Geometry of non-equilibrium thermodynamics: a homogeneous symplectic approach

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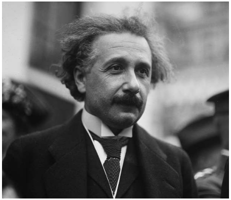
Famous quote on classical, macroscopic, thermodynamics taken from Albert Einstein's autobiographical notes:

A theory is more impressive the greater the simplicity of its premises, the more different things it relates, and the more extended its area of applicability. Hence the deep impression that classical thermodynamics made upon me.
It is the only physical theory of universal content concerning which I am convinced that, within the framework of the applicability of its basic concepts, it will never be overthrown.



Note: thermodynamics directly originates from engineering (maximal efficiency of steam engines, ..).

Geometric modeling of thermodynamic systems

Whereas the geometry of Equilibrium Thermodynamics is well-known (Gibbs, Maxwell (1880s), Hermann (1960s), Arnold (1989), Mrugala (1970s) ..), there are several competing formulations for geometric irreversible thermodynamics:

- Metriplectic/GENERIC (Grmela, Öttinger et al.,)
- Irreversible Port Hamiltonian systems (Ramirez et al., 2013)
- variational formulations (Gay-Balmaz & Yoshimura, 2017)
- contact control Hamiltonian systems (Eberard et al. 2007 ...)

embedding the energy and entropy balance equations !

Recent interest in mathematical physics (black-hole thermodynamics, ..), information theory (thermodynamically consistent machine learning ..), as well as in engineering (thermal/hysteresis effects in mechatronics, heat networks, chemical engineering, .. nonlinear control).

Our motivation: to formulate a geometric, coordinate-free theory of irreversible thermodynamic systems and their interconnections, generalizing the port-Hamiltonian formulation of multi-physics systems.

Main points

- Starting from Gibbs' relation contact geometry has been recognized as appropriate geometric framework for thermodynamics: $(n+1)$ extensive - n intensive thermodynamical variables.
- Contact manifolds are canonically symplectized: gauge variable, projective geometry.
- Irreversible thermodynamical processes are defined by homogeneous Hamiltonian functions

Leads to unifying symplectic geometric formulation of (irreversible) thermodynamic processes which :

- unifies of energy and entropy representations
- eases computations
- leads to a natural definition of ports

Outline

1. Gibbs and contact geometry
2. From contact geometry to homogeneous symplectic geometry
3. Definition of port-thermodynamic systems
4. Examples
5. Conclusions

Simplest context: consider a *closed* thermodynamic system:

extensive variables: volume V and entropy S, internal energy E

intensive variables: pressure P, temperature T

Its thermodynamic properties are formalized by Gibbs' relation

$$dE = TdS - PdV$$

More generally for mixtures:

extensive variables, V, S, E and number of moles $N_1, \cdots, N_m$,

intensive variables P, T and chemical potentials $\mu_1, \cdots, \mu_m$,

Gibbs' relation

$$dE = TdS - PdV + \mu_1 dN_1 + \cdots + \mu_m dN_m,$$

What does Gibbs' relation $dE = TdS - PdV$ mean?

Pragmatic answer: If E is expressed as function of the other two extensive variables V, S

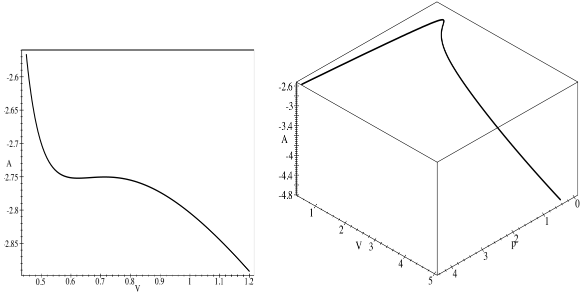
$$E = E(V, S),$$

then the two intensive variables $-P$, T are determined as

$$-P = \frac{\partial E}{\partial V}(V, S), \quad T = \frac{\partial E}{\partial S}(V, S)$$

Geometric point of view: Gibbs' equation (in the isentropic case) defines the submanifold $L \subset \mathbb{R}^3$ given as

$$L = \{(V, E, -P) \in \mathbb{R}^5 \mid E = E(V), -P = \frac{\partial E}{\partial V}\}$$



(Figures taken from Ph.D. thesis of L.Bennayoun, 1999)

Geometric point of view: Gibbs' equation defines the submanifold $L \subset \mathbb{R}^5$ given as

$$L = \{(V, S, E, -P, T) \in \mathbb{R}^5 \mid E = E(V,S), -P = \frac{\partial E}{\partial V}, T = \frac{\partial E}{\partial S}\}$$

Different ways of locally parametrizing given by thermodynamic potentials obtained by Legendre transformation of $E(V,S)$

$$\begin{array}{rcll} F(V,T) & = & E(V,S) - TS, & \text{Helmholtz energy} \quad \text{coord. } V, T \\ H(P,S) & = & E(V,S) + PV, & \text{enthalpy} \quad \text{coord. } P, S \\ G(P,T) & = & H(P,S) - TS, & \text{Gibbs' free energy} \quad \text{coord. } P, T \end{array}$$

Contact geometric point of view

On the space $\mathbb{R}^5 \ni (V, S, E, -P, T)$ of extensive and intensive variables, consider the contact form

$$\theta := dE - TdS + PdV,$$

State properties are described by maximal submanifolds L restricted to which θ is zero; i.e., on L

$$0 = \theta_L = dE - TdS + PdV \quad \text{i.e., Gibbs' relation}$$

Any such L is 2-dimensional.

L is called a Legendre submanifold of $(\mathbb{R}^5, \theta)$.

Thus the thermodynamic properties are defined by a Legendre submanifold of $\mathbb{R}^5$.

For any such L there exists locally at least one parametrization by $E(V,S), F(V,T), H(-P,S)$, or $G(-P,T)$, such that

$$L = \{(V,S,E,-P,T) \mid E = E(V,S), -P = \frac{\partial E}{\partial V}, T = \frac{\partial E}{\partial S}\}$$

or

$$L = \{(V,S,E,-P,T) \mid E = F(V,T) - T\frac{\partial F}{\partial T}, -P = \frac{\partial F}{\partial V}, S = -\frac{\partial F}{\partial T}\}$$

or

$$L = \{(V,S,E,-P,T) \mid E = H(-P,S) + P\frac{\partial H}{\partial(-P)}, T = \frac{\partial H}{\partial S}, V = -\frac{\partial H}{\partial(-P)}\}$$

or

$$L = \{(V,S,E,-P,T) \mid E = G(-P,T) - T\frac{\partial G}{\partial T} + P\frac{\partial G}{\partial P}, V = -\frac{\partial G}{\partial(-P)}, S = -\frac{\partial G}{\partial T}\}$$

E, F, H, G are called generating functions for L.

NB Can get complicated: Maxwell spent 1874 summer on making a plaster model for $E = E(V,S)$ (explaining discontinuous phase transitions)

θ is special type of 1-form: a contact form

The 1-form $\theta = dE - TdS + PdV$ satisfies the non-degeneracy condition

$$\begin{aligned} d\theta \wedge d\theta \wedge \theta &= (-dT \wedge dS + dP \wedge dV) \wedge (-dT \wedge dS + dP \wedge dV) \\ &\quad \wedge (dE - TdS + PdV) \\ &= -2dT \wedge dS \wedge dP \wedge dV \wedge dE \neq 0 \end{aligned}$$

θ is called maximally non-integrable:

maximal manifolds on which θ is zero have minimal dimension; i.e., 2.

Such 1-forms are called contact forms and are 'as far as possible' from integrable 1-forms such as dK, for some $K : \mathbb{R}^5 \to \mathbb{R}$.

(NB: maximal manifolds on which dK is zero have dimension 4 instead.)

Standard starting point of contact geometry

By Darboux's theorem for any 1-form on $\mathbb{R}^5$ satisfying

$$d\theta \wedge d\theta \wedge \theta \neq 0 \quad \text{contact form}$$

there exist coordinates

$$q_0, q_1, q_2, \gamma_1, \gamma_2$$

such that

$$\theta = dq_0 - \gamma_1 dq_1 - \gamma_2 dq_2$$

Any Legendre submanifold L of $(\mathbb{R}^5, \theta)$ is locally represented as

$$L = \{(q_0, q_1, q_2, \gamma_1, \gamma_2) \mid q_0 = F - \gamma_J \frac{\partial F}{\partial \gamma_J}, \gamma_I = \frac{\partial F}{\partial q_I}, \; q_J = -\frac{\partial F}{\partial \gamma_J}, \}$$

for some generating function $F(q_I, \gamma_J)$, $\{1,2\} = I \cup J$.
Conversely, any such L is Legendre submanifold.
Is immediately generalized to general contact manifolds.

Definition

A contact manifold is a $(2n+1)$-dimensional manifold $\mathcal{M}$ with (a locally defined) 1-form θ satisfying $\theta \wedge (d\theta)^n \neq 0$.

By Darboux's theorem $\exists$ coordinates $q_0, q_1, \cdots, q_n, \gamma_1, \cdots, \gamma_n$ for $\mathcal{M}$ s.t.

$$\theta = dq_0 - \sum_{i=1}^{n} \gamma_i dq_i,$$

$q_0, q_1, \cdots, q_n$ extensive and $\gamma_1, \cdots, \gamma_n$ intensive variables. A Legendre submanifold L is integral manifold of θ of maximal dimension $(= n)$.

Any Legendre submanifold L of $(\mathcal{M}, \theta)$ is locally represented as

$$L = \{(q_0, q_1, \cdots, q_n, \gamma_1, \cdots, \gamma_n) \mid q_0 = F - \gamma_J \frac{\partial F}{\partial \gamma_J}, \gamma_I = \frac{\partial F}{\partial q_I}, \ q_J = -\frac{\partial F}{\partial \gamma_J}, \}$$

for some generating function $F(q_I, \gamma_J)$, $\{1, \cdots, n\} = I \cup J$.

As a result, since the 1970s (Hermann, Mrugala, ..) contact geometry has been recognized as appropriate geometric framework for thermodynamics.

Thermodynamically consistent transformations are naturally expressed by contact transformations; e.g. $\phi : \mathbb{R}^5 \to \mathbb{R}^5$ such that $\phi^* \theta = \tau \theta$ for some nowhere vanishing function τ.

Infinitesimal contact transformations are the contact vector fields X satisfying

$$\mathbb{L}_X \theta = \rho \theta$$

for some function ρ. The corresponding contact Hamiltonian is the function $\theta(X)$.

Mrugala has shown that a contact vector field X leaves a Legendre submanifold L invariant if and only its contact Hamiltonian $\theta(X)$ is zero on L.
This corresponds to leave the thermodynamic (equilibrium) properties of the system invariant !

This leads to the theory of thermodynamic transformations:

- reversible transformations as developed by Mrugala, Benayou, $\cdots$
- irreversible transformations by Grmela, Balian, Valentin
- controlled irreversible systems by Maschke, van der Schaft, Eberard, Favache, Ramirez, ...

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Summarizing:

- Gibbs' relation immediately leads to contact geometry.
- State properties are described by Legendre submanifolds.
- Contact transformations are natural tools.

Actually thermodynamic properties may also be written in entropy representation where the properties are derived from the expression of the entropy function

$$S = S(V, E),$$

leading to the intensive variables, the reciprocal temperature $\frac{1}{T} and \frac{P}{T}$

$$\frac{1}{T} = \frac{\partial S}{\partial E}(V, E), \quad \frac{P}{T} = \frac{\partial S}{\partial V}(V, E)$$

This results from rewriting Gibbs' relation as $dS = \frac{1}{T}dE + \frac{P}{T}dV$,
and defining the associated 'entropy' contact form

$$\tilde{\theta} = dS - \frac{1}{T}dE - \frac{P}{T}dV$$

This is a different contact form ! (although 'conformally equivalent' to θ) where the Legendre submanifolds defining the thermodynamic properties are generated by Massieu's functions.

Basic message (Balian & Valentin, 2001): multiply Gibbs' contact form

$$\theta = dE - TdS + PdV$$

on $\mathbb{R}^5$ by an extra (gauge) variable p_E to obtain

$$p_E dE - p_E TdS + p_E PdV,$$

defining the Liouville form on the cotangent bundle $T^*\mathbb{R}^3 = \mathbb{R}^6$

$$\alpha := p_E dE + p_S dS + p_V dV, \quad p_S := -p_E T, \ p_V := p_E P$$

Then

$$\frac{p_S}{-p_E} = T, \quad \frac{p_V}{-p_E} = -P$$

corresponds to energy representation, while

$$\frac{p_E}{-p_S} = \frac{1}{T}, \quad \frac{p_V}{-p_S} = \frac{P}{T}$$

corresponds to entropy representation.

Thus we have replaced the intensive variables

$$T, \ -P \qquad \text{energy representation}$$

or

$$\frac{1}{T}, \ \frac{P}{T} \qquad \text{entropy representation}$$

by the homogeneous coordinates

$$p_V, p_S, p_E$$

In this way we replace the contact manifold $\mathbb{R}^5$ with contact form θ or $\tilde{\theta}$ by the symplectic manifold $\mathbb{R}^6 = T^*\mathbb{R}^3$, with $\mathbb{R}^3$ the space of extensive variables (V, S, E), and co-extensive variables (p_V, p_S, p_E).

In this way the energy and entropy representation are unified (main motivation for Balian & Valentin). But there are many more advantages !

Symplectization of contact manifolds (cf. Arnold, Libermann & Marle)

Start with $(n+1)$-dimensional manifold Q *of all extensive variables*.

Denote by $\mathcal{T}^*Q$ the $(2n+2)$-dimensional cotangent bundle T^*Q without its zero-section.

Coordinates for the cotangent space will be homogeneous coordinates for the space of intensive variables.

Define $\mathbb{P}(T^*Q)$ as the projectivization of $\mathcal{T}^*Q$:
the $(2n+1)$-dimensional fiber bundle over Q with fiber at any point $q \in Q$ given by the n-dimensional projective space $\mathbb{P}(T^*_q Q)$.

Then $\mathbb{P}(T^*Q)$ is contact manifold, defining the thermodynamic phase space of extensive and intensive variables.

Intermezzo: $\mathbb{P}(T^*Q)$ as contact manifold

Indeed; let Q be $(n+1)$-dimensional. Take any point $q \in Q$, and consider the set of n-dimensional subspaces S of the $(n+1)$-dimensional tangent space $T_q Q$.

This defines an $(2n+1)$-dimensional manifold $\mathcal{M}$, which is a fiber bundle over Q with projection $\Pi : \mathcal{M} \to Q$.

Define a field of hyperplanes on $\mathcal{M}$ by considering at each point $(q, S) \in \mathcal{M}$, with $q \in Q$ and S an n-dimensional subspace of $T_q Q$, the subspace of all tangent vectors at (q, S) to $\mathcal{M}$ which are such that the projection to $T_q Q$ (under Π) is contained in S.

It can be checked that this defines a contact structure on $\mathcal{M}$: i.e., this field of hyperplanes is the kernel of a (locally defined) contact form.

$\mathbb{P}(T^*Q)$ as contact manifold; cont'd

But an n-dimensional subspace S of the tangent space T_qQ can be identified with the set of all non-zero multiples of some cotangent vector in T_q^*Q whose kernel equals this subspace.

Hence, the contact manifold $\mathcal{M}$ as above is equal to

$$\mathcal{M} = \mathbb{P}(T^*Q),$$

i.e., the fiber bundle over Q with fiber at any point $q \in Q$ given by the projective space $\mathbb{P}(T_q^*Q)$.

Conversely, $\mathcal{T}^*Q$ is the symplectization of the contact manifold $\mathbb{P}(T^*Q)$.

Furthermore by Darboux's theorem any other $(2n+1)$-dimensional contact manifold is locally contactomorphic to the contact manifold $\mathbb{P}(T^*Q)$ for some $(n+1)$-dimensional manifold Q.

Hence any contact manifold is locally $\mathbb{P}(T^*Q)$ for some Q.

$\mathbb{P}(T^*Q)$ as contact manifold; cont'd

Summarizing, the canonical contact manifold (thermodynamic phase space) is the $(2n+1)$-dimensional manifold $\mathbb{P}(T^*Q)$,

obtained from the $(2n+2)$-dimensional symplectic cotangent bundle $\mathcal{T}^*Q$.

Furthermore, objects on the thermodynamic phase space $\mathbb{P}(T^*Q)$ can be derived from corresponding objects on $\mathcal{T}^*Q$ having additional homogeneity properties.

Advantages:

- Unification of energy, entropy, $\cdots$, representations.
- All computations etc. will be much easier on $\mathcal{T}^*Q$.
- Will allow for a simple definition of power and rate of entropy ports.

Objects on $\mathbb{P}(T^*Q)$ from homogeneous objects on T^*Q

Definition

A function $K : T^*Q \to \mathbb{R}$ is homogeneous of degree r (in p) if

$$K(q_0, q_1, \cdots, q_n, \lambda p_0, \lambda p_1, \cdots, \lambda p_n) = \lambda^r K(q_0, q_1, \cdots, q_n, p_0, p_1, \cdots, p_n), \quad \forall \lambda \neq 0$$

Theorem (Euler)

Differentiable function $K : T^*Q \to \mathbb{R}$ is homogeneous of degree r iff

$$\sum_{i=0}^{n} p_i \frac{\partial K}{\partial p_i}(q,p) = r\, K(q,p), \qquad \textit{for all } (q,p) \in T^*Q$$

Furthermore, if K is homogeneous of degree r, then its derivatives $\frac{\partial K}{\partial p_i}$, $i = 0, 1, \cdots, n$, are homogeneous of degree $r-1$.

Correspondence between Legendre submanifolds of $\mathbb{P}(T^*Q)$ and homogeneous Lagrangian submanifolds of $\mathcal{T}^*Q$

$\mathcal{T}^*Q$ is endowed with the Liouville 1-form

$$\alpha = p_0 dq_0 + p_1 dq_1 + \cdots p_n dq_n$$

and the symplectic form

$$\omega = d\alpha = dp_0 \wedge dq_0 + dp_1 \wedge dq_1 + \cdots dp_n \wedge dq_n$$

A Lagrangian submanifold is a maximal submanifold $\mathcal{L} \subset \mathcal{T}^*Q$ restricted to which ω is zero.

$\mathcal{L} \subset \mathcal{T}^*Q$ is called homogeneous if whenever $(q,p) \in \mathcal{L}$ then also $(q, \lambda p) \in \mathcal{L}$ for any $0 \neq \lambda \in \mathbb{R}$.

Consider the canonical projection

$$\pi : \mathcal{T}^*Q \to \mathbb{P}(T^*Q)$$

Then: any Legendre submanifold $L \subset \mathbb{P}(T^*Q)$ defines a homogeneous Lagrangian submanifold

$$\mathcal{L} := \pi^{-1}L \subset \mathcal{T}^*Q,$$

and conversely any homogeneous Lagrangian submanifold is of this type.

Furthermore ! :

Theorem

Homogeneous Lagrangian submanifolds $\mathcal{L} \subset \mathcal{T}^*Q$ are maximal submanifolds restricted to which the Liouville form α is zero.

(Hence, not only $\omega := d\alpha$ is zero on $\mathcal{L}$, but in fact α is zero on $\mathcal{L}$!)

Simplest case

(q, S, E, p, p_S, p_E) can. coordinates for $\mathcal{T}^* Q^e$, $Q^e = Q \times \mathbb{R} \times \mathbb{R}$.

Generating function of homogeneous Lagrangian submanifold $\mathcal{L}$ in energy representation

$$-p_E E(q, S)$$

yielding

$$\begin{aligned} \mathcal{L} &= \{(q, S, E, p, p_S, p_E) \mid E = E(q, S), \\ &\qquad p = -p_E \frac{\partial E}{\partial q}(q, S), p_S = -p_E \frac{\partial E}{\partial S}(q, S)\} \end{aligned}$$

In the entropy representation, homogeneous generating function of $\mathcal{L}$ is

$$-p_S S(q, E)$$

yielding

$$\begin{aligned} \mathcal{L} &= \{(q, S, E, p, p_S, p_E) \mid S = S(q, E), \\ &\qquad p = -p_S \frac{\partial S}{\partial q}(q, E), p_E = -p_S \frac{\partial S}{\partial E}(q, E)\} \end{aligned}$$

General case

Any Legendre submanifold L of a contact manifold with coordinates

$$q_0, q_1, \cdots, q_n, \gamma_1, \cdots, \gamma_n, \quad \theta = dq_0 - \gamma_1 dq_1 \cdots - \gamma_n dq_n$$

with generating function $F(q_I, \gamma_J)$ (with $I \cup J = \{1, \cdots, n\}$)is

$$\begin{aligned} L &= \{(q_0, q_1, \cdots, q_n, \gamma_1, \cdots, \gamma_n) \mid q_0 = F - \gamma_J \tfrac{\partial F}{\partial \gamma_J}, \\ &\quad q_J = -\tfrac{\partial F}{\partial \gamma_J}, \gamma_I = \tfrac{\partial F}{\partial q_I}\} \end{aligned}$$

Then the homogeneous Lagrangian submanifold $\mathcal{L} = \pi^{-1}(L)$ is defined by the homogeneous degree 1 generating function

$$G(q_0, \cdots, q_n, p_0, \cdots, p_n) = -p_0 F(q_I, \frac{p_J}{-p_0})$$

i.e.,

$$\mathcal{L} = \{(q_0, \cdots, q_n, p_0, \cdots, p_n) \mid q_0 = -\tfrac{\partial G}{\partial p_0}, q_J = -\tfrac{\partial G}{\partial p_J}, p_I = \tfrac{\partial G}{\partial q_I}\}$$

Contact and homogeneous Hamiltonian vector fields

Take Hamiltonian $K : \mathcal{T}^*Q \to \mathbb{R}$. Then Hamiltonian vector field X_K on $\mathcal{T}^*Q$ is

$$\dot{q} = \frac{\partial K}{\partial p}, \quad \dot{p} = -\frac{\partial K}{\partial q}, \quad (q,p) \text{ canonical coordinates}$$

Any Hamiltonian vector field X_K is characterized by the property that the Lie-derivative $\mathbb{L}_{X_K}\omega = 0$.

A Hamiltonian vector field X_K on $\mathcal{T}^*Q$ with K homogeneous of degree 1 not only satisfies $\mathbb{L}_{X_K}\omega = 0$, but in fact $\mathbb{L}_{X_K}\alpha = 0$

$$\mathbb{L}_{X_K}\alpha = i_X d\alpha + d(\alpha(X_K)) = -dK + dK = 0$$

Conversely, if $\mathbb{L}_{X_K}\alpha = 0$, then by homogeneity $\alpha(X_K) = K$, and thus

$$0 = \mathbb{L}_{X_K}\alpha = i_X d\alpha + d(\alpha(X_K)) = i_X d\alpha + dK$$

implying that K, up to a constant, is homogeneous of degree 1.

Contact and homogeneous Hamiltonian vector fields

Furthermore, any such Hamiltonian vector field X_K with K homogeneous of degree 1 projects to a contact vector field $X_{\widehat{K}} = \pi_* X_K$ on the contact manifold $\mathbb{P}(T^*Q)$, i.e.,

$$\mathbb{L}_{X_{\widehat{K}}} \theta = \rho \theta, \quad \text{for some function } \rho$$

Correspondence between homogeneous Hamiltonian K on $\mathcal{T}^*Q$ and contact Hamiltonian $\widehat{K}$ on $\mathbb{P}(T^*Q)$ is given as

$$K(q_0, \cdots, q_n, p_0, \cdots, p_n) = p_0 \widehat{K}(q_0, \cdots, q_n, \frac{p_1}{-p_0}, \cdots, \frac{p_n}{-p_0})$$

Recall that a contact vector field X leaves a Legendre submanifold L invariant if and only if its contact Hamiltonian $\widehat{K} = \theta(X)$ is zero on L.

Similarly, a homogeneous Lagrangian submanifold $\mathcal{L}$ is left invariant by X_K with K homogeneous of degree 1 if and only if K is zero on $\mathcal{L}$.
(Thus *Mrugala's theory of thermodynamic transformations can be immediately translated to the homogeneous symplectic formulation*.)

Furthermore, the Poisson bracket

$$\{K^1, K^2\}$$

of two degree 1 Hamiltonians K_1, K_2 on $\mathcal{T}^*Q$ is also of degree 1, and corresponds to the Jacobi bracket $\{\cdot, \cdot\}_J$ of the corresponding contact Hamiltonians $\widehat{K}_1, \widehat{K}_2$ on $\mathbb{P}(T^*Q)$:

$$\{\widehat{K}^1, \widehat{K}^2\}_J = \{\widehat{K^1, K^2}\}$$

(This will allow to set up an easy theory of controllability and observability for port-thermodynamic systems as discussed hereafter.)

Excursion to optimal control[1]

Consider the optimal control problem of minimizing

$$\int_0^T L(x(t), u(t))dt, \quad x(0) = x_0,\ x \in \mathbb{R}^n,$$

over all input functions $u : [0, T] \to \mathbb{R}^m$ for the dynamics $\dot{x} = f(x, u)$.

Define x_0 such that $\dot{x}_0 = L(x, u),\ x_0(0) = 0$ ('Mayer problem').

Define the Hamiltonian $H : T^*\mathbb{R}^{n+1} \times \mathbb{R}^m \to \mathbb{R}$ as the canonical lifting of the total dynamics

$$H(x_0, x, \lambda_0, \lambda, u) = \lambda^T f(x, u) + \lambda_0 L(x, u),$$

which is homogeneous in (λ_0, λ).

[1] See Ohsawa, Joszwikowski & Respondek for the contact formulation

The corresponding Hamiltonian vector field X_H (parametrized by u) is

$$\begin{aligned} \dot{x}_0 &= L(x,u) \\ \dot{x} &= f(x,u) \\ \dot{\lambda}_0 &= 0 \\ \dot{\lambda} &= -\lambda^T \tfrac{\partial f(x,u)}{\partial x} - \lambda_0 \tfrac{\partial L(x,u)}{\partial x} \end{aligned}$$

Thus λ_0 is constant. $\lambda_0 = 0$ is the so-called abnormal case. For $\lambda_0 \neq 0$ the standard co-state variables are defined as

$$p = \frac{\lambda}{-\lambda_0},$$

resulting in the standard equations of Pontryagin's Maximum principle.

For the infinite-horizon optimal control problem ($T \to \infty$), the stationary Hamilton-Jacobi-Bellman equation corresponds to a homogeneous Lagrangian submanifold $\mathcal{L} \subset T^*\mathbb{R}^{n+1}$, with generating function

$$-\lambda_0 V(x)$$

where V is Bellman's value function, i.e.,

$$\mathcal{L} = \{(x_0, x, \lambda_0, \lambda) \mid x_0 = V(x), \lambda = -\lambda_0 \frac{\partial V}{\partial x}(x)\}$$

and

$$\min_u H(V(x), x, \lambda_0, -\lambda_0 \frac{\partial V}{\partial x}(x), u) = 0$$

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Towards definition of port-thermodynamic systems

(1) Thermodynamic properties are described by a Legendre submanifold $L \subset \mathbb{P}(T^*Q)$ or the homogeneous Lagrangian submanifold $\mathcal{L} \subset \mathcal{T}^*Q$.

(2) Any thermodynamically consistent dynamics should leave the thermodynamic properties invariant, i.e., should leave the Legendre submanifold $L \subset \mathbb{P}(T^*Q)$ or the homogeneous Lagrangian submanifold $\mathcal{L} \subset \mathcal{T}^*Q$ invariant.

(3) How to define the dynamics on L or $\mathcal{L}$?

(4) How to define interaction ports of a thermodynamic system ?

Change of paradigm: the thermodynamic phase space is *not* an ordinary state space

State properties of the thermodynamic system are described by Gibbs' relation: relation between all extensive and intensive variables.

Thus the Legendre submanifold $L \subset \mathbb{P}(T^*Q)$ or the homogeneous Lagrangian submanifold $\mathcal{L} \subset \mathcal{T}^*Q$ describes the actual state space of the thermodynamic system !

Thus in principle there is no need to consider points of $\mathbb{P}(T^*Q)$ outside L, and the dynamics of the thermodynamic system necessarily leaves $L \subset \mathbb{P}(T^*Q)$ invariant !

Similarly, in the homogeneous symplectic formulation there is no need to consider points of $\mathcal{T}^*Q$ outside $\mathcal{L}$, and the dynamics of the thermodynamic system necessarily leaves $\mathcal{L} \subset \mathcal{T}^*Q$ invariant.

Change of paradigm: a simple analogy

Situation regarding invariance of L or $\mathcal{L}$ may be compared with description of, e.g.,an electrical capacitor: its 'state properties' are

$$E = E(Q)\ (= \frac{1}{2C}Q^2), \quad V = \frac{dE}{dQ}(Q)\ (= \frac{Q}{C})$$

From a geometric 'thermodynamic point of view' this corresponds to 1-dimensional Legendre submanifold L of the 'thermodynamic phase space' of the capacitor $\mathbb{R}^3 \ni (Q, E, V)$

$$L = \{(Q, E, V) \mid E = E(Q),\ V = \frac{dE}{dQ}(Q)\},$$

instead of the common 1-dimensional vector space $\mathbb{R}$ with coordinate Q or V.

Definition of port-thermodynamic system

Introduce new notation emphasizing special role extensive variables S, E:

Define $Q^e = Q \times \mathbb{R} \times \mathbb{R}$ as the manifold of all extensive variables, with coordinates for Q^e denoted by

$$q^e = (q, S, E),$$

with q coordinates for Q: remaining extensive variables (such as $V, N_1, \cdots, N_m$).

Cotangent bundle coordinates for $\mathcal{T}^* Q^e$ will be denoted by

$$(q^e, p^e) = (q, S, E, p, p_S, p_E)$$

Consider the state properties defined by $\mathcal{L} \subset \mathcal{T}^* Q^e$, or equivalently $L \subset \mathbb{P}(T^* Q^e)$, which should be left invariant by the dynamics of the thermodynamic system.

Definition of port-thermodynamic system; cont'd

This leads to defining the dynamics of a port-thermodynamic system with state properties $\mathcal{L} \subset \mathcal{T}^* Q^e$ by a homogeneous (degree 1 in p^e) Hamiltonian, parametrized by $u \in \mathbb{R}^m$

$$K := K^a + K^c u : \mathcal{T}^* Q^e \to \mathbb{R}, \quad u \in \mathbb{R}^m,$$

with K^a (drift Hamiltonian) and $K_j^c, j = 1, \cdots, m$ (input Hamiltonians), which are all zero restricted to $\mathcal{L}$, and hence leave $\mathcal{L}$ invariant.

By Euler's Theorem, homogeneity implies

$$K^a = p^T f + p_S f_S + p_E f_E, \qquad f = \frac{\partial K^a}{\partial p}, f_S = \frac{\partial K^a}{\partial p_S}, f_E = \frac{\partial K^a}{\partial p_E}$$

$$K^c = p^T g + p_S g_S + p_E g_E, \quad g = \frac{\partial K^c}{\partial p}, g_S = \frac{\partial K^c}{\partial p_S}, g_E = \frac{\partial K^c}{\partial p_E}$$

where the functions f, f_S, f_E, g, g_S, g_E are all homogeneous of degree 0;

defining the dynamics of the extensive variables.

Additional conditions on the drift part K^a

First Law of Thermodynamics additionally imposes

$$f_E|_{\mathcal{L}} = 0,$$

i.e., conservation of energy when no interaction with the environment takes place.

Second Law of Thermodynamics imposes

$$f_S|_{\mathcal{L}} \geq 0,$$

i.e., entropy increases when no interaction with the environment takes place: $f_S|_{\mathcal{L}}$ is irreversible entropy production.

Symplectization leads to formalization of interaction with environment through ports

Define the outputs (homogeneous degree 0)

$$y_p := g_E|_{\mathcal{L}}, \quad \text{homogeneous degree 0},$$

leading to the power balance $\frac{d}{dt}E|_{\mathcal{L}} = y_p u$.

(u, y_p) defines a power port.

Alternative entropy-conjugate outputs are defined as

$$y_e := g_S|_{\mathcal{L}}, \quad \text{homogeneous degree 0},$$

leading to the rate of entropy balance $\frac{d}{dt}S|_{\mathcal{L}} \geq y_e u$.

(u, y_e) defines a rate of entropy port.

Some additional observations

- Note that the Hamiltonians K^a and K^c are (physically) dimension-less.
- On the other hand, in the energy representation the contact Hamiltonians $\widehat{K}^a$ and $\widehat{K}^c$ have dimension of power; and in the entropy representation dimension of rate of entropy.
- One could also define ports with respect to the other extensive variables; e.g., volume V.

Outline

1. Gibbs and contact geometry
2. From contact geometry to homogeneous symplectic geometry
3. Definition of port-thermodynamic systems
4. Examples
5. Conclusions

Example (Mass-spring-damper system)

Consider extensive variables z (extension of the spring), π (momentum) and entropy S. State properties are described by Lagrangian submanifold $\mathcal{L}$ with generating function

$$-p_E\left(\frac{1}{2}kz^2+\frac{\pi^2}{2m}+U(S)\right),$$

defining the state properties

$$\begin{aligned}\mathcal{L} \;=\; & \{(z,\pi,S,E,p_z,p_\pi,p_S,p_E) \mid E=\tfrac{1}{2}kz^2+\tfrac{\pi^2}{2m}+U(S),\\ & p_z=-p_E kz, p_\pi=-p_E\tfrac{\pi}{m}, p_S=-p_E U'(S)\}\end{aligned}$$

Dynamics is given by the homogeneous Hamiltonian

$$K=p_z\frac{\pi}{m}+p_\pi\left(-kz-d\frac{\pi}{m}\right)+p_S\frac{d(\frac{\pi}{m})^2}{U'(S)}+\left(p_\pi+p_E\frac{\pi}{m}\right)u$$

The power-conjugate output $y_p=\frac{\pi}{m}$ is the velocity of the mass.

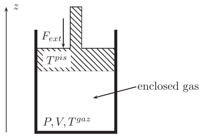
Example (Gas-piston-damper system)

This system is analogous to previous example, replacing z by volume V and the partial energy $\frac{1}{2}kz^2 + U(S)$ by internal energy of the gas $U(V,S)$.

Dynamics is defined by the Hamiltonian

$$K = p_z \frac{\pi}{m} + p_\pi \left(-\frac{\partial U}{\partial V} - d\frac{\pi}{m} \right) + p_S \frac{d(\frac{\pi}{m})^2}{\frac{\partial U}{\partial S}} + \left(p_\pi + p_E \frac{\pi}{m} \right) u,$$

where the power-conjugate output $y_p = \frac{\pi}{m}$ is the velocity of the piston.



Example (Heat exchanger)

Extensive variables S_1, S_2 (entropies of the two compartments) and E (total energy). The state properties are described by

$$\begin{aligned} \mathcal{L} &= \{(S_1, S_2, E, p_{S_1}, p_{S_2}, p_E) \mid E = E_1(S_1) + E_2(S_2), \\ & \quad p_{S_1} = -p_E E_1'(S_1),\ p_{S_2} = -p_E E_2'(S_2)\}, \end{aligned}$$

corresponding to generating function $-p_E(E_1(S_1) + E_2(S_2))$, with E_1, E_2 energies of the two compartments. Denoting the temperatures $T_1 = E_1'(S_1)$, $T_2 = E_2'(S_2)$, the dynamics is given by Hamiltonian

$$K^a = \lambda(\frac{1}{T_1} - \frac{1}{T_2})(p_{S_1} T_2 - p_{S_2} T_1)$$

with λ Fourier's conduction coefficient. Dynamics on $\mathcal{L}$ satisfies

$$\dot{S}_1 + \dot{S}_2 = \lambda(\frac{1}{T_1} - \frac{1}{T_2})(T_2 - T_1) \geq 0$$

Example (Carnot cycle for a gas)

$$\mathcal{L} = \{(V, S, E, p_V, p_S, p_E) \mid E = E(V, S), p_V = -p_E \frac{\partial E}{\partial V}, p_S = -p_E \frac{\partial E}{\partial S}\}$$

Assuming reversibility $K^a = 0$. Furthermore, consider input Hamiltonians

$$K_V^c = p_V + p_E \frac{\partial E}{\partial V}, \quad K_q^c = p_E + p_S \frac{\partial S}{\partial E}$$

with inputs u_V rate of extension of the volume, and u_q heat flow.

In case of an ideal gas

$$E(V, S) = C_V e^{\frac{S}{C_V}} V e^{-\frac{R}{C_V}},$$

with C_V heat capacity (at constant volume), and R universal gas constant.

Adiabatic process corresponds to $K_V^c u_V$, and isothermal process to a combination of $K_V^c u_V$ and $K_q^c u_q$ such that $T = \frac{\partial E}{\partial S}$ remains constant.

Interconnection of port-thermodynamic systems

Consider two port-thermodynamic systems with phase space

$$(q_i, p_i, S_i, p_{S_i}, E_i, p_{E_i}) \in T^*Q_i \times T^*\mathbb{R} \times T^*\mathbb{R}, \quad i = 1, 2,$$

and Liouville one-forms $\alpha_i = p_i dq_i + p_{S_i} dS_i + p_{E_i} dE_I$ on the space of extensive and co-extensive variables $T^*Q_i \times T^*\mathbb{R} \times T^*\mathbb{R}$.

Impose the constraint

$$p_{E_1} = p_{E_2} =: p_E$$

This leads to the summation of the Liouville forms α_1 and α_2:

$$\alpha_{\mathrm{sum}} := p_1 dq_1 + p_2 dq_2 + p_{S_1} dS_1 + p_{S_2} dS_2 + p_E d(E_1 + E_2)$$

on the composed space defined as

$$\begin{aligned} T^*Q_1^e \circ T^*Q_2^e \quad := \quad & \{(q_1, p_1, q_2, p_2, S_1, p_{S_1}, S_2, p_{S_2}, E, p_E) \\ & \in T^*Q_1 \times T^*Q_2 \times T^*\mathbb{R} \times T^*\mathbb{R} \times T^*\mathbb{R}\} \end{aligned}$$

Let the state properties of the two individual systems be defined by homogeneous Lagrangian submanifolds

$$\mathcal{L}_i \subset T^*Q_i \times T^*\mathbb{R}_i \times T^*\mathbb{R}_i, \quad i = 1, 2,$$

with generating functions $-p_{E_i} E_i(q_i, S_i), i = 1, 2$.

The state properties of the composed system are defined by homogeneous Lagrangian submanifold

$$\begin{aligned} \mathcal{L}_1 \circ \mathcal{L}_2 \quad := \quad & \{(q_1, q_2, p_1, p_2, S_1, p_{S_1}, S_2, p_{S_2}, E, p_E \mid E = E_1 + E_2, \\ & (q_i, p_i, S_i, p_{S_i}, E_i, p_{E_i}) \in \mathcal{L}_i, \ i = 1, 2\}, \end{aligned}$$

with generating function $-p_E \left[E_1(q_1, S_1) + E_2(q_2, S_2)\right]$.

Consider the dynamics on $\mathcal{L}_i$ defined by Hamiltonians $K_i = K_i^a + K_i^c u_i, i = 1, 2.$

Assume K_i do not depend on $E_i, i = 1, 2$. Then

$$K_1 + K_2$$

is well-defined on $\mathcal{L}_1 \circ \mathcal{L}_2$ for all u_1, u_2.

Imposing interconnection constraints on the power-port variables u_1, u_2, y_{p1}, y_{p2} satisfying

$$y_{p1} u_1 + y_{2p} u_2 = 0,$$

yields the closed-loop dynamics on $\mathcal{L}_1 \circ \mathcal{L}_2$.

Similarly for interconnection via rate of entropy flow ports, imposing interconnection constraints satisfying

$$y_{e1} u_1 + y_{e2} u_2 \geq 0,$$

For example, the mass-spring-damper system can be built up from power interconnection of 'thermodynamic' subsystems:
(1) mass, (2) spring, (3) damper.

Outline

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- Gibbs' relation describes state properties, and corresponds to Legendre submanifold of contact manifold.
- Contact geometry can be symplectized. This allows easy switching between entropy and energy representation, and simplifies picture (e.g., extensive and intensive variables) and computations.
- Thermodynamic systems defined by $\mathcal{L}$ (state properties) and by $K = K^a + K^c u$ which is zero on $\mathcal{L}$.
- Leads to simple definition of power ports and rate of entropy flow ports for thermodynamic systems; and thereby interconnection theory of port-thermodynamic systems.
- Allows for nonlinear controllability and observability analysis of thermodynamic systems: Poisson bracket $\{K_1, K_2\}$ of homogeneous K_i is again homogeneous.
- Additional geometry: intrinsically defined Riemannian metric on $\mathcal{L}$, generalizing the Weinhold and Ruppeiner metrics.
- Homogeneity with respect to the extensive variables can be added: Gibbs-Duhem relations.
- Open problem: 'Canonical' form of K^a and K^c is yet unknown.

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