The geometric formulation of non-equilibrium macroscopic thermodynamics

From network modeling to control

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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.

Thermodynamics is especially interesting for systems and control, since it directly originates in engineering (maximal efficiency of steam engines, ..), and always considers systems in interaction with others.

Geometric modeling of thermodynamic systems

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

Compared with geometric mechanics not much work has been done.

In the finite-dimensional case by Gibbs, Hermann (1960s), Mrugala (1970s), Gay-Balmaz & Yoshimura, $\cdots$,
and (also in infinite-dimensional case) by Grmela, Öttinger et al., GENERIC, $\cdots$.

Recently, increasing interest in (geometric) thermodynamics, both in engineering (thermal effects in high-precision mechatronics, heat networks, chemical engineering, ..) as well as mathematical physics (black-hole thermodynamics, links with information theory, ..).

Outline

Consider a simple thermodynamic system:

extensive variables V, S, E

intensive variables $-P$, T

Its state properties are formalized by Gibbs' relation

$$dE = TdS - PdV$$

More generally:

extensive variables, $V, N_1, \cdots, N_m, S, E$

intensive variables $-P, \mu_1, \cdots, \mu_m, T$

Gibbs' relation

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

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

Answer: If E is expressed as function of the other extensive variables V, S

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

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

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

By Legendre transformation of $E(V,S)$, one obtains other thermodynamic potentials

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

Just different ways of locally parametrizing the submanifold L given as

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

On the other hand, not all parametrizations may be possible !

Another quote:

Every mathematician knows that it is impossible to understand any elementary course in thermodynamics.
The reason is that the thermodynamics is based,
- as Gibbs has explicitly proclaimed -,
on a rather complicated mathematical theory,
on the contact geometry.

Vladimir I. Arnold,
Contact geometry: the geometrical method of Gibbs's thermodynamics,

(Proc. of the Gibbs Symposium, American Mathematical Society, 1989)

Basic contact geometry

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

$$0 = dE - TdS + PdV \qquad \text{Gibbs' relation}$$

Any such L is 2-dimensional.

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

How complicated can it get !

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

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.

(Maximal manifolds on which dK is zero have dimension 4.)

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.

Outline

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

On the other hand, contact geometry does not intrinsically distinguish between extensive and intensive variables, and state properties may also be written in entropy representation (instead of in energy representation)

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

together with the accompanying relations

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

This results from rewriting Gibbs' relation as

$$dS = \frac{1}{T}dE + \frac{P}{T}dV,$$

leading to different intensive variables $\frac{1}{T}, \frac{P}{T}$, and different contact form

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

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

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

which we rewrite as the Liouville form

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

on the cotangent bundle $T^*\mathbb{R}^3 = \mathbb{R}^6$. 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:
(p_V, p_S, p_E) *are homogeneous coordinates for space of intensive variables.*

General geometric picture

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.

$\mathbb{P}(T^*Q)$ as contact manifold (see e.g. Arnold's Classical Mechanics, Appendix 4)

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_qQ.

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_qQ, the subspace of all tangent vectors at (q, S) to $\mathcal{M}$ which are such that the projection to T_qQ (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 $\mathbb{P}(T_q^*Q)$.

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

Furthermore by Darboux's theorem any $(2n+1)$-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 $\mathbb{P}(T^*Q)$.

Summarizing, the canonical contact manifold 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 $\mathbb{P}(T^*Q)$ can be derived from corresponding objects on $\mathcal{T}^*Q$ having additional homogeneity properties.

All computations etc. will be much easier on $\mathcal{T}^*Q$!

Additional advantages as well: unifies energy and entropy representations, and crucial for 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 $\mathcal{L}$!)

Example: denote

(q, S, E, p, p_S, p_E) 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 is homogeneous

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

yielding

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

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

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

yielding

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

Outline

Gibbs' relation describes state properties: relation between all extensive and intensive variables.
Thus Legendre submanifold $L \subset \mathbb{P}(T^*Q)$ or Lagrangian submanifold $\mathcal{L} \subset \mathcal{T}^*Q$ describes actual state space of the system !

Situation may be compared with description of capacitor: 'state properties' of the capacitor are

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

From a geometric 'thermodynamic point of view' one would write

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

Thus 'thermodynamic phase space' of capacitor is $\mathbb{R}^3$, with state properties given by 1-dimensional Legendre submanifold L !

Thus there is no need to consider points of $\mathbb{R}^3$ outside L, and the dynamics of the capacitor necessarily leaves $L \subset \mathbb{R}^3$ invariant !
In this sense, the terminology thermodynamic phase space for the contact manifold $\mathbb{P}(T^*Q)$ is confusing !

Towards definition of port-thermodynamic systems

Note:

(1) Warning: Most of theory on thermodynamics is actually thermostatics:

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

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

Recall that given $K : \mathcal{T}^* Q \to \mathbb{R}$ the Hamiltonian vector field X_K on $\mathcal{T}^* Q$ with coordinates (q, p) is

$$\dot{q} = \frac{\partial K}{\partial p}, \quad \dot{p} = -\frac{\partial K}{\partial q}$$

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

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

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

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, possibly modified by a constant, is homogeneous of degree 1.

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

$$\mathbb{L}_{\pi_* X_K} \theta = \rho \theta$$

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

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

Summary: correspondence between *contact* and *homogeneous symplectic* geometry and dynamics

- Contact manifold $\mathbb{P}(T^*Q) \leftrightarrow$ symplectized manifold $\mathcal{T}^*Q$
- Locally defined contact form θ on $\mathbb{P}(T^*Q) \leftrightarrow$ Liouville form α on $\mathcal{T}^*Q$
- Functions on $\mathbb{P}(T^*Q) \leftrightarrow$ functions on $\mathcal{T}^*Q$ that are homogeneous of degree 0 in p
- Legendre submanifold $L \leftrightarrow$ homogeneous Lagrangian submanifold $\mathcal{L}$
- Generating function for $L \leftrightarrow$ homogeneous generating function for $\mathcal{L}$
- Contact Hamiltonian $\widehat{K} \leftrightarrow$ homogeneous Hamiltonian K
- Contact vector field $X_{\widehat{K}} \leftrightarrow$ Hamiltonian vector field X_K with $\mathbb{L}_{X_K}\alpha = 0$
- invariance of L: $\widehat{K}$ zero on $L \leftrightarrow$ invariance of $\mathcal{L}$: K zero on $\mathcal{L}$

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.

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.

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 $\mathcal{L}$.

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 ('conservation of energy') additionally imposes

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

Second Law of Thermodynamics ('increase of entropy') imposes

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

Symplectization leads to formalization of interaction with environment through ports

Define the outputs (homogeneous degree 0)

$$y_p := g_E|_{\mathcal{L}},$$

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

(u, y_p) defines a power port.

Entropy-conjugate outputs (again homogeneous degree 0) are defined as

$$y_e := g_S|_{\mathcal{L}},$$

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.

Note that $K = K^a + K^c u$ is dimension-less.

Outline

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

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

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

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

Interconnection of port-thermodynamic systems

Consider two port-thermodynamic systems with extensive variables

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

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 α_1 and α_2:

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

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

- 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 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.
- Basic examples are given; much more to be done !

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Consider two heat compartments, interacting by heat flow through conducting wall. The two systems, indexed by 1 and 2, exchange a heat flow q given by Fourier's law

$$q = \lambda(T_1 - T_2),$$

with temperatures

$$T_i = \frac{\partial E_i}{\partial S_i}(S_i), \quad i = 1, 2,$$

with $U_1(S_1), U_2(S_2)$ the internal energies of the two compartments.

Leads to pseudo port-Hamiltonian system

$$\begin{bmatrix} \dot{S}_1 \\ \dot{S}_2 \end{bmatrix} = \begin{bmatrix} -\frac{q}{T_1} \\ \frac{q}{T_2} \end{bmatrix} = \begin{bmatrix} -\lambda \frac{T_1 - T_2}{T_1} \\ \lambda \frac{T_1 - T_2}{T_2} \end{bmatrix} = \begin{bmatrix} 0 & \lambda(\frac{1}{T_1} - \frac{1}{T_2}) \\ -\lambda(\frac{1}{T_1} - \frac{1}{T_2}) & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial U}{\partial S_1} \\ \frac{\partial E}{\partial S_2} \end{bmatrix}$$

with total energy $E(S_1, S_2) := E_1(S_1) + E_1(S_2)$.