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A symplectic formulation of open thermodynamic systems

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***Abstract*— In this work we expand on the symplectic formulation of thermodynamic systems exposed in [30], [16], and inspired by [3]. The main novel contribution is the geometric formulation of *open* thermodynamic systems as a homogeneous Lagrangian submanifold of the product of the symplectized thermodynamic phase space and a space of external variables. This leads to a natural property of shifted passivity to be used for analysis and control. Furthermore, it will be discussed how this homogeneous Lagrangian submanifold admits a natural (singular) Riemannian metric.**

I. Extended Abstract

A. Introduction

The geometric formulation of mechanical systems has spurred *symplectic geometry*; see e.g. the classical textbooks [2], [1], [14]. Symplectic geometry was also underlying the formulation of *Hamiltonian input-output systems*, starting with the ground-breaking paper [5] and continued in e.g. [25], [28], [26]. By generalizing symplectic and Poisson structures to Dirac structures, and by emphasizing port-based modeling of multi-physics systems, this also led to the theory of *port-Hamiltonian systems*; see e.g. [15], [29], and the introductory survey [31].

The geometric formulation of thermodynamics has remained more elusive. Starting from Gibbs fundamental relation, *contact geometry* was recognized as an appropriate geometric framework; see [13], [18], [19], [20], [21], [6]. Recently, the interest in contact-geometric descriptions of thermodynamics has been intensified; see e.g. [17], [4], [12],[11], [9]. In particular, this has led to the theory of *contact control systems*, see [7], [8], [22], [23], [24].

On the other hand, it is well-known in geometry that contact manifolds can be naturally *symplectized* to symplectic manifolds with an additional structure of *homogeneity*; see [2], [14] for textbook expositions. Nevertheless, the applications of this symplectization procedure appear to be largely confined to *time-dependent* Hamiltonian mechanics [14] and partial differential equations [2]. Only in [3] it was argued that the symplectization of contact manifolds provides an insightful viewpoint to thermodynamic systems as well.

Inspired by [3], and motivated by control problems in physical systems with thermodynamic components, our recent work [30], [16] expands the symplectization point of view. In [30] the definition of *homogeneous Hamiltonian control systems* was provided, by symplectization of the notion of contact control systems developed in [6], [7], [8], [22], [23], [24], [17]. Furthermore, in the companion paper [16] a number of examples of multi-physics and thermodynamical systems was treated within this geometric framework.

In this talk we will continue on the work in [30], [16] by focussing on the geometric formalization of the state properties of open thermodynamic systems as homogeneous Lagrangian submanifolds of the product of the symplectized thermodynamic phase space with the space of external variables.

B. The geometric framework

Recall the definition of a *contact manifold*; see [2], [14]. A contact manifold is a $(2n+1)$-dimensional manifold M equipped with a maximally non-integrable field of hyperplanes ξ. This means that $\xi = \ker \theta \subset TM$ for a, possibly only locally defined, 1-form θ on M satisfying

$$\theta \wedge (d\theta)^n \neq 0 \tag{1}$$

By Darboux's theorem there exist local coordinates $q^0, q^1, \cdots, q^n, \gamma_1, \cdots, \gamma_n$ for M such that

$$\theta = dq^0 - \sum_{i=1}^{n} \gamma_i dq^i \tag{2}$$

The canonical example of a contact manifold is the following; see e.g. [2]. Consider an $(n+1)$-dimensional manifold Q, and consider at any point $q \in Q$ the set of n-dimensional subspaces of the $(n+1)$-dimensional tangent space T_qQ. This defines an $(2n+1)$-dimensional manifold M, which is a fiber bundle over the base space manifold Q. A field of hyperplanes ξ on M is defined by considering at each point $(q, S) \in M$, with $q \in Q$ and S an n-dimensional subspace of T_qQ, the subspace of all tangent vectors at (q, S) which are such that the projection to T_qQ is contained in the n-dimensional subspace S. It can be readily verified that the thus defined field of hyperplanes ξ is indeed maximally non-integrable. Obviously, any n-dimensional subspace of the tangent space T_qQ can be identified with all non-zero multiples of some cotangent vector in T_q^*Q, whose kernel equals this subspace. Hence it follows that the thus defined canonical contact manifold is equal to the projectivization $\mathbb{P}(T^*Q)$ of the cotangent bundle T^*Q, i.e., the fiber bundle over Q with fiber at any point $q \in Q$ given by the projective space $\mathbb{P}(T_q^*Q)$. (Recall that elements of $\mathbb{P}(T_q^*Q)$ are identified with rays in T_q^*Q, i.e., non-zero multiples of non-zero cotangent vectors.) Furthermore, $q^0, \cdots, q^n$ in (2) can be taken to be coordinates for Q. Finally, from Darboux's theorem it follows that any $(2n+1)$-dimensional manifold M

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is locally *contactomorphic* to a canonical contact manifold $\mathbb{P}(T^*Q)$ with $\dim Q = n+1$.

Any $(2n+1)$-dimensional contact manifold M can be *symplectized* to a $(2n+2)$-dimensional symplectic manifold; see [2], [14]. In case of $M = \mathbb{P}(T^*Q)$ this is very clear: the symplectization of $\mathbb{P}(T^*Q)$ is simply given by the cotangent bundle T^*Q without its zero-section; denoted by T_0^*Q. The projection from T_0^*Q to $\mathbb{P}(T^*Q)$, taking non-zero cotangent vectors to the corresponding equivalence classes (rays) in the cotangent space will be denoted by

$$\pi : T_0^*Q \to \mathbb{P}(T^*Q) \tag{3}$$

The cotangent bundle T^*Q, as well as T_0^*Q, is endowed with its *canonical* 1*-form* α, in natural coordinates

$$(q,p) = (q^0, q^1, \cdots, q^n, p_0, p_1, \ \cdots, p_n) \tag{4}$$

for T^*Q given by

$$\alpha = \sum_{i=0}^{n} p_i dq^i, \tag{5}$$

as well as its *canonical symplectic form* $\omega := d\alpha$ expressed as

$$\omega = d\alpha = \sum_{i=0}^{n} dp_i \wedge dq^i \tag{6}$$

Note that the contact form θ on $\mathbb{P}(T^*Q)$, as well as the local Darboux coordinates as in (2) for θ, are obtained from α and the natural coordinates (4) for T_0^*Q as follows. Consider local coordinates $q^0, q^1, \cdots, q^n, p_0, p_1, \ \cdots, p_n$ as in (4), and consider a neighborhood where e.g. $p_0 \neq 0$. Then define

$$\gamma_i := -\frac{p_i}{p_0}, \qquad i = 1, \cdots, n \tag{7}$$

It follows that

$$\alpha = p_0(dq^0 - \sum_{i=1}^{n} \gamma_i dq^i) = p_0\theta \tag{8}$$

Performing the same construction for *any* coordinate $p_j \neq 0$ (instead of p_0) this yields different definitions for $\gamma_1, \cdots, \gamma_n$. This corresponds in the case of thermodynamical systems to the choice of different representations; e.g. the *energy representation* of a thermodynamical systems instead of its *entropy representation*; see [16] for the treatment of a number of examples.

C. Homogeneity and correspondence between $\mathbb{P}(T^*Q)$ and T_0^*Q

It turns out that there is a one-to-one correspondence between *contact Hamiltonian* vector fields on $\mathbb{P}(T^*Q)$ and ordinary Hamiltonian vector fields on the symplectic manifold T_0^*Q by restricting the Hamiltonians on T_0^*Q to Hamiltonians that are homogeneous of degree 1 in the p-variables. Similarly, there is a correspondence between *Legendre submanifolds* of $\mathbb{P}(T^*Q)$ and *Lagrangian submanifolds* of T_0^*Q satisfying a homogeneity property.

Definition 1.1: A function $h : T_0^*Q \to \mathbb{R}$ is called homogeneous (of degree 1 in $p_0, \cdots, p_n$) if

$$\begin{aligned} &h(q^0, q^1, \cdots, q^n, \lambda p_0, \lambda p_1, \cdots, \lambda p_n) = \\ &\lambda h(q^0, q^1, \cdots, q^n, p_0, p_1, \cdots, p_n), \quad \forall \lambda \neq 0 \end{aligned} \tag{9}$$

Homogeneity is characterized by *Euler's theorem*. First, consider T_0^*Q with its canonical 1-form α. Define the dilation vector field D by

$$i_D d\alpha = \alpha \tag{10}$$

Proposition 1.2: A differentiable function $h : T_0^*Q \to \mathbb{R}$ is homogeneous if and only if

$$\sum_{i=0}^{n} p_i \frac{\partial h}{\partial p_i}(q,p) = h(q,p), \qquad \text{for all } (q,p) \in T_0^*Q \tag{11}$$

or equivalently $\mathcal{L}_D h = h$, with $\mathcal{L}$ denoting the Lie derivative.

Furthermore [30], if $h : T_0^*Q \to \mathbb{R}$ is homogeneous then the ordinary Hamiltonian vector field X_h on T_0^*Q generated by h satisfies

$$\mathcal{L}_{X_h}\alpha = 0 \tag{12}$$

Conversely, if $\mathcal{L}_{X_h}\alpha = 0$ then h up to a constant is homogeneous.

Recall that a vector field X on a contact manifold is called a *contact vector field* if

$$\mathcal{L}_X\theta = \rho\theta \tag{13}$$

for some function ρ. Furthermore, the function $K := \theta(X)$ is called the *contact Hamiltonian* of the contact vector field X. Conversely, for any differentiable function K it can be shown that there exists a unique contact vector field X such that $K = \theta(X)$, and we denote this contact vector field by X_K.

It can be shown that every contact Hamiltonian vector field on the contact manifold $\mathbb{P}(T^*Q)$ can be *lifted* to an ordinary Hamiltonian vector field X_h on T_0^*Q with a homogeneous Hamiltonian h, and conversely, that every ordinary Hamiltonian vector field X_h on T_0^*Q with homogeneous Hamiltonian h projects (under π) to a contact vector field on $\mathbb{P}(T^*Q)$ with contact Hamiltonian K given by the projection of the homogeneous Hamiltonian h. Furthermore, this correspondence is such that the *Jacobi bracket* of two contact Hamiltonians corresponds to the *Poisson bracket* of the corresponding homogeneous Hamiltonians [2].

With regard to the correspondence between Legendre submanifolds of $\mathbb{P}(T^*Q)$ and Lagrangian submanifolds of T_0^*Q the story is as follows. Recall that a *Legendre submanifold* L of the contact manifold $\mathbb{P}(T^*Q)$ is an integral manifold of θ of maximal dimension. It follows that for an $(n+1)$-dimensional Q the dimension of a Legendre submanifold of $\mathbb{P}(T^*Q)$ is n. On the other hand, a *Lagrangian submanifold* L_s of the symplectic space T_0^*Q is a manifold of maximal dimension restricted to which the symplectic form $\omega = d\alpha$ is zero. For Q being $(n+1)$-dimensional the dimension of a Lagrangian submanifold $L_s \subset T_0^*Q$ is $n+1$.

Definition 1.3: A Lagrangian submanifold $L_s \subset T_0^*Q$ is called homogeneous if $(q,p) \in L_s$ implies $(q, \lambda p) \in L_s$ for

every $\lambda \neq 0$, or equivalently, the dilation vector field D is tangent to L_s everywhere.
Homogeneity of L_s can be nicely characterized as follows.

Proposition 1.4: A Lagrangian submanifold $L_s \subset T_0^*Q$ is homogeneous if and only if α restricted to L_s is zero.
We mention that homogeneity of Lagrangian submanifolds equivalently can be expressed in terms of homogeneity of their *generating functions*, and this was in fact the point of view taken in [3].

Overall, it follows that the *contact-geometric* formulation of thermodynamic systems can be immediately translated to a *symplectic* formulation, with Hamiltonians and Lagrangian submanifolds that are *homogeneous* (with an extra 'gauge' variable p_0). The symplectization not only simplifies the structure of the theory and the computations, but also offers a natural framework for defining the state properties of *open* thermodynamic systems as indicated in the next subsection.

D. State properties of open thermodynamic systems

As discussed in [3], see [30], [16] for an in-depth geometric exposition, the *state properties* of a thermodynamic system are specified by a homogeneous Lagrangian submanifold $L_s \subset T_0^*Q$. The generating function of this Lagrangian submanifold corresponds to a thermodynamic potential such as internal energy or entropy. In the present talk we will extend this point of view to the geometric characterization of an *open* thermodynamic system, where next to the thermodynamic potential the interaction port of the thermodynamic system with its environment is explicitly modeled. This is captured by a homogeneous Lagrangian submanifold of the product of T_0^*Q with the set of external (port) variables.

Such definition naturally leads to a uniform *shifted passivity* property of open thermodynamical systems, with storage function given by the *availability function* corresponding to the thermodynamic potential of the homogeneous Lagrangian submanifold. (The availability function is also called the *shifted storage function* [27], or Bregman divergence, in the context of passive systems.) Obviously, this has immediate implications for analysis and control. Furthermore, we will characterize the *invariance* of this Lagrangian submanifold with respect to external processes. Finally we will show how the homogeneous Lagrangian submanifold is endowed with a (singular) Riemannian metric (see also [19] and references therein), which plays an important role in the stability analysis.

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