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The geometric structure of interconnected thermo-mechanical systems. ⋆

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Abstract: This contribution reports on an ongoing research project aimed in developing a unified theoretical framework for the description of interconnected thermo-mechanical systems with a particular emphasis on thermodynamic engines. We analyse from the geometrical viewpoint the structure of thermodynamic and mechanical interconnection and propose an approach to the unified description of thermo-mechanical systems. The theoretical results are illustrated by a physical example.

Keywords: Hamiltonian systems, Mathematical modelling, Equilibrium thermodynamics, Contact geometry, Interconnected Systems

1. INTRODUCTION

During the last decades there have been a growing interest in geometrical description and interpretation of thermodynamic systems. We refer the interested reader to the works Mrugała et al. (1991); Eberard et al. (2007); Merker and Krüger (2013); Delvenne and Sandberg (2014); Gromov and Caines (2015) and references therein for an overview of different directions of research within this broad field.

One particularly important application of thermodynamics is the design and optimisation of thermodynamic (heat) engines, that is systems that transform heat energy into the mechanic energy. By now, dozens of heat engines have been developed working according to different schemes (i.e., implementing different thermodynamic cycles). However, there is one aspect common for any heat engine: the interaction between the thermodynamic subsystem and the mechanical one. We believe that the geometrical analysis of the interconnection structure of these two systems may allow us to better understand and optimise the overall system in order to achieve maximal possible efficiency.

The main obstacle in developing this programme is that thermodynamic and mechanical systems "live in different worlds": a mechanical system evolves on an even-dimensional symplectic manifold while a thermodynamic system evolves on an odd-dimensional submanifold of a contact manifold (often referred to as the thermodynamic phase space). Recently, there have been several attempts to reconcile these representations. In particular, it was shown that contact vector fields can be used to describe the evolution of dissipative Hamiltonian systems (see Bravetti et al. (2016) and references therein). On the other hand, there are a number of results that attempt to describe thermodynamic systems using the Hamiltonian (symplectic) framework (see, e.g., Morrison (1998); Öttinger (2005)). However, despite many theoretical advances there have not been substantial progress in the geometrical description of interconnected thermo-mechanical systems so far.

In this contribution we use the approach based upon the symplectification of the thermodynamic evolution. It is shown formally that the thermodynamic evolutionary equations can be obtained in the same way as the ones generated by a mechanical Hamiltonian.This approach leads to certain loss of information. However, we argue that this does not restrict the applicability of the approach as we retain most important information. The developed approach is illustrated by a simple, but physically relevant example.

The paper is organized as follows. Section 2 gives a brief overview of modelling Hamiltonian systems with constraints. Section 3 presents necessary facts about the description of thermodynamic evolution and discusses in detail the bundle isomorphism induced by the thermodynamic contact 1-form. In Sec. 4 we discuss different approaches to the description of interconnected systems while Sec. 5 presents an example.

2. HAMILTONIAN SYSTEMS WITH CONSTRAINTS

Consider a controlled mechanical system with the Hamiltonian $H(q,p) : T^*Q \to \mathbb{R}$, where Q is the configuration space which we assume to be equal to $\mathbb{R}^n$. Let there be a number of, generally, non-holonomic constraints expressed as a distribution $C(q) \in T_qQ$ restricting the evolution of the system. We assume that the distribution C is generated by a set of linearly independent 1-forms $\phi^i(q) \in T^*Q$, $i = 1,\dots,k$. This implies that the admissible velocity vectors $\dot{q}$ belong to the kernel of a smooth k-dimensional co-distribution $C^* \subset T^*Q$, i.e. $\dot{q} \in \ker C^*$, which is expressed as $\langle \dot{q}, \sigma\rangle = 0$ with $\sigma \in C^*$ and $\langle\cdot,\cdot\rangle : TQ \times T^*Q \to \mathbb{R}$

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the standard pairing operation or, in algebraic notation, as $C^T(q)\dot{q} = 0$, where $C(q)$ is an $[n \times k]$ matrix whose columns are the components of the 1-forms spanning C^* written in local coordinates.

The distribution C is said to be *involutive* if $X, Y \in C \Rightarrow [X, Y] \in C$, where the square brackets denote the Lie commutator of two vector fields. By Frobenius theorem an involutive distribution can be integrated to yield k smooth functions $c(q)$ such that $X(c) = 0$. These functions are referred to as the first integrals. In this case we say that the respective constraints (2b) are *holonomic*. Otherwise, the constraints are said to be *non-holonomic*. In practice, the set of constraints include both holonomic and non-holonomic constraints.

An unconstrained Hamiltonian system evolves on the state space manifold T^*Q which is endowed with the canonical symplectic form $\omega = dq^i \wedge dp_i$ (here and henceforth the Einstein summation convention is implied). This symplectic form defines a canonical isomorphism between the tangent and cotangent bundles: $\Omega : T(T^*Q) \to T^*(T^*Q)$ defined by $\Omega(X)(\cdot) = \omega(X, \cdot)$. The vector field, corresponding to the Hamiltonian H, is defined as $X_H = \Omega^{-1}(dH)$, i.e. $\omega(X_H, \cdot) = dH$.

When dealing with the constrained system, the Hamiltonian function has to be augmented to take into account the constraints. Thus, we define the constrained vector field as follows:

$$X_{H,\phi} = \Omega^{-1}(dH + \lambda_i \pi_Q^* \phi^i), \tag{1}$$

where $\pi_Q : T^*Q \to Q$ is the projection of the cotangent bundle on its base and π_Q^* is the pull-back of π_Q which lifts ϕ^i to $T^*(T^*Q)$.

In local coordinates, the dynamics of a port-Hamiltonian system with constraints is described by a set of differential-algebraic equations of the form (Neimark and Fufaev, 1972; Arnold et al., 2006; Castaños et al., 2013):

$$\dot{x} = J\nabla H(x) + \hat{C}(x)\lambda + \hat{g}(x)u \tag{2a}$$

$$\mathbf{0} = C^T(q)\nabla_p H(x) \tag{2b}$$

$$y = \nabla^T H(x)\hat{g}(x)\ , \tag{2c}$$

where H is the Hamiltonian (energy) function of the unconstrained system, the state is given by $x^T = \begin{pmatrix} q^T & p^T \end{pmatrix}$ with $r \in Q$ and $p \in T_r^*Q$ the positions and momenta, respectively; $\hat{C}(x) = \begin{pmatrix} \mathbf{0}_{[k\times n]} & C^T(x) \end{pmatrix}^T$, $\lambda \in \mathbb{R}^k$ is the vector of implicit variables that enforce the constraints; $(u, y) \in \mathbb{R}^{*m} \times \mathbb{R}^m$ are the conjugated external port variables, and $\hat{g}(x) = \begin{pmatrix} \mathbf{0}_{[m\times n]} & g^T(x) \end{pmatrix}^T$ is a $(2n \times m)$-matrix such that $\operatorname{rank} \hat{g}(x) = m$ for all $x \in \mathbb{R}^n \times \mathbb{R}^{*n}$. The $[2n \times 2n]$-matrix J is the one associated with the canonical symplectic form,

$$J = \begin{pmatrix} 0_n & I_n \\ -I_n & 0_n \end{pmatrix}\ .$$

Here and forth all functions are assumed to be smooth enough and the gradient is assumed to be a column vector.

The vector field $X \in T(T^*\mathbb{R}^n)$ is written as

$$X = D_H + D_c\lambda + X_g u \tag{3}$$

where

$$D_H = \Omega^{-1}(dH) = \frac{\partial H}{\partial p_i}\frac{\partial}{\partial q^i} - \frac{\partial H}{\partial q^i}\frac{\partial}{\partial p_i} \tag{4}$$

is the Hamiltonian vector field,

$$D_C\lambda = C_i^j(q)\lambda_j \frac{\partial}{\partial p_i} \tag{5}$$

is the vector field of the internal (constraint) forces, and

$$X_g u = g_i^j u_j \frac{\partial}{\partial p_i}$$

is the control vector field.

Equation (2b) constrains the configuration space of (2) and can be written as $D_C(H) = 0$. This is equivalent to saying that the internal forces do not produce work as there is no displacement in the direction of the constraint forces and hence they do not alter the total energy of the system. However, this may not be true in general, when non-holonomic constraints of general form are considered (see, e.g., (Bloch, 2003; Baruh, 1999)).

3. THERMODYNAMIC CONTACT VECTOR FIELDS

In this section, we present a brief overview of the geometric approach to the description of thermodynamic systems' evolution. For a more detailed treatment see Callen (1985); Kondepudi and Prigogine (1998) for thermodynamics, Geiges (2008); Arnold (1989) for contact geometry, and Mrugała et al. (1991); Gromov and Caines (2015) for the contact description of thermodynamics.

3.1 Contact geometry basics

In the following, we will consider single phase, single component homogeneous thermodynamic systems that do not undergo any chemical transformations. The state space of such a system can be represented as an embedded manifold in the thermodynamic phase space $\mathcal{M}$. This manifold is shown to be an integral (*Legendre*) manifold corresponding to a specific contact 1-form.

Definition 1. Let $(x^0, x^1, \ldots, x^n, y_1, \ldots, y_n)$ be the local coordinates on $\mathcal{M}$. The *canonical thermodynamic contact 1-form* is defined as

$$\alpha = dx^0 - y_i dx^i, \qquad 1 \le i \le n. \tag{6}$$

Each Legendre manifold on $(\mathcal{M}, \alpha)$ is uniquely determined by a particular function.

Lemma 2. (Arnold (1989)). Let $\mathcal{N} = \{1, \ldots, n\}$ be the set of indices. Given the contact form (6), a disjoint partitioning $I, J \subset \mathcal{N}$, $I \cap J = \emptyset$, $I \cup J = \mathcal{N}$ with n_I and n_J components, $n_I + n_J = n$, and a smooth function $\zeta(x^i, y_j)$, $i \in I, j \in J$, the following equations define the Legendre manifold $\mathcal{L}_\zeta$ on $(\mathcal{M}, \alpha)$:

$$\lambda^0(x, y) = x^0 - \zeta + y_j \frac{\partial \zeta}{\partial y_j} = 0, \tag{7a}$$

$$\lambda^j(x, y) = x^j + \frac{\partial \zeta}{\partial y_j} = 0, \tag{7b}$$

$$\lambda_i(x, y) = y_i - \frac{\partial \zeta}{\partial x^i} = 0. \tag{7c}$$

The variables (x^i, y_j), $i \in I, j \in J$ can be chosen as local coordinates in some open neighbourhood of $a \in \mathcal{L}_\zeta$. The