPLE 4. *A gas in a cylinder under a piston.* Consider in this example a gas contained in a cylinder closed by a piston subject to gravity (see Fig. 1).

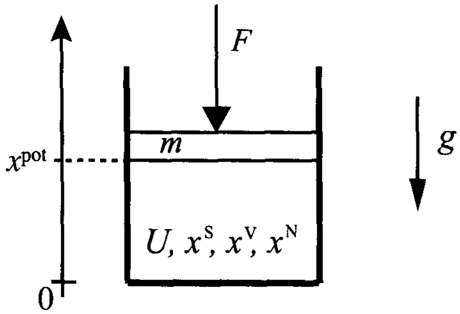

Fig. 1. A gas in a cylinder under a piston.

The thermodynamic properties of this system may be decomposed into the properties of the piston in the gravitation field and the properties of the perfect gas. The properties of the piston in the gravity field are defined by the sum of the potential and kinetic energies:

$$H_0 = \frac{1}{2m} x^{\mathrm{kin}2} + mgx^{\mathrm{pot}},$$

where x^{pot} denotes the height of the piston and x^{kin} its kinetic momentum. The properties of the perfect gas may be defined by its internal energy $U(x^S, x^V, x^N)$ where x^S denotes the entropy variable, x^V the volume variable and x^N the number of moles. The properties of the total system gas and piston are defined in the TPS

$$\mathcal{T}_{\mathrm{GP}} = \mathbb{R} \times \mathbb{R}^{10} \ni \{x^0, x^S, x^V, x^N, x^{\mathrm{pot}}, x^{\mathrm{kin}}, p_S, p_V, p_N, p_{\mathrm{pot}}, p_{\mathrm{kin}}\}, \tag{37}$$

and are given by the potential $H(x') = U(x^S, x^V, x^N) + H_0(x^{\mathrm{pot}}, x^{\mathrm{kin}})$. The Legendre submanifold $\mathcal{L}$ generated by H is given by

$$\begin{aligned}
p_S|_{\mathcal{L}} &= \left.\frac{\partial U}{\partial S}\right|_{\mathcal{L}} \triangleq T, \\
p_V|_{\mathcal{L}} &= -\left.\frac{\partial U}{\partial V}\right|_{\mathcal{L}} \triangleq -P, \\
p_N|_{\mathcal{L}} &= \left.\frac{\partial U}{\partial N}\right|_{\mathcal{L}} \triangleq \mu, \\
p_{\mathrm{pot}}|_{\mathcal{L}} &= mg \triangleq F, \\
p_{\mathrm{kin}}|_{\mathcal{L}} &= \frac{x^{\mathrm{kin}}}{m} \triangleq v,
\end{aligned} \tag{38}$$

where T is the temperature, P the pressure, μ the chemical potential of the gas, F the gravity force, and v the velocity of the piston.

The gas in the cylinder under the piston may undergo a **nonreversible transformation** when the piston moves. We assume that in this case a nonadiabatic transformation due to mechanical friction[8], and that the *dissipated mechanical energy is converted entirely into a heat flow in the gas.* Consider the contact Hamiltonian

$$K_{\text{tot}} = K_{\text{mec}} - (p_V + P)\,Av - (p_{\text{kin}} - v)\,AP + \left(p_{\text{kin}} - \frac{p_S}{T}\,v\right)\nu\,v, \tag{39}$$

where ν is the friction coefficient defining the mechanical energy dissipation, P, v and T are the functions defined in (38), and

$$K_{\text{mec}} = -(p_{\text{pot}},\, p_{\text{kin}})\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} F \\ v \end{pmatrix}. \tag{40}$$

This contact Hamiltonian is composed of four terms. The first one is precisely the contact Hamiltonian associated with the piston moving in the gravity field alone, that is the contact Hamiltonian K_0 in (20) of a lifted Hamiltonian system. The last term is a quadratic term in the velocity v associated with the mechanical friction, analogous to the nonlinear term of the contact Hamiltonian (31) associated with dissipative Hamiltonian systems. The second and third terms are associated with the coupling between the piston and the gas by relating the force F^{e} and pressure P on the piston and the velocity v of the piston and the variation of volume f_V^{e}

$$\begin{pmatrix} f_V^{\text{e}} \\ F^{\text{e}} \end{pmatrix} = \begin{pmatrix} 0 & A \\ -A & 0 \end{pmatrix}\begin{pmatrix} (-P) \\ v \end{pmatrix} \tag{41}$$

where A denotes the area of the piston.

It is immediately seen that the contact Hamiltonian satisfies the invariance condition $K_{\text{irr}}|_{\mathcal{L}} = 0$. The dynamics restricted to the Legendre submanifold and projected on the extensive coordinates is

$$\begin{aligned}
\left.\frac{dx^S}{dt}\right|_{\mathcal{L}} &= \frac{dS}{dt} = -\frac{\partial K_{\text{tot}}}{\partial p_S} = \frac{1}{T}\nu v^2 \triangleq \sigma, \\
\left.\frac{dx^V}{dt}\right|_{\mathcal{L}} &= \frac{dV}{dt} = -\frac{\partial K_{\text{tot}}}{\partial p_V} = A\,v, \\
\left.\frac{dx^N}{dt}\right|_{\mathcal{L}} &= \frac{dN}{dt} = -\frac{\partial K_{\text{tot}}}{\partial p_N} = 0, \\
\left.\frac{dx^{\text{pot}}}{dt}\right|_{\mathcal{L}} &= \frac{dz}{dt} = -\frac{\partial K_{\text{tot}}}{\partial p_{\text{pot}}} = v, \\
\left.\frac{dx^{\text{kin}}}{dt}\right|_{\mathcal{L}} &= \frac{d\pi}{dt} = -\frac{\partial K_{\text{tot}}}{\partial p_{\text{kin}}} = -F + A\,P = -mg + AP,
\end{aligned} \tag{42}$$

[8]Notice that another (equivalent) way to model irreversibility is to introduce the *viscosity coefficient* of the gas, providing the same dynamics.

where z denotes the height, and σ the irreversible entropy creation associated with the mechanical friction. The last equation is simply Newton's law applied to the piston, the fourth is the definition of the velocity. The third equation indicates that the system is closed (there is no exchange of matter). The second equation indicates that the motion of the piston induces a variation of the volume of the gas. And the first one is the entropy balance where irreversible creation of entropy due to mechanical friction is transformed into an entropy flow in the gas.

It is interesting to note that this formulation of an irreversible transformation of a gas-cylinder system encompasses the formulation of reversible transformation using a port Hamiltonian system defined on a Dirac structure proposed in [19] (by setting $\nu = 0$, the entropy variation becomes $\dot{x}^S = 0$, hence characterizes reversible transformations).

The next example concerns a classical example of irreversible system: heat conduction with Fourier's law.

EXAMPLE 5. *Heat conduction.* 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 thermodynamic properties of each ideal gas are described in the composed TPS

$$\mathcal{T} = \mathbb{R} \times \mathbb{R}^{12} \ni x' = (x^0, x_i^j, p_{j_i})_{i=1,2\, j=1,\dots,3} \tag{43}$$

where the x_i^j denote the coordinates of the extensive variables and p_{j_i} of the conjugated intensive variables of the system i. Assume that the thermodynamic properties of each system are generated by the internal energy $U_i(x_i^j)$ for $i = 1, 2$ and $j = 1, \dots, 3$ (for an ideal gas given in Example 2). The thermodynamic properties of the composed system are simply obtained by considering the Legendre submanifold $\mathcal{L}_U$ generated by the potential $U = U_1 + U_2$.

The two systems may exchange a heat flux $\dot{Q}$ according to Fourier's law $\dot{Q} = \lambda(T_1 - T_2)$, where $\lambda \in \mathbb{R}_+^*$ denotes Fourier's heat conduction coefficient. The heat transfer dynamics is described by the conservative contact system on $\mathcal{L}$ with the internal contact Hamiltonian

$$K_0(x') = (p_{1_1}, p_{1_2})^t R(p_{1_1}, p_{1_2}) \Lambda^\sharp\big((T_1, T_2)^t\big) = R(p)\Lambda(p, T), \tag{44}$$

where

$$R(p) = \lambda\left(\frac{1}{p_{1_2}} - \frac{1}{p_{1_1}}\right), \qquad T_i = \frac{\partial U_i}{\partial p_{1_i}}(x_i^j), \qquad i = 1, 2,$$

and $\Lambda^\sharp$ denotes the vector bundle map associated with the canonical symplectic Poisson tensor Λ on $\mathbb{R}^2$. Note that this multiplicative R destroys the Hamiltonian structure (Poisson or Dirac structure) and allows to take into account *entropy production* via nonlinear generating flux laws. By construction, the contact Hamiltonian K_0 satisfies the invariance condition of Theorem 2, and leaves invariant the Legendre submanifold $\mathcal{L}$, that is, it satisfies Gibbs' relation. Let us now write the restriction of the vector field X_{K_0} to the Legendre submanifold $\mathcal{L}$. Consider first its projection on the temperature coordinates p_{1_1}, p_{1_2}. Using the fact that the systems are isochore together with the definition of the calorific capacitance $C_V = \frac{\partial U}{\partial T}$, one obtains

$$\frac{d}{dt}(p_{1_1}, p_{1_2})^t\bigg|_{\mathcal{L}} = (\dot{T}_1, \dot{T}_2) = \left(\frac{\partial K_0}{\partial x^1{}_1}, \frac{\partial K_0}{\partial x^1{}_2}\right)^t\bigg|_{\mathcal{L}} = \begin{pmatrix} -C_{V1}{}^{-1}\lambda(T_1 - T_2) \\ C_{V2}{}^{-1}\lambda(T_1 - T_2) \end{pmatrix}. \tag{45}$$

These two equations are simply the energy balance equations written in terms of the temperature and using the calorimetric relations, for each of the simple thermodynamical systems 1 and 2. Consider now the projection on the entropy coordinates,

$$\frac{d}{dt}(x^1{}_1, x^1{}_2)\bigg|_{\mathcal{L}} = (\dot{S}_1, \dot{S}_2) = -\left(\frac{\partial K_0}{\partial p_{1_1}}, \frac{\partial K_0}{\partial p_{1_2}}\right)^t\bigg|_{\mathcal{L}} = \begin{pmatrix} -\dfrac{\lambda(T_1 - T_2)}{T_1} \\ \dfrac{\lambda(T_1 - T_2)}{T_2} \end{pmatrix}, \tag{46}$$

which corresponds to the entropy balance equation written for each simple thermodynamic system. It may be seen that this system resembles a Hamiltonian system, however the multiplicative modulus

$$R(T_1, T_2) = \lambda\left(\frac{1}{T_2} - \frac{1}{T_1}\right) \tag{47}$$

renders the relation between the entropy flows dS/dt and the temperatures *nonlinear*. This is again an illustration in which sense the contact formulation allows to encompass irreversible phenomena in opposite to Hamiltonian systems. Finally, we may consider the projection on the energy coordinate x^0,

$$\frac{dx^0}{dt}\bigg|_{\mathcal{L}} = -\left(R(T_1, T_2) + \frac{\partial R}{\partial p_1}^t \frac{\partial U}{\partial x^1}\right) \wedge \left(\begin{pmatrix} T_1 \\ T_2 \end{pmatrix}, \begin{pmatrix} T_1 \\ T_2 \end{pmatrix}\right) = 0, \tag{48}$$

which indicates that the potential U, i.e. the internal energy, is conserved on trajectories on the Legendre submanifold. Furthermore, it is worth noting that the entropy source term, given by

$$\sigma = \dot{S}_1 + \dot{S}_2 = \dot{Q}\left(\frac{1}{T_2} - \frac{1}{T_1}\right) \geq 0, \tag{49}$$

is a positive term which vanishes at the thermodynamic equilibrium ($T_1 = T_2$).

4.2. Nonisolated systems

In this section, we shall extend the previously defined conservative contact systems in order to cope with models of *open* thermodynamical systems. Therefore we shall follow a construction very similar to the definition of Hamiltonian control systems [4, 36, 32]. Namely we shall introduce additional contact Hamiltonians, called *interaction contact Hamiltonians*, which will represent the interactions of the system with its environment. First, we shall give the definition of these conservative control contact systems and illustrate it with simple examples. Second, we shall define pairs of conjugated port variables by considering a power balance equation.

Let us first extend the definition of conservative contract systems to control systems as follows.

DEFINITION 4. A *conservative control contact system* is defined as a conservative contact system together with input vector fields, i.e. as the set $(\mathcal{M}, \theta, \mathcal{L}, \mathcal{U}, K_0, \dots, K_m)$ where $(\mathcal{M}, \theta)$ is a contact manifold, $\mathcal{L}$ a Legendre submanifold, $\mathcal{U}$ the input space, with $m+1$ contact Hamiltonians satisfying the invariance condition

$$K_{j|\mathcal{L}} = 0, \qquad j = 0, \dots, m, \tag{50}$$

and the dynamics is given by the differential equation

$$\frac{dx'}{dt} = X_{K_0}(x') + \sum_{j=1}^{m} X_{K_j}(x', u_j) = X(x', u). \tag{51}$$

The system's dynamics is composed of two terms. The first term consists of the drift dynamics X_{K_0} which defines precisely a conservative contact system with respect to the Legendre submanifold $\mathcal{L}$ in the sense of Definition 3. The second term is composed by the linear combination of m contact fields generating also m conservative contact systems with respect to the Legendre submanifold $\mathcal{L}$. All these vector fields satisfy the invariance condition of Theorem 2 with respect to the Legendre submanifold $\mathcal{L}$. Obviously, their linear combination $X(x', u)$ satisfies as well the invariance condition, and leaves $\mathcal{L}$ invariant.

In the context of thermodynamic systems, this system may be interpreted as follows. The Legendre submanifold $\mathcal{L}$ represents the thermodynamic properties of the system. The internal contact Hamiltonian K_0 represents the law giving the fluxes in the closed system due to nonequilibrium conditions *in* the system (for instance due to heat conduction or chemical reaction kinetics). Finally the interaction contact Hamiltonians K_j give the fluxes due to the nonequilibrium of the system with its environment. The invariance conditions guarantee the fundamental thermodynamic principle: thermodynamic properties are invariant under the dynamics. In other words, Gibbs' relations are satisfied along irreversible transformations.

In order to illustrate this definition, let us consider the following examples.

EXAMPLE 6. *Lift of a port Hamiltonian system as conservative control contact system.* The lift of a port Hamiltonian system to its TPS is a conservative control contact system with the internal contact Hamiltonian given by (20), and interaction contact Hamiltonians (21). Notice that the interaction contact Hamiltonians are linear in the input functions u_i.

The second example consists in Example 5 (heat conduction between two simple thermodynamic systems) which is now assumed to interact with an external thermostat.

EXAMPLE 7. *Heat conduction continued.* Consider again the example of two simple thermodynamic systems, indexed by 1 and 2 (for instance two ideal gases) which may interact through a heat flow through a conducting wall. But consider now that one of the systems, indexed by 2, interacts through a heat flow with a thermostat with constant temperature T_e; the heat conduction coefficient will be denoted λ_e. The interaction with the thermostat at temperature T_e is given by the interaction contact Hamiltonian

$$K_{\text{int}}(x', T_e) = \lambda_e \left[(p_{12} - T_2) + \left(T_e \ln \left(\frac{T_2}{p_{12}} \right) \right) \right]. \tag{52}$$

Notice that this interaction contact Hamiltonian is affine in the control variable T_e. By construction, it satisfies the invariance condition of Theorem 2. The restriction of its associated vector field to the Legendre submanifold projected on the energy coordinate is

$$\left. \frac{dx^0}{dt} \right|_{\mathcal{L}} = \frac{dU}{dt} = \lambda_e \, (T_e - p_{12}), \tag{53}$$

which is simply the energy balance equation. The projection on the temperature coordinates, using the fact that the systems are isochore and $C_{Vi} = \frac{\partial U}{\partial T}$, gives

$$\left. \frac{d}{dt}(p_{11}, p_{12})^t \right|_{\mathcal{L}} = (\dot{T}_1, \dot{T}_2)^t = \begin{pmatrix} -C_{V1}{}^{-1} \lambda(T_1 - T_2) \\ C_{V2}{}^{-1} \lambda(T_1 - T_2) \end{pmatrix} + \begin{pmatrix} 0 \\ C_{V2}{}^{-1} \lambda_e(T_e - T_2) \end{pmatrix}, \tag{54}$$

which is precisely the dynamics of the isolated system (45) augmented with the second term corresponding to the heat flux from the environment into the system 2. The projection on the entropy coordinates gives:

$$\left. \frac{dx^1{}_i}{dt} \right|_{\mathcal{L}} = \frac{dS_i}{dt} = \lambda \left(\frac{1}{T_2} - \frac{1}{T_1} \right) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} T_1 \\ T_2 \end{pmatrix} + \begin{pmatrix} 0 \\ \lambda_e \, (1/T_2 - 1/T_e) \; T_e \end{pmatrix} \tag{55}$$

which are the entropy balance equation (46) of the isolated system augmented with a second term which describes the entropy flow in the system 2 due to the heat flow from the thermostat.

The third example concerns a gas in a cylinder with moving boundary, that is a subpart of Example 4.

EXAMPLE 8. *Gas in a cylinder with moving boundary.* The dynamics of an ideal gas in a cylinder with a moving boundary (the surface of the piston) undergoing some mechanical work, may be defined as a conservative control contact system. This system is defined on the TPS $\mathcal{T}_{\text{gas}} = \mathbb{R} \times \mathbb{R}^6 \ni (x^0, x^j, p_j)$ where x^i denote the extensive variables and p_i the conjugated intensive variables. Its thermodynamic properties are given by the Legendre submanifold already defined in (9). As the gas is considered to be in equilibrium with the control volume, the drift dynamics is of course zero. And the external mechanical work provided by an external pressure

P^e, and variation of volume f_V^e leads to the interaction contact Hamiltonian

$$K_{\text{gas}}^i = (p_2 - P)\, f_V^e, \tag{56}$$

where by definition the pressure of the gas is $P = p_2|_{\mathcal{L}}$. The restriction of the system to the Legendre submanifold followed by a projection on the extensive variables gives the dynamics

$$\begin{aligned} \frac{dS}{dt} &= 0, \\ \frac{dV}{dt} &= -f_V^e, \\ \frac{dN}{dt} &= 0. \end{aligned} \tag{57}$$

4.3. Energy balance equation and port variables

In this paragraph we conclude with some considerations on the definition of output variables conjugated to the input variables in the sense that they define a *power balance equation*. Indeed, the definition of control Hamiltonian systems and the time variation of the Hamiltonian function (or some Legendre transformation with respect to the inputs) lead to the definition of outputs conjugated to the inputs, and include these systems in the class of dissipative systems [41, 4, 36, 39]. From a thermodynamic point of view, each pair of conjugated variables consists of an intensive variable and the rate of its conjugated extensive variable, such as for instance the pair entropy flow and temperature, or the pair molar flow and enthalpy. Any pair has the property that it allows to express either continuity or discontinuity of some flows, or the equilibrium or nonequilibrium conditions at the boundary of the system.

In order to define such pairs of conjugated variables, let us first write the time derivative of an arbitrary function $V \in C^\infty(\mathcal{M})$. A straightforward calculation leads to the following equality [12],

$$\frac{dV}{dt} = s_V^0 + \sum_{j=1}^{m} s_V^j, \tag{58}$$

where s_V^0 is the *internal source term* defined by

$$s_V^0 = \{K_0, V\} + V\frac{\partial K_0}{\partial x^0}, \tag{59}$$

and s_V^j is the *external source term associated with the input* u_j

$$s_V^j = \{K_j, V\} + V\frac{\partial K_j}{\partial x^0}. \tag{60}$$

If, furthermore, there exists a function $y_V^j(x', u_j)$ such that $s_V^j = u_j\, y_V^j$, then (58) may be written in the form

$$\frac{dV}{dt} = \sum_{j=1}^{m} u_j\, y_V^j + s_V, \tag{61}$$

and y_V^j is called the V*-conjugate output variable.*

REMARK 3. If the interaction contact Hamiltonians are linear functions of the inputs, that is, there exists a function $\bar{K}_j$ such that $K_j(x', u_j) = \bar{K}_j(x)\, u_j$, then there exists a port-conjugate output variable

$$y_V^j = \{\bar{K}_j, V\} + V \frac{\partial \bar{K}_j}{\partial x^0}. \tag{62}$$

This is the case of the lift of a port Hamiltonian system, and the gas in a cylinder with moving piston.

If, on the whole TPS, the equality (61) is satisfied with the following conditions: (i) the function V is bounded from below, (ii) the source term s_V is smaller or equal to 0, then the control contact system would be dissipative and the function V is then called a *storage function* [41, 38]. In the particular case when the source term is zero, the system is said to be *lossless*. However, through a few examples we shall see that for thermodynamic systems, the definition of conjugate output variables and the balance equation should be rather considered on the restriction of the control conservative contact system to its Legendre submanifold.

Let us first consider the lift of a port Hamiltonian system considered in Section 3.1.

EXAMPLE 9. *Port-conjugate variable and power balance equation of a lifted port Hamiltonian system.* Consider as a first case the lifted port Hamiltonian system (20)–(22), and the time derivative of the internal Hamiltonian H_0. Then the source term writes

$$s_{H_0} = \Lambda(d_x H_0(x), d_x H_0(x)) = 0. \tag{63}$$

Hence the source term s_{H_0} is zero on the *whole* thermodynamic phase space, and this amounts to saying that the internal Hamiltonian is a conserved quantity on the whole thermodynamic phase space. It is remarkable that the nullity of the source term s_{H_0} (*everywhere on the TPS*) is equivalent to the invariance condition of the contact field $K_{0|\mathcal{L}} = 0$. The H_0-conjugate output defined by the interaction contact Hamiltonian $K_j = \langle dH_0 - p, g_j \rangle$ reads

$$y_{H_0}^j = \mathcal{L}(g_j) H_0. \tag{64}$$

Notice that they are precisely the *port outputs* of a port Hamiltonian system defined in (17). Hence, the power balance equation (18) is satisfied both for the port Hamiltonian system and its lift to the TPS.

Consider now an example including an irreversible system like the heat conduction in Example 5.

EXAMPLE 10. *Heat conduction with thermostat: port-output and power balance equation.* We shall consider example of the heat conduction between two simple thermodynamic systems and with a thermostat as treated in the Examples 5 and 7. We shall analyze here the variation of a natural candidate function for a power balance equation: the internal energy U of the system. A straightforward calculation shows that the source term with respect to the internal energy is

$$\begin{aligned} s_U &= R(p_1)\Lambda\left(\begin{pmatrix} T_1 \\ T_2 \end{pmatrix}, \begin{pmatrix} T_1 \\ T_2 \end{pmatrix}\right) + \left(\frac{\partial U}{\partial x}^T \frac{\partial R}{\partial p}\right)\Lambda\left(\begin{pmatrix} p_{11} \\ p_{12} \end{pmatrix}, \begin{pmatrix} T_1 \\ T_2 \end{pmatrix}\right) \\ &= \left(\frac{\partial U}{\partial x}^T \frac{\partial R}{\partial p}\right)\Lambda\left(\begin{pmatrix} p_{11} \\ p_{12} \end{pmatrix}, \begin{pmatrix} T_1 \\ T_2 \end{pmatrix}\right). \end{aligned} \tag{65}$$

This time, the source term does not vanish on the whole TPS, but it does when *restricted to the Legendre submanifold* $\mathcal{L}_U$, which is the only physically meaningful dynamics.

Consider now the port-conjugate output with respect to the internal energy U of the system

$$\frac{\partial K_{\text{int}}}{\partial p_{12}} \frac{\partial U}{\partial x_2^2} = \lambda_e \frac{p_{12} - T_2}{p_{12}} T_2 = \left[\lambda_e \left(\frac{1}{T_e} - \frac{1}{p_{12}}\right) T_2\right] T_e. \tag{66}$$

This leads us to define the port-conjugate output

$$y_{U_{\text{tot}}} = \lambda_e \left(\frac{1}{T_e} - \frac{1}{p_{12}}\right) T_2, \tag{67}$$

the restriction of which to the Legendre submanifold is precisely the entropy flow into the environment $-\lambda_e\,(T_e - T_2)/T_e$ conjugated to its temperature T_e.

5. Conclusion

In the first instance we have defined a class of contact systems, called *conservative contact systems*, allowing us to describe the dynamics of isolated irreversible thermodynamic systems. They are defined on some contact manifold by two objects: a Legendre submanifold of the contact structure, and a contact vector field. In the context of physical systems' modeling, these objects may be interpreted as follows. The Legendre submanifold describes thermodynamic properties of some physical system according to the classical differential-geometric formulation of equilibrium thermodynamics. The contact vector field is associated with some phenomenological laws induced by some thermodynamical nonequilibrium conditions in the system, and are generated by contact Hamiltonians being the virtual power associated with these phenomena. Furthermore this contact Hamiltonian should satisfy a compatibility condition with the Legendre submanifold, actually should vanish on it, hereby ensuring the invariance of the thermodynamic properties along the trajectories. The class of conservative contact systems has been shown to encompass models such as reversible Hamiltonian systems, and reversible as well as irreversible thermodynamic transformations.

In the second instance we have completed this class of systems in order to cope with models of *open thermodynamic systems*. Therefore we have defined an interaction contact Hamiltonian associated with phenomenological laws describing the interaction of the system with its environment according to some phenomenological laws associated with nonequilibrium conditions between the system and its environment. We have shown that this class of systems, called *control conservative contact systems*, encompasses the class of port Hamiltonian systems as well as coupled mechanical and thermodynamical systems. Finally, we have defined pairs of power conjugated variables associated with the energy flow at the boundary of the system when restricted to the Legendre submanifold.

In our perspective, the definition of the class of conservative contact systems opens the way for further investigations in two main directions. It remains open to define some additional characterizations of a class of contact Hamiltonians (and related Legendre submanifolds) which agree with the second principle of thermodynamics in the sense that one may deduce an entropy creation term. Moreover, the definition of irreversible transformations using contact functions, could also open the way for the definition of irreversible phenomenological laws far from equilibrium and the investigation of global stability properties of irreversible thermodynamic systems. Another open investigation aera concerns the nonlinear control of physical systems. Indeed, the definition of nonlinear contact Hamiltonians opens the way for the definition of power continuous interconnection structures generalizing the interconnection of Hamiltonian systems using Dirac structures [40, 37]. As a consequence the class of nonlinear control laws used in the so-called Passivity Based Control — Interconnection and Damping Assignment [34] could also be generalized and leads to novel stabilizing controllers.

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