On a geometrical formulation of open thermodynamical systems

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- Contact geometry and thermostatics.
- Dynamics of thermodynamic systems; control contact systems.
- Lifting of port-Hamiltonian systems to contact manifold

Thermostatics and contact geometry

(Hermann, Mrugala)

The *thermodynamic phase space*, on which the thermodynamic properties of a system are defined, is a **contact manifold** endowed with a **contact structure**.

Typical example of a contact manifold:

Let $\mathcal{N}$ be an n-dimensional manifold. Define the associated thermodynamic phase space $\mathcal{T}$ as $\mathbb{R} \times T^*\mathcal{N}$ whose elements are denoted (x^0, x, p). It has a canonical contact structure defined by the contact form

$$\theta = \mathrm{d}x^0 - \sum_{k=1}^{n} p_k \mathrm{d}x^k,$$

where d denotes the exterior derivative.

General definition of a contact manifold

Definition 1 *A* 1*-form* θ *on a* $2n+1$*-dimensional manifold* $\mathcal{T}$ *is a contact form if* $\theta \wedge (d\theta)^n$ *is a volume form. Then the pair* $(\mathcal{T}, \theta)$ *is called a contact manifold.*

Proposition 2 *Given a contact form* θ *on a* $2n+1$*-dimensional manifold* $\mathcal{T}$*. Then there exists local coordinates* (x^0, x, p) *for* $\mathcal{T}$ *such that*

$$\theta = dx^0 - \sum_{k=1}^{n} p_k dx^k,$$

In thermodynamic systems x^0 is associated with a thermodynamic potential, such as the energy U, the enthalpy H, etc., and (x^i, p_i) denotes the pairs of conjugated extensive and intensives variables, such as the pairs of volume V and pressure P, entropy S and temperature T, number of moles N_i and chemical potentials μ_i.

The Gibbs' relation

$$\mathrm{d}U = T\mathrm{d}S - P\mathrm{d}V + \mu_i \mathrm{d}N^i$$

corresponds to the definition of a canonical submanifold of a contact manifold, called *Legendre submanifold*.

Definition 1 *A* Legendre submanifold *of a contact manifold* $(\mathcal{T}, \theta)$ *is an* n*-dimensional submanifold of* $\mathcal{T}$ *that is an integral manifold of* θ*.*

Legendre submanifolds are locally generated by a *generating function*.

Theorem 1 *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 formulas*

$$x^0 = F - p_J \frac{\partial F}{\partial p_J}, \quad x^J = -\frac{\partial F}{\partial p_J}, \quad p_I = \frac{\partial F}{\partial x^I} \tag{1}$$

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

Consider the particular case of a generating function F which is a differentiable function on $\mathcal{N}$. The Legendre submanifold is then the set

$$\mathcal{L}_F := \left\{ x^0 = F(x), x, p = \frac{\partial F}{\partial x}(x) \right\}$$

For thermodynamic systems, the generating functions are potentials such as U, G, etc., while the associated Legendre submanifold defines the thermodynamic properties of the system, an ideal gas.

Example 3 *Consider an ideal gas. One way to express its thermodynamic properties is to use the contact form*

$$\theta_G := dG + SdT - VdP - \mu dN$$

with generating function being the Gibbs free energy G (where R is the ideal gas constant):

$$G(T,P,N) = \frac{5}{2}R(1 - \ln(\frac{T}{T_0})) - NT(S_0 - R\ln(\frac{P}{P_0})$$

The generated Legendre submanifold is

$$\begin{aligned}
x^0 &= G(T,P,N) \\
p_1 &= -S(T,P,N) = \tfrac{\partial G}{\partial T} = NS_0 + 5/2NR\ln(\tfrac{T}{T_0}) - NR\ln(\tfrac{P}{P_0}) = S \\
p_2 &= V(T,P,N) = \tfrac{\partial G}{\partial P} = NR\tfrac{T}{P} \\
p_3 &= \mu(T,P,N) = \tfrac{\partial G}{\partial N} = 5/2RT - T\tfrac{S}{N}
\end{aligned}$$

However, one may also take as coordinates for the Legendre submanifold the extensive variables S, V, N. In this case the generating function is the internal energy U obtained by the Legendre transform of G as

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

where

$$\gamma(S,V,N) = (S - NS_0 + NRln(NRT_0) - NR\ln(VP_0))/(\frac{3}{2}NR)$$

with the contact form given as

$$\theta = dU - TdS + PdV - \mu dN$$

Thermo**dynamics**

Definition 4 *A vector field X on $(\mathcal{T}, \theta)$ is a* **contact vector field** *if and only if there exists a differentiable function ρ such that*

$$L_X \, \theta = \rho \, \theta,$$

where L_X denotes the Lie derivative with respect to the vector field X.

The set of contact vector fields forms a Lie subalgebra of the Lie algebra of vector fields.

There exists a mapping between contact vector fields and differentiable functions on $\mathcal{T}$. To every contact vector field X one associates the function $\mathcal{T}$

$$f = \theta(X)$$

This function f is called the *contact Hamiltonian*. Conversely, to every function f there corresponds the contact vector field X_f given as

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

The mapping $f \to X_f$ defines an isomorphism from the Lie algebra structure of the contact vector fields to the Lie algebra structure on the space of contact Hamiltonians defined by the following bracket ('*Jacobi bracket*'):

$$\{f, g\} = \theta([X_f, X_g])$$

where $[\cdot, \cdot]$ is the usual Lie bracket.

(This replaces the usual isomorphism between the Lie algebra of Hamiltonian vector fields and the Lie algebra of functions with respect to the Poisson bracket (modulo $\mathbb{R}$), on any symplectic manifold (e.g. a cotangent bundle $T^*\mathcal{N}$)).

Theorem 2 (Mrugala) *Let* $(\mathcal{T}, \theta)$ *be a contact manifold and* $\mathcal{L}$ *a Legendre submanifold. Then* X_K *is tangent to* $\mathcal{L}$ *if and only if* K *is identically zero on* $\mathcal{L}$.

Example 5 *Let the generating function of* $\mathcal{L}$ *be* $U(x^i, p_j), i \in I, j \notin I, I \subset \{1, \cdots, n\}$. *Consider the contact Hamiltonian*

$$K = x^0 - U + p_j \frac{\partial U}{\partial p_j}$$

This generates a reversible transformation. In the example of the ideal gas

$$K = PV - NRT$$

'Real' dynamics corresponds to the case where the contact Hamiltonian K represents the (irreversible) dynamics in the system due to non-equilibrium conditions (e.g., due to heat conduction or chemical reaction kinetics).

Control contact systems

Definition 2 *Let* $(\mathcal{T}, \theta)$ *be a contact manifold and* $\mathcal{L}$ *a Legendre submanifold. A* control contact system *on* $\mathcal{T}$ *is determined by an input space* $\mathcal{U} = \mathbb{R}^m$ *and inputs* $u_j,\ j = 1, .., m$*, together with* $m + 1$ *contact Hamiltonian functions :* K_0 *the internal contact Hamiltonian and* $K_j,\ j = 1, \ldots, m$ *the interaction contact Hamiltonians, all satisfying the invariance condition :* $K_{l|\mathcal{L}} \equiv 0$*,* $l = 0, \ldots, m$*. The dynamics of the control contact system is given by*

$$X_{K_0} + \sum_{j=1}^{m} u_j \, X_{K_j} \, .$$

- The Legendre submanifold $\mathcal{L}$ represents the thermodynamic properties of the system.
- The internal contact Hamiltonian K_0 represents the law giving the dynamics due to non-equilibrium conditions *in* the system (for instance due to heat conduction or chemical reaction kinetics).
- The interaction contact Hamiltonians K_j provide the flows due to the non-equilibrium of the system with its environment.

Example 6 (Ideal gas in a cylinder with moving piston)
Define the interaction contact Hamiltonian

$$K(x,p) = (P - p_2)$$

This leads to $\frac{dV}{dt} = u$.

How to merge thermodynamical systems with port-Hamiltonian systems ?

Lifting of conservative systems on $\mathcal{N}$ to $\mathbb{R} \times T^*\mathcal{N}$

Consider a closed dynamical system on $\mathcal{N}$:

$$\dot{x} = f(x), x \in \mathcal{N}$$

This can be *lifted* to the contact vector field X_{K_f} on $\mathbb{R} \times T^*\mathcal{N}$ with contact Hamiltonian

$$K_f(x^0, x, p) = -p^T f(x)$$

Lemma 7 *Consider a Legendre submanifold $\mathcal{L}_H$ with generating function $H(x)$. Then K_f is zero restricted to $\mathcal{L}_H$ if and only if*

$$\dot{H} = L_f H = 0$$

Thus: X_{K_f} defines a dynamics on $\mathcal{L}_H$ if and only if $\dot{x} = f(x)$ is conservative with respect to H.

Remark 8 *In this case the dynamics X_{K_f} on $\mathcal{L}_H$ can be described in terms of the extensive variables x as*

$$\dot{x} = f(x),$$

and equally well in terms of the intensive variables p, provided that the map

$$p = \frac{\partial H}{\partial x}(x)$$

is injective. The dynamics in extensive variables p is then given by

$$\dot{p} = -\frac{\partial K}{\partial x} = -(Df)^T(x)p$$

with Df the Jacobian of f. (For LC-circuits this yields the **Brayton-Moser equations***.)*

In particular, the Hamiltonian dynamics

$$\dot{x} = J(x)\frac{\partial H}{\partial x}(x)$$

can be lifted to a contact vector field with contact Hamiltonian

$$K(x,p) = -p^T J(x)\frac{\partial H}{\partial x}(x)$$

which is clearly zero on the Legendre submanifold

$$\mathcal{L}_H := \left\{ x^0 = H(x), x, p = \frac{\partial H}{\partial x}(x) \right\}.$$

Note that the contact Hamiltonian has the dimension of **power** (and not of **energy**).

A Hamiltonian dynamics **with** energy dissipation

$$\dot{x} = [J(x) - R(x)]\frac{\partial H}{\partial x}(x)$$

may be also lifted to a contact vector field by adding an extra extensive variable S ('entropy'), and defining the contact Hamiltonian

$$K(x, S, p, T) = -p^T[J(x) - R(x)]\frac{\partial H}{\partial x}(x) - \frac{T}{T_0}\frac{\partial H}{\partial x}(x)R(x)\frac{\partial H}{\partial x}(x)$$

which obviously is zero on the Legendre submanifold

$$\left\{x^0 = H(x), x, S, p = \frac{\partial H}{\partial x}(x), T = T_0\right\}.$$

Finally, port-Hamiltonian systems with inputs

$$\dot{x} = [J(x) - R(x)]\frac{\partial H}{\partial x}(x) + \sum g_j(x)u_j$$

are lifted to control contact systems by defining the interaction contact Hamiltonians

$$K_j(x,p) = g_j^T(x)[\frac{\partial H}{\partial x}(x) - p]$$

Port contact systems

Compute the time derivative of a function V on $\mathcal{T}$ with respect to a control contact system:

$$\frac{\mathrm{d}V}{\mathrm{d}t} = \sum_{j=1}^{m} u_j \, y_V^j + \sigma_V \, ,$$

where y_V^j is the V-*conjugated output variable* :

$$y_V^j = \{K_j, V\} + V \frac{\partial K_j}{\partial x^0}, \tag{2}$$

and σ_V is a *source term* defined by :

$$\sigma_V = \{K_0, V\} + V \frac{\partial K_0}{\partial x^0}.$$

Definition 3 *A* conserved quantity *of a control contact system is a function* V *on* $\mathcal{T}$ *such that* $\sigma_{V|\mathcal{L}} = 0$.

Using the definition of a conjugated output (2), we are now able to define a *port contact system* as follows:

Definition 4 *A* port contact system *is a control contact system, with the additional condition that there exists a generating function U of a Legendre submanifold that is a conserved quantity (i.e. $\sigma_{U|\mathcal{L}_U} = 0$), completed with the U-conjugated outputs defined in (2). The port contact system is denoted by $(\mathcal{T}, U, K_j)$.*

Conclusions

- Definition of the thermodynamic phase space and Legendre submanifold corresponding to thermo**statics**.
- Thermo**dynamics** defined by contact vector fields with contact Hamiltonian zero on the Legendre submanifold.
- Lifting of conservative, in particular Hamiltonian, systems to the Legendre submanifold.
- Lifting of Hamiltonian dynamics with energy dissipation.
- Mixed 'thermodynamical' and 'non-thermodynamical' systems.