Dirac structures in nonequilibrium thermodynamics

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Plan of our talk

- Some background: We will focus on the geometric structure and variational formulations behind thermodynamics, in particular, we will see the cases of open thermodynamics and interconnected systems of mechanical and thermodynamic subsystems. Then we will see what are our main problems.

- Dirac formulation: Second, we will make a brief review on Dirac formulation for the case of mechanics. Then we will see how to extend it to nonequilibrium thermodynamics for the case of adiabatically closed systems, where we will use the specific feature of constraints appeared in thermodynamics, called the nonlinear constraints of thermodynamic type.

- Dirac formulation of open thermodynamics: Third, we will further extend it to the case of simple open systems in the context of the time-dependent nonlinear nonholonomic mechanics by using the Dirac structure and the associated dynamical system, together with the variational formulation over the covariant Pontryagin bundle.

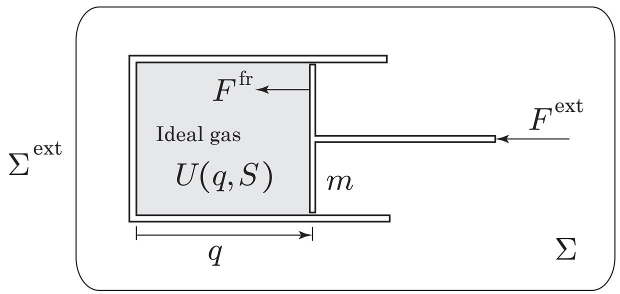
- Some examples of thermodynamics: Last, we will illustrate our theory with two examples, one is an interconnected system with mechanical constraints and thermodynamic nonlinear constraints. The other is an open system of the forced piston with ports, through which the matter and heat power exchanges with exterior.

Background in thermodynamics

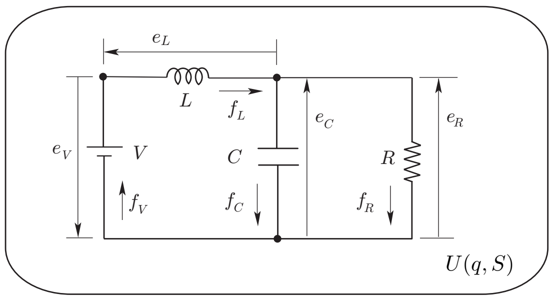
□ Nonequilibrium thermodynamic systems

- Thermodynamics is a phenomenological theory which aims to identify and describe the relations between the macroscopic properties of a system, treats almost exclusively equilibrium states and quasi-static transition from one equilibrium state to another and is governed by the first and second laws.
- On the other hand, classical mechanics, fluid dynamics as well as electromagnetism CANNOT be treated in the context of the classical equilibrium thermodynamics, because they belong to the subject of nonequilibrium thermodynamics, which treats the time evolution of dynamical systems.
- Here we have two typical examples of the nonequilibrium thermodynamic systems:

An adiabatic piston system with an ideal gas



A resistive circuit with internal entropy production



- Surprisingly, we have not well established a unified approach to treat such nonequilibrium thermodynamic systems, consistently with the traditional Hamilton's principle in mechanics.

Geometry in thermodynamics

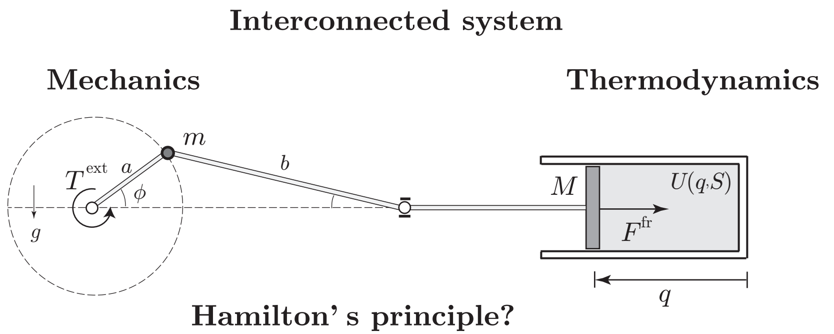
- The geometry of **equilibrium thermodynamics** has been traditionally described by contact geometry (Gibbs[1873], Caratheodry[1909], Hermann[1973], others) using the Gibbs form $\theta = dx^0 - p_i dx^i$ such as

$$\theta = dU - TdS + pdV - \mu dN,$$

  which characterizes the **thermodynamic phase space**, where x^0 denotes the energy and (x^i, p_i) are pairs of conjugated extensive and intensive variables.

- The ideas have been **extended to nonequilibrium thermodynamics**, where thermodynamic properties are encoded by **Legendre submanifolds** of the thermodynamic phase space (Mrugala[1978,1980]), and a geometric formulation of irreversible processes was made in Eberard, Maschke, and van der Schaft[2007] by lifting **port-Hamiltonian systems** to the thermodynamic phase space.

- On the other hand, there have been still a gap between mechanics and thermodynamics, because the geometric structures in mechanics are in general given by symplectic, Poisson or Dirac structures, together with the variational formulation based on Hamilton's principle.



- So the question is: what is the unified geometric and variational approach to the dynamics of the interconnected system of mechanical and thermodynamic subsystems as shown below?

□ Variational principles in thermodynamics

- As is well known, there are conventional variational principles called principle of least dissipation of energy (Onsager and Machlup [1953]) and principle of minimum entropy production (Prigogine [1947], Glansdorff and Prigogine [1971]), so that the power function associated with the internal entropy production

$$P = \boldsymbol{J}_i \boldsymbol{X}_j$$

becomes minimum with some boundary, where $\boldsymbol{J}_i = L_{ij} \boldsymbol{X}_j$ (with symmetric properties $L_{ij} = L_{ji}$) are given phenomenological relations.

- However, we do not know how to incorporate the principle of least dissipation of energy or the principle of minimum entropy production into the conventional Hamilton's principle in mechanics, which is needed to formulate an interconnected system that consists of mechanical and thermodynamical systems.

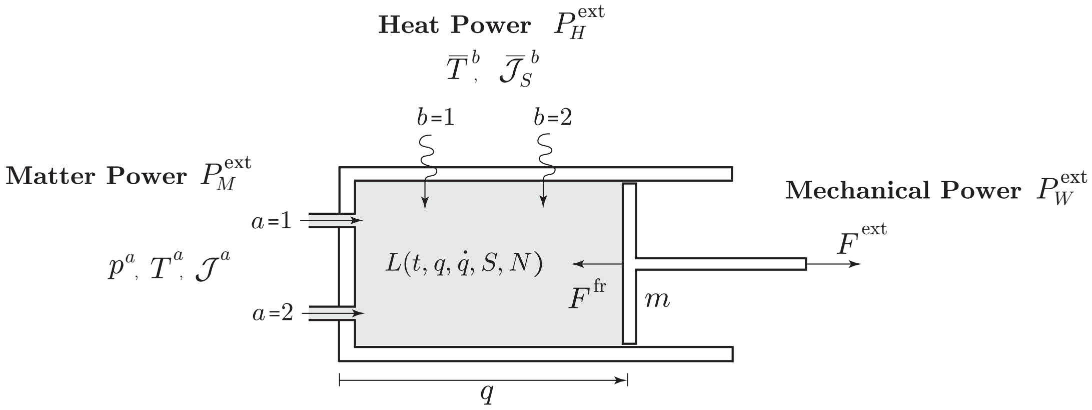
- Then the second question is: what is the unified variational principle for nonequilibrium thermodynamics including the conventional Hamilton's principle in mechanics?

$$\delta \int_{t_1}^{t_2} L(q(t), \dot{q}(t)) dt = 0$$

  - A Lagrangian variational formulation for nonequilibrium thermodynamics that is an extension of Hamilton's variational principle in mechanics has been proposed by GB-Yo(2016).
  - Regarding geometry in nonequilibrium thermodynamics, it has been shown that there exist Dirac structures for the isolated cases, consistently with variational structures; see GB-Yo(2018).

□ Open systems that exchange matter and heat power with exterior

- We are mainly concerned with a general class of open thermodynamic systems such as a forced-piston with ports, through which exchanges matter and heat power with exterior and hence $P_H^{\rm ext} \neq P_M^{\rm ext} \neq P_W^{\rm ext} \neq 0$.



This class of thermodynamic systems is very important for understanding biological systems such as cells.

- Again, the geometry and variational formulation of such an open system have not been well understood.

- Thus our talk will be as follows:

  – We clarify underlying geometry of open nonequilibrium thermodynamics using "time-dependent Dirac structures" in an extended context of time-dependent nonlinear nonholonomic mechanics.

  – Associated with Dirac geometry, we show the variational formulation of time-dependent Dirac dynamical systems by extending the Lagrange-d'Alembert-Pontryagin principle.

  – Finally, we illustrate our theory by an example of open systems, namely, a forced-piston with exchanging matter and heat power with exterior through ports.

Variational formulation of simple closed systems (GBYo[2016])

- Consider an simple closed system ($P_M^{\rm ext}=0$) described by an entropy S and mechanical variables $(q^i,\dot q^i)$ with Lagrangian $L=L(q,\dot q,S):TQ\times\mathbb{R}\to\mathbb{R}$, an exterior force $F^{\rm ext}(q,\dot q,S)$and a friction force $F^{\rm fr}(q,\dot q,S)$.

Consider the critical condition of the action integral

$$\delta\int_{t_1}^{t_2}L(q,\dot q,S)dt+\int_{t_1}^{t_2}\left\langle F^{\rm ext}(q,\dot q,S),\delta q\right\rangle=0,\qquad \text{Variational condition}$$

subject to

$$\frac{\partial L}{\partial S}(q,\dot q,S)\delta S=\left\langle F^{\rm fr}(q,\dot q,S),\delta q\right\rangle,\qquad \text{Variational constraint } C_V$$

and with

$$\frac{\partial L}{\partial S}(q,\dot q,S)\dot S=\underbrace{\left\langle F^{\rm fr}(q,\dot q,S),\dot q\right\rangle}_{\text{nonlinear constraint}}-P_H^{\rm ext}.\qquad \text{Phenomenological constraint } C_K$$

- If a curve $(q(t),S(t))$ on $Q\times\mathbb{R}$ is the critical curve, then it satisfies the evolution equations:

$$\begin{cases}\dfrac{d}{dt}\dfrac{\partial L}{\partial\dot q}-\dfrac{\partial L}{\partial q}=F^{\rm ext}(q,\dot q,S)+\underbrace{F^{\rm fr}(q,\dot q,S)}_{\text{friction}},\\[2ex] \underbrace{\dfrac{\partial L}{\partial S}\dot S}_{\text{thermodynamic power}}=\underbrace{\left\langle F^{\rm fr}(q,\dot q,S),\dot q\right\rangle}_{\text{friction power}}-P_H^{\rm ext}.\end{cases}$$

- First law and second laws are recovered:

$$\frac{d}{dt}E(q(t),S(t))=\underbrace{\left\langle F^{\rm ext},\dot q\right\rangle}_{=P_W^{\rm ext}}+P_H^{\rm ext}\quad\text{and}\quad \dot S(t)=\frac{1}{T}\left\langle\lambda(q,S)\dot q,\dot q\right\rangle\geq 0$$

Dirac dynamical formulation in mechanics

- Before going into detail on the Dirac formulation of thermodynamics, let us recall the Dirac formulation of nonholonomic mechanics.

- The geometry of nonholonomic mechanics is well understood in the context of (almost) Dirac structures, which is a unified geometric object of presymplectic and almost Poisson structures.

- The Dirac structure plays a central role in formulating the constrained mechanical system such as an interconnected system (Kron [1963]) of circuits, rolling balls, and multibody systems, where the Dirac structure indicates how the energy flow is regulated among system elements.

- In mechanics, the nonholonomic constraints are usually given by linear in velocities, which are expressed by a distribution $\Delta_Q \subset TQ$ (here we call "mechanical constraints") as

$$\Delta_Q(q) = \{(q,\dot{q}) \in T_qQ \mid \langle \omega^a(q), \dot{q} \rangle = 0, \ a = 1, ..., m < n\},$$

where $\omega^a(q) = \sum_{i=1}^n \omega_i^a(q) dq^i$ are m one-forms on a finite dimensional configuration manifold Q.

- Example: Given a two-form $\omega_M \in \Lambda^2(M)$ and a distribution Δ_M (nonholonomic constraints) on M, an (almost) Dirac structure $D_{\Delta_M} \subset TM \oplus T^*M$ on M is defined by:

$$D_{\Delta_M}(m) := \Big\{ (v_m, \alpha_m) \in T_mM \times T_m^*M \ \mid \ v_m \in \Delta_M(m) \text{ and } \langle \alpha_m, w_m \rangle = \omega_M(m)(v_m, w_m) \ \text{ for all } \ w_m \in \Delta_M(m) \Big\}.$$

- In mechanics, we have the Dirac dynamical systems on the Pontryagin bundle $M = TQ \oplus T^*Q$ (YoMa[2006]):

$$(\dot{x}(t), \mathbf{d}E(x(t))) \in D_{\Delta_M}(x(t)), \quad \text{for each } x(t) = (q(t), v(t), p(t)) \in M,$$

- Associated with this Dirac dynamical system, there is a natural variational formulation called the Lagrange-d'Alembert-Pontryagin principle:

$$\begin{aligned}
&\delta \int_{t_1}^{t_2} \left[L(q(t), v_q(t)) + \langle p_q(t), \dot{q}(t) - v_q(t) \rangle \right] dt \\
&= \delta \int_{t_1}^{t_2} \left[\langle p_q(t), \dot{q}(t) \rangle - E(q(t), v_q(t), p_q(t)) \right] dt = 0,
\end{aligned}$$

subject to the variational constraint

$$\delta q(t) \in \Delta_Q(q(t))$$

and with the kinematic constraint ("linear" in velocities)

$$\dot{q}(t) \in \Delta_Q(q(t)).$$

– This yields the Lagrange-d'Alembert-Pontryagin equations:

$$p_q = \frac{\partial L}{\partial v_q}, \quad \dot{q} = v_q \in \Delta_Q(q), \quad \text{and} \quad \dot{p}_q - \frac{\partial L}{\partial q} \in \Delta_Q^\circ(q).$$

- Problem in thermodynamics: there exists some difficulty of how to incorporate nonlinear nonholonomic constraints appeared in the entropy production into the context of symplectic, Poisson and Dirac structures:

$$\underbrace{\frac{\partial L}{\partial S} \dot{S}}_{\text{thermodynamic power}} = \underbrace{\left\langle F^{\mathrm{fr}}(q, \dot{q}, S), \dot{q} \right\rangle}_{\text{friction power}} - P_H^{\mathrm{ext}},$$

since it can't be directly treated as fiber-wise linear relations of symplectic, Poisson and Dirac structures !

Generalized LDA principle for nonlinear nonholonomic constraints

- In our theory, we can avoid this difficulty in thermodynamics by using the specific feature existing in the variational and kinematic constraints.

Definition 1 (Nonlinear constraints of thermodynamic type: GBYo(2017)) Consider a variational constraint $C_V \subset TQ \times_Q TQ$ over a configuration manifold Q, such that, at each $(\mathsf{q},\mathsf{v}) \in T_{\mathsf{q}}Q$, the subspace

$$C_V(\mathsf{q},\mathsf{v}) := \{(\mathsf{q},\delta\mathsf{q}) \mid (\mathsf{q},\mathsf{v},\delta\mathsf{q}) \in C_V \cap (\{(\mathsf{q},\mathsf{v})\} \times T_{\mathsf{q}}Q)\} \subset TQ$$

defines the nonlinear constraint of thermodynamic type $C_K \subset TQ$ as

$$C_K := \{(\mathsf{q},\mathsf{v}) \in TQ \mid (\mathsf{q},\mathsf{v}) \in C_V(\mathsf{q},\mathsf{v})\}.$$

- For a Lagrangian $L : TQ \to \mathbb{R}$ and a given external force $F^{\rm ext} : TQ \to T^*Q$, consider the generalized Lagrange-d'Alembert-Pontryagin principle:

$$\delta \int_{t_1}^{t_2} [L(\mathsf{q}(t),\mathsf{v}(t)) + \langle \mathsf{p}, \dot{\mathsf{q}}(\mathsf{t}) - \mathsf{v}(\mathsf{t})\rangle]\, dt + \int_{t_1}^{t_2} \left\langle F^{\rm ext}(\mathsf{q}(t),\dot{\mathsf{q}}(t)), \delta\mathsf{q}(t)\right\rangle dt = 0,$$

subject to $\delta\mathsf{q}(t) \in C_V(\mathsf{q}(t),\dot{\mathsf{q}}(t)) \subset T_{\mathsf{q}(t)}Q$ and with $(\mathsf{q}(t),\dot{\mathsf{q}}(t)) \in C_K$.

- This yields

$$\mathsf{p} = \frac{\partial L}{\partial \mathsf{v}}, \quad (\mathsf{q},\dot{\mathsf{q}}) \in C_V(\mathsf{q},\dot{\mathsf{q}}), \quad \dot{\mathsf{q}} = \mathsf{v} \quad \text{and} \quad \dot{\mathsf{p}} - \frac{\partial L}{\partial \mathsf{q}} - F^{\rm ext} \in C_V(\mathsf{q},\dot{\mathsf{q}})^\circ.$$

- Since this special relation is always satisfied in thermodynamics, a Dirac structure and the Dirac dynamical system can be always constructed in association with the generalized Lagrange-d'Alembert-Pontryagin equations.

- Consider an adiabatically closed system ($P_M^{\rm ext} = P_H^{\rm ext} = 0$) with a thermodynamic configuration space $\mathcal{Q} = Q \times \mathbb{R}$ with $\mathsf{q} = (q, S) \in \mathcal{Q}$.

  – Assume that the variational constraint for thermodynamics $C_V^{\rm th} \subset T\mathcal{Q} \times T\mathcal{Q}$ is given by

$$C_V^{\rm th} = \left\{ (q, S, v_q, v_S, \delta q, \delta S) \in T\mathcal{Q} \times_{\mathcal{Q}} T\mathcal{Q} \;\middle|\; \frac{\partial L}{\partial S}(q, v_q, S)\delta S = \left\langle F^{\rm fr}(q, v_q, S), \delta q \right\rangle \right\}.$$

  Assume also that there are mechanical constraints

$$\Delta_Q(q) = \{(q, v_q) \in TQ \mid \langle \omega^r(q), v_q \rangle = 0,\ r = 1, ..., m < n\} \subset TQ,$$

  from which, we define the mechanical variational constraint $C_V^{\rm mech} \subset T\mathcal{Q} \times_{\mathcal{Q}} T\mathcal{Q}$ as

$$C_V^{\rm mech} = T\mathcal{Q} \times_{\mathcal{Q}} \Delta_{\mathcal{Q}} = T\mathcal{Q} \times_{\mathcal{Q}} (T\pi_{(\mathcal{Q},Q)})^{-1}(\Delta_Q).$$

  – Thus, we can develop the variational constraint for the thermodynamic system as

$$C_V := C_V^{\rm th} \cap C_V^{\rm mech} \subset T\mathcal{Q} \times_{\mathcal{Q}} T\mathcal{Q},$$

  which is locally described by

$$C_V = \left\{ (q, S, v_q, v_S, \delta q, \delta S) \;\middle|\; (q, \delta q) \in \Delta_Q(q) \ \text{ and } \ \frac{\partial L}{\partial S}(q, v_q, S)\delta S = \left\langle F^{\rm fr}(q, v_q, S), \delta q \right\rangle \right\},$$

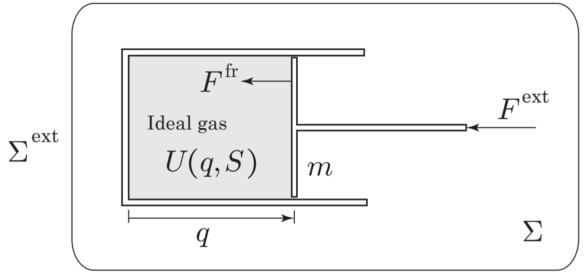
  and the annihilator of $C_V(q, S, v_q, v_S) \subset T_{(q,S)}\mathcal{Q}$ is given by

$$C_V(q, S, v_q, v_S)^\circ = \left\{ (q, S, \alpha, \mathcal{T}) \;\middle|\; \frac{\partial L}{\partial S}\alpha + \mathcal{T} F^{\rm fr} \in \Delta_Q(q)^\circ \right\} \subset T^*\mathcal{Q}.$$

  – For the nonlinear kinematic constraint $C_K \subset T\mathcal{Q}$, we can obtain C_K from C_V as

$$C_K = \left\{ (q, S, \dot{q}, \dot{S}) \;\middle|\; (q, S, \dot{q}, \dot{S}) \in C_V(q, S, \dot{q}, \dot{S}) \right\}.$$

Example: a forced piston system with an ideal gas



- Consider a piston-cylinder system $\mathbf{\Sigma}$ with $\mathcal{Q} = \mathbb{R} \times \mathbb{R} \ni (q, S)$ with an external force $F^{\rm ext}$ and the Lagrangian

$$L(q, v, S) = \frac{1}{2} m \dot{q}^2 - U(q, S),$$

where $U(q, S)$ is the internal energy of gas. Assume that the friction force is given by $F^{\rm fr}(q, v, S) = -\lambda(q, S) v$.

- The variational condition reads

$$\delta \int_{t_1}^{t_2} \left[L(q, v, S) + p(t) \left(\dot{q} - v \right) \right] dt + \int_{t_1}^{t_2} F^{\rm ext}(q, v) \delta x dt = 0,$$

subject to the variational constraint and phenomenological constraint is

$$\frac{\partial U}{\partial S}(q, S) \delta S = \lambda(q, S) \dot{q} \; \delta q \quad \text{and} \quad \frac{\partial U}{\partial S}(q, S) \dot{S} = \lambda(q, S) \dot{q}^2$$

- The solution curve satisfies the evolution equations, where we also recover the second law:

$$p = m v, \quad \dot{q} = v, \quad \dot{p} = P(q, S) A - \lambda(x, S) \dot{q} + F^{\rm ext}(q, \dot{q}), \quad \dot{S} = \frac{1}{T} \lambda(q, S) \dot{q}^2 > 0.$$

- One can easily verify the first law of energy balance $\dot{E} = F^{\rm ext}(q, \dot{q}) \dot{q}$ along the solution curve $(q(t), S(t))$.

Dirac structures on the Pontryagin bundle $\mathcal{P} = T\mathcal{Q} \oplus T^*\mathcal{Q}$

- Let $\mathcal{P} = T\mathcal{Q} \oplus T^*\mathcal{Q}$ be the Pontryagin bundle over a thermodynamic configuration space $\mathcal{Q} = Q \times \mathbb{R}$:

$$\pi_{(\mathcal{P},\mathcal{Q})} : \mathcal{P} = T\mathcal{Q} \oplus T^*\mathcal{Q} \to \mathcal{Q}; \quad x = (q, S, v_q, v_S, p_q, p_S) \mapsto \mathsf{q} = (q, S),$$

and define an induced distribution $\Delta_{\mathcal{P}}$ on $\mathcal{P}$ from the given variational constraint $C_V(\mathsf{q}, \mathsf{v}) \subset \mathsf{T}_{\mathsf{q}}\mathcal{Q}$ by

$$\Delta_{\mathcal{P}}(x) := (T_x\pi_{(\mathcal{P},\mathcal{Q})})^{-1}(C_V(q, S, v_q, v_S)) \subset T_x\mathcal{P},$$

which is locally given by, for each $x = (q, S, v_q, v_S, p_q, p_S) \in \mathcal{P}$,

$$\Delta_{\mathcal{P}}(x) := \left\{ (x, \delta x) \in T_x\mathcal{P} \;\middle|\; (q, \delta q) \in \Delta_Q(q) \;\text{ and }\; \frac{\partial L}{\partial S}(q, v, S)\delta S = \left\langle F^{\mathrm{fr}}(q, v, S), \delta q \right\rangle \right\}.$$

- Using $\Omega_{T^*\mathcal{Q}}$ on $T^*\mathcal{Q}$, the presymplectic form on $\mathcal{P}$ is induced by $\omega_{\mathcal{P}}(x) = \pi^*_{(\mathcal{P},T^*\mathcal{Q})}\Omega_{T^*\mathcal{Q}}$, locally denoted by

$$\omega_{\mathcal{P}} = dq^i \wedge dp_i + dS \wedge dp_S.$$

- From $\Delta_{\mathcal{P}}$ and $\omega_{\mathcal{P}}$, an induced Dirac structure $D_{\Delta_{\mathcal{P}}} \subset T\mathcal{P} \oplus T^*\mathcal{P}$ on $\mathcal{P}$ is defined as

$$D_{\Delta_{\mathcal{P}}}(x) := \big\{ (v_x, \alpha_x) \in T_x\mathcal{P} \times T^*_x\mathcal{P} \;\mid\; v_x \in \Delta_{\mathcal{P}}(x) \text{ and }$$
$$\langle \alpha_x, w_x \rangle = \omega_{\mathcal{P}}(x)(v_x, w_x) \;\text{ for all }\; w_x \in \Delta_{\mathcal{P}}(x) \big\}.$$

Dirac systems on $\mathcal{P}=T\mathcal{Q}\oplus T^*\mathcal{Q}$ (adiabatically closed systems)

Theorem 1 For a given Lagrangian L on $TQ\times\mathbb{R}$ and $F^{\mathrm{fr}}, F^{\mathrm{ext}}: TQ\times\mathbb{R}\to T^*Q$, a generalized energy is defined on $\mathcal{P}=T\mathcal{Q}\oplus T^*\mathcal{Q}$ as

$$\mathcal{E}(q,S,v_q,v_S,p_q,p_S)=\langle p_q,v_q\rangle+p_S v_S-L(q,v,S).$$

A curve $x(t)=(q(t),S(t),v_q(t),v_S(t),p_q(t),p_S(t))\in\mathcal{P}$ is the solution curve of the Dirac thermodynamic system:

$$\big((x,\dot{x}),\mathbf{d}\mathcal{E}(x)-\widetilde{F}^{\mathrm{ext}}(x)\big)\in D_{\Delta_{\mathcal{P}}}(x),$$

if and only if $x(t)$ satisfies the intrinsic Dirac thermodynamic equations on $\mathcal{P}$:

$$\mathbf{i}_{\dot{x}}\omega_{\mathcal{P}}(x)-\mathbf{d}\mathcal{E}(x)+\widetilde{F}^{\mathrm{ext}}(x)\in\Delta_{\mathcal{P}}(x)^\circ,\quad \dot{x}\in\Delta_{\mathcal{P}}(x).$$

- The bundle picture is given as follows:

$$\begin{tikzcd}
& & D_{\Delta_{\mathcal{P}}}\subset T\mathcal{P}\oplus T^*\mathcal{P} \arrow[dl, "\rho_{T^*\mathcal{P}}"'] \arrow[dd, "\rho_{\mathcal{P}}"] \arrow[dr, "\rho_{T\mathcal{P}}"] & & \\
& T^*\mathcal{P} \arrow[dr, shift left, "\pi_{\mathcal{P}}"] & & T\mathcal{P} \arrow[dl, "\tau_{\mathcal{P}}"'] & \\
\mathbb{R} & & \mathcal{P}=T\mathcal{Q}\times_{\mathcal{Q}}T^*\mathcal{Q} \arrow[ll, "\mathcal{E}"'] \arrow[ul, shift left, "\mathbf{d}\mathcal{E}"] \arrow[dr, "\pi_{(\mathcal{P},T\mathcal{Q})}"] \arrow[dd, "\pi_{(\mathcal{P},\mathcal{Q})}"] & & \\
& & & T\mathcal{Q} \arrow[dl, "\tau_{\mathcal{Q}}"] \arrow[r, "\widetilde{L}"] & \mathbb{R} \\
& & \mathcal{Q}=Q\times\mathbb{R} & &
\end{tikzcd}$$

- The associated variational formulation is given by generalized Lagrange-d'Alembert-Pontryagin principle:

$$\delta \int_{t_1}^{t_2} \Big[\langle \theta_{\mathcal{P}}(x), \dot{x}\rangle - \mathcal{E}(x)\Big] dt + \int_{t_1}^{t_2} \widetilde{F}^{\mathrm{ext}}(x(t)) \cdot \delta x(t) dt = 0,$$

  which is locally denoted by

$$\delta \int_{t_1}^{t_2} \Big[\langle p_q, \dot{q} - v_q\rangle + p_S(\dot{S} - v_S) + L(q, v_q, S)\Big]\, dt + \int_{t_1}^{t_2} \big\langle F^{\mathrm{ext}}(q, \dot{q}, S), \delta q\big\rangle\, dt = 0,$$

  with respect to variations $\delta x \in \Delta_{\mathcal{P}}(x)$ and with the constraint $\dot{x} \in \Delta_{\mathcal{P}}(x)$.

- This variational formulation also deduces the intrinsic Dirac thermodynamic equations:

$$\mathbf{i}_{\dot{x}}\omega_{\mathcal{P}}(x) - \mathbf{d}\mathcal{E}(x) + \widetilde{F}^{\mathrm{ext}}(x) \in \Delta_{\mathcal{P}}(x)^{\circ}, \quad \dot{x} \in \Delta_{\mathcal{P}}(x),$$

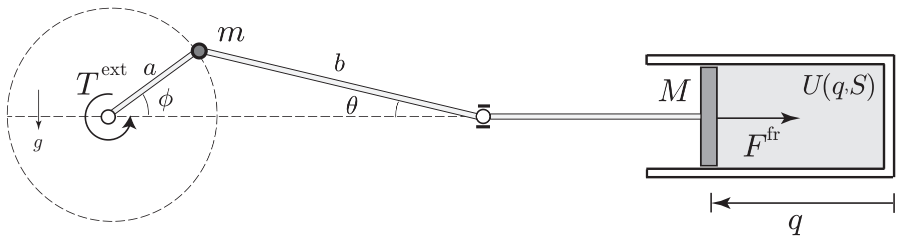
  which are locally denoted by

$$\left\{ \begin{array}{l} \dot{p}_q - \dfrac{\partial L}{\partial q}(q, v_q, S) - F^{\mathrm{ext}}(q, v_q, S) - F^{\mathrm{fr}}(q, v_q, S) \in \Delta_Q(q)^{\circ}, \\[2ex] \dot{q} = v_q \in \Delta_Q(q), \quad \dot{S} = v_S, \quad \dfrac{\partial L}{\partial S} = \underbrace{\big\langle F^{\mathrm{fr}}(q, \dot{q}, S), \dot{q}\big\rangle}_{\text{nonlinear constraint}}, \quad p_q = \dfrac{\partial L}{\partial v_q}, \quad p_S = 0 \end{array} \right.$$

- The **energy conservation (first law)** holds along the curve $x(t)$ as

$$\frac{d}{dt}\mathcal{E}(x(t)) = \Big\langle \widetilde{F}^{\mathrm{ext}}(x(t)), \dot{x}(t) \Big\rangle.$$

Example: a forced piston-cylinder system with an ideal gas



- Consider a forced piston-cylinder system with $Q = \mathbb{R} \times S^1 \ni (q, \phi)$ and with L on $TQ \times \mathbb{R}$ given by

$$L(q, \phi, v_q, v_\phi, S) = \frac{1}{2} M v_q^2 + \frac{1}{2} m a^2 v_\phi^2 - \mathsf{U}(q, \phi, S),$$

where $\mathsf{U}(q, \phi, S)$ consists of the internal energy $U(q, S)$ as well as the gravity potential.

- The mechanical constraint $\Delta_Q \subset TQ$ is given by (see, Sommerfeld[1964])

$$\Delta_Q = \{(q, \phi, \delta q, \delta\phi) \mid \delta q + \alpha(\phi)\delta\phi = 0\}, \quad \text{where} \quad \alpha(\phi) = a \sin\phi \left(1 + \frac{\frac{a}{b}\cos\phi}{\sqrt{1 - \left(\frac{a}{b}\right)^2 \sin^2\phi}} \right).$$

The variational constraint $C_V \subset T\mathcal{Q} \times_{\mathcal{Q}} T\mathcal{Q}$ for both mechanical and thermodynamic constraints is

$$C_V = \left\{ (q, \phi, S, v_q, v_\phi, v_S, \delta q, \delta\phi, \delta S) \;\middle|\; \underbrace{\delta q + \alpha(\phi)\delta\phi = 0}_{\text{mechanical constraint}} \text{ and } \underbrace{\frac{\partial L}{\partial S}(q, \phi, v_q, v_\phi, S)\delta S = \left\langle F^{\mathrm{fr}}(q, \phi, v_q, v_\phi, S), \delta q \right\rangle}_{\text{thermodynamic constraint}} \right\}.$$

- Associated to $D_{\Delta_{\mathcal{P}}} \subset T\mathcal{P} \oplus T^*\mathcal{P}$, the Dirac system on $\mathcal{P}$ is given by, for $x = (q, \phi, S, v_q, v_\phi, v_S, p_q, p_\phi, p_S) \in \mathcal{P}$,

$$\left((x, \dot{x}), \mathbf{d}\mathcal{E}(x) - \widetilde{T}^{\mathrm{ext}}(x)\right) \in D_{\Delta_M}(x).$$

- The associated variational condition reads

$$\delta \int_{t_1}^{t_2} \left[\frac{1}{2} M v_q^2 + \frac{1}{2} m a^2 v_\phi^2 - U(q, \phi, S) + \langle p_q, \dot{q} - v_q \rangle + \left\langle p_\phi, \dot{\phi} - v_\phi \right\rangle \right] dt + \int_{t_1}^{t_2} \left\langle T^{\text{ext}}(q, \phi, S, v_q, v_\phi, v_S), \delta\phi \right\rangle dt = 0,$$

subject to the variational constraints

$$\delta q + \alpha(\phi)\delta\phi = 0 \quad \text{and} \quad \frac{\partial L}{\partial S}(q, \phi, v_q, v_\phi, S)\delta S = \left\langle F^{\text{fr}}(q, \phi, v_q, v_\phi, S), \delta q \right\rangle$$

and with the nonlinear constraints

$$\delta q + \alpha(\phi)\dot{\phi} = 0 \quad \text{and} \quad \frac{\partial L}{\partial S}(q, \phi, v_q, v_\phi, S)\dot{S} = \left\langle F^{\text{fr}}(q, \phi, v_q, v_\phi, S), \dot{q} \right\rangle.$$

- Thus, we get the coupled mechanical and thermal evolution equations of the piston-cylinder system:

$$\begin{cases} p_q = M v_q, \quad \dot{p}_q - p(x, S)A - r\dot{q} = \mu, \quad \dot{q} = v_q, \\ p_\phi = m a^2 v_\phi, \quad \dot{p}_\phi + m g a \sin\phi = \alpha(\phi)\mu + T^{\text{ext}}, \quad \dot{\phi} = v_\phi, & \text{Lagrange-d'Alembert equations} \\ \dot{q} = -\alpha(\phi)\dot{\phi}, & \text{mechanical constraint} \\ \dot{S} = \dfrac{1}{T}\langle r\dot{q}, \dot{q} \rangle \geq 0, & \text{internal entropy production (second law)} \end{cases}$$

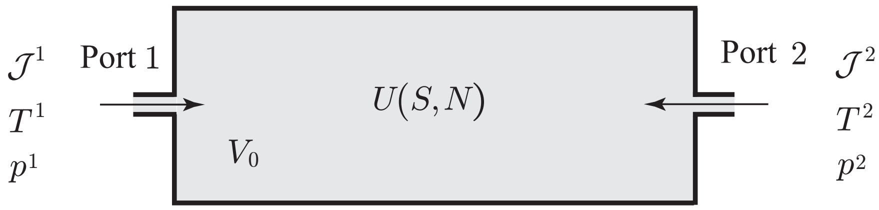
where $F^{\text{fr}}(q, \dot{q}, S) = -r\dot{q}$ and $T = -\frac{\partial L}{\partial S}(q, v, S)$, where $r > 0$ denotes the friction coefficient factor and $\frac{\partial U_{\text{gas}}}{\partial q} = -\mathsf{p}(x, S)A$, where $\mathsf{p}(x, S)$ is the pressure of the ideal gas.

- One can easily verify the first law of energy conservation along the solution curve as

$$\frac{d}{dt} E_L(t) = \left\langle T^{\text{ext}}(t), \dot{q}(t) \right\rangle.$$

Fundamental setting of open thermodynamics

- Consider an open system with external ports $a = 1, ..., A$, through which matter can flow into or out of the system. Suppose that the system has one chemical species with N the number of moles.



(1) Mass balance: The mole balance equation is given by

$$\frac{d}{dt}N = \sum_{a=1}^{A} \mathcal{J}^a,$$

where $\mathcal{J}^a$ is the molar flux (molar flow rate) through the a-th port; $\mathcal{J}^a > 0$ (flow into) and $\mathcal{J}^a < 0$ (flow out).

- As matter enters or leaves the system at the a-th port, it carries its internal energy $\mathsf{U}^a \mathcal{J}^a$, which is the product of the energy per mole (or molar energy) U^a and the molar flux $\mathcal{J}^a$ at the a-th port.

- Associated with matter flowing through the a-th port, the power flow due to the pressure is given as $p^a \mathsf{V}^a \mathcal{J}^a$, where p^a and V^a denote the pressure and the molar volume of the substance at the a-th port.

(2) First law: The power exchange due to the mass transfer is expressed by

$$\frac{d}{dt}U = \sum_{a=1}^{A} \mathcal{J}^a(\mathsf{U}^a + p^a \mathsf{V}^a) = \sum_{a=1}^{A} \mathcal{J}^a \mathsf{H}^a = P_M^{\mathrm{ext}},$$

where $\mathsf{H}^a = \mathsf{U}^a + p^a \mathsf{V}^a$ is the molar enthalpy at the a-th port.

(3) Second Law: One obtains the equations for the rate of change of the entropy of the system as

$$\frac{d}{dt}S = I + \sum_{a=1}^{A} \mathsf{S}^a \mathcal{J}^a,$$

where S^a is the molar entropy at the a-th port and I is the rate of internal entropy production given by

$$I = \frac{1}{T} \sum_{a=1}^{A} \left[\mathcal{J}_S^a (T^a - T) + \mathcal{J}^a (\mu^a - \mu) \right],$$

where $T = \frac{\partial U}{\partial S}$ the temperature, $\mu = \frac{\partial U}{\partial N}$ the chemical potential, and the entropy flow rate

$$\mathcal{J}_S^a := \mathsf{S}^a \mathcal{J}^a$$

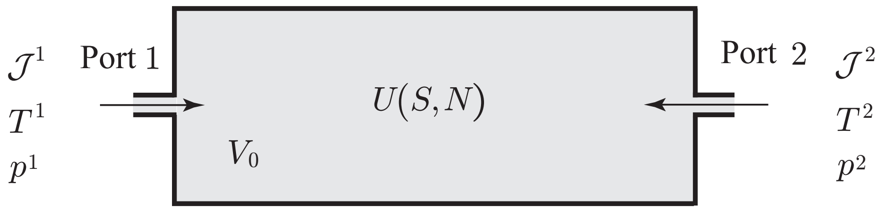
and with the expressions for the enthalpy

$$\mathsf{H}^a (= \mathsf{U}^a + p^a \mathsf{V}^a) = \mu^a + T^a \mathsf{S}^a.$$

(4) External ports: The external thermodynamic quantities at the ports are usually given by the pressure and the temperature p^a, T^a as functions of time t, from which other quantities may be described as

$$\mu^a = \mu^a(p^a(t), T^a(t)) \quad \text{or} \quad \mathsf{S}^a = \mathsf{S}^a(p^a(t), T^a(t))$$

So, we want to formulate dynamics of open systems in the context of the time-dependent mechanics.



Time-dependent constraints of open thermodynamic type

- Given a configuration manifold $\mathcal{Q}$, define the extended configuration manifold including the space of time:

$$\mathcal{Y} := \mathbb{R} \times \mathcal{Q} \ni (t, x).$$

- From the viewpoint of classical field theories, the extended configuration manifold is the trivial bundle

$$\mathcal{Y} = \mathbb{R} \times \mathcal{Q} \to \mathcal{X} = \mathbb{R}, \ (t, x) \mapsto t$$

and we use the first jet bundle, the dual first jet bundle (affine dual) and the Π bundle (dual to $J^1\mathcal{Y}$):

$$(t, x, v) \in J^1\mathcal{Y} \cong \mathbb{R} \times T\mathcal{Q}, \quad (t, x, \mathsf{p}, p) \in J^1\mathcal{Y}^\star \cong T^*\mathcal{Y} = T^*(\mathbb{R} \times \mathcal{Q}), \quad (t, x, p) \in \Pi\mathcal{Y} \cong \mathbb{R} \times T^*\mathcal{Q}.$$

Definition 2 Consider a time-dependent variational constraint $C_V \subset J^1\mathcal{Y} \times_{\mathcal{Y}} T\mathcal{Y}$ as

$$C_V = \big\{(t, x, v, \delta t, \delta x) \in J^1\mathcal{Y} \times_{\mathcal{Y}} T\mathcal{Y} \mid \sum_{i=1}^{n} A_i^r(t, x, v)\delta x^i + B^r(t, x, v)\delta t = 0, \ r = 1, ..., m\big\}.$$

Then, the associated time-dependent kinematic constraint C_K of thermodynamic type reads

$$C_K = \big\{(t, x, \dot{t}, \dot{x}) \in T\mathcal{Y} \mid \sum_{i=1}^{n} A_i^r(t, x, \dot{x})\dot{x}^i + B^r(t, x, \dot{x})\dot{t} = 0, \ r = 1, ..., m\big\},$$

where C_K and C_V are called time-dependent nonlinear constraints of thermodynamic type, because there exists the special relation:

$$C_K = \big\{(t, x, \dot{t}, \dot{x}) \in T\mathcal{Y} \mid (t, x, \dot{t}, \dot{x}) \in C_V(t, x, \dot{x})\big\} \subset T\mathcal{Y}.$$

Dirac structures on covariant Pontryagin bundles

- By analogy with the case of time-independent cases, consider the covariant Pontryagin bundle over the extended configuration manifold $\mathcal{Y} = \mathbb{R} \times \mathcal{Q}$ as

$$\pi_{(\mathcal{P},\mathcal{Y})} : \mathcal{P} = (\mathbb{R} \times T\mathcal{Q}) \times_{\mathcal{Y}} T^*\mathcal{Y} \to \mathcal{Y} = \mathbb{R} \times \mathcal{Q}; \qquad (v, \mathsf{p}, p) \mapsto (t, x).$$

- From $C_V \subset J^1\mathcal{Y} \times_{\mathcal{Y}} T\mathcal{Y}$ (recall $J^1\mathcal{Y} \cong \mathbb{R} \times T\mathcal{Q}$), define the induced distribution $\Delta_{\mathcal{P}}$ on $\mathcal{P}$ by

$$\Delta_{\mathcal{P}}(t, x, v, \mathsf{p}, p) := \left(T_{(t,x,v,\mathsf{p},p)}\pi_{(\mathcal{P},\mathcal{Y})}\right)^{-1}(C_V(t, x, v)) \subset T_{(t,x,v,\mathsf{p},p)}\mathcal{P},$$

which is locally given by

$$\Delta_{\mathcal{P}}(t, x, v, \mathsf{p}, p) = \left\{ (\delta t, \delta x, \delta v, \delta \mathsf{p}, \delta p) \in T_{(t,x,v,\mathsf{p},p)}\mathcal{P} \;\middle|\; \sum_{i=1}^{n} A_i^r(t, x, v)\delta x^i + B^r(t, x, v)\delta t = 0, \quad r = 1, ..., m \right\}.$$

- Given the canonical one-form $\Theta_{T^*\mathcal{Y}} = p_i dx^i + \mathsf{p}dt$, define the canonical symplectic form on $T^*\mathcal{Y}$ given by

$$\Omega_{T^*\mathcal{Y}} = -\mathbf{d}\Theta_{T^*\mathcal{Y}} = dx^i \wedge dp_i + dt \wedge d\mathsf{p}.$$

Using the projection $\pi_{(\mathcal{P},T^*\mathcal{Y})} : \mathcal{P} \to T^*\mathcal{Y}$, we get the presymplectic form on the covariant Pontryagin bundle

$$\omega_{\mathcal{P}} = \pi^*_{(\mathcal{P},T^*\mathcal{Y})}\Omega_{T^*\mathcal{Y}}.$$

- From $\Delta_{\mathcal{P}}$ and $\omega_{\mathcal{P}}$, define the time-dependent Dirac structure $D_{\Delta_{\mathcal{P}}}$ on $\mathcal{P}$ by, for each $\mathrm{x} \in \mathcal{P}$,

$$D_{\Delta_{\mathcal{P}}}(\mathrm{x}) = \left\{ (\mathfrak{u}_{\mathrm{x}}, \mathfrak{a}_{\mathrm{x}}) \in T_{\mathrm{x}}\mathcal{P} \times T^*_{\mathrm{x}}\mathcal{P} \mid \mathfrak{u}_x \in \Delta_{\mathcal{P}}(\mathrm{x}), \quad \langle \mathfrak{a}_{\mathrm{x}}, \mathfrak{v}_{\mathrm{x}} \rangle = \Omega_{\mathcal{P}}(\mathrm{x})(\mathfrak{u}_{\mathrm{x}}, \mathfrak{v}_{\mathrm{x}}), \quad \forall\, \mathfrak{v}_{\mathrm{x}} \in \Delta_{\mathcal{P}}(\mathrm{x}) \right\}.$$

Time-dependent Dirac systems on covariant Pontryagin bundles

- For the covariant Pontryagin bundle $\mathcal{P} = J^1\mathcal{Y} \times_{\mathcal{Y}} J^1\mathcal{Y}^\star \to \mathcal{Y} = \mathbb{R} \times \mathcal{Q}$, recall an element in the fiber at $y = (t, x) \in \mathcal{Y}$ is denoted by (v, p, p).

- Given a time-dependent Lagrangian $\mathcal{L}$ on $\mathbb{R} \times T\mathcal{Q}$, the covariant generalized energy $\mathcal{E} : \mathcal{P} \to \mathbb{R}$ is defined as

$$\mathcal{E}(t, x, v, \mathsf{p}, p) = \mathsf{p} + \langle p, v\rangle - \mathcal{L}(t, x, v),$$

which consists of the covariant Hamiltonian and the generalized energy $E : \mathbb{R} \times (T\mathcal{Q} \oplus T^*\mathcal{Q}) \to \mathbb{R}$ by

$$E(t, x, v, p) = \langle p, v\rangle - \mathcal{L}(t, x, v).$$

- **Proposition 1** Given $\Delta_{\mathcal{P}}$ and $\mathcal{L}$, a curve ("section") $\mathrm{x}(t) = (t, x(t), v(t), \mathsf{p}(t), p(t))$ on the covariant Pontryagin bundle $\mathcal{P}$ is a solution of the time-dependent Dirac dynamical system for a curve of the form

$$\big(\dot{\mathrm{x}}(t), \mathbf{d}\mathcal{E}(\mathrm{x}(t))\big) \in D_{\Delta_{\mathcal{P}}}(\mathrm{x}(t)).$$

if and only if $\mathrm{x}(t)$ satisfies the Lagrange-d'Alembert-Pontryagin equations:

$$\mathbf{i}_{\dot{\mathrm{x}}}\Omega_{\mathcal{P}} - \mathbf{d}\mathcal{E}(\mathrm{x}) \in \Delta_{\mathcal{P}}(\mathrm{x})^\circ, \;\; \dot{\mathrm{x}} \in \Delta_{\mathcal{P}}(\mathrm{x}),$$

which locally yields the following evolution equations:

$$\begin{cases} \dot{x} = v, \qquad \dot{t} = 1, \qquad p = \dfrac{\partial \mathcal{L}}{\partial v}, \\ (t, x, \dot{t}, \dot{x}) \in C_V(t, x, v), \qquad \left(\dot{\mathsf{p}} - \dfrac{\partial \mathcal{L}}{\partial t}, \dot{p} - \dfrac{\partial \mathcal{L}}{\partial x}\right) \in C_V(t, x, v)^\circ. \end{cases}$$

- In finite dimension, the coordinate expression of the Lagrange-d'Alembert-Pontryagin equations is given by:

$$\begin{cases} \dot{x}^i = v^i, \qquad \dot{t} = 1, \qquad p_i - \dfrac{\partial \mathcal{L}}{\partial v^i} = 0, \quad i = 1, ..., n, \\ \displaystyle\sum_{i=1}^{n} A_i^r(t, x, v)\dot{x}^i + B^r(t, x, v) = 0, \quad r = 1, ..., m, \\ \dot{p}_i - \dfrac{\partial \mathcal{L}}{\partial x^i} = \displaystyle\sum_{r=1}^{m} \lambda_r A^r(t, x, v), \qquad \dot{\mathsf{p}} - \dfrac{\partial \mathcal{L}}{\partial t} = \displaystyle\sum_{r=1}^{m} \lambda_r B^r(t, x, v), \end{cases}$$

which finally recovers the time-dependent Lagrange-d'Alembert equations for the curve $x(t) \in \mathcal{Q}$:

$$\begin{cases} \dfrac{d}{dt}\dfrac{\partial \mathcal{L}}{\partial \dot{x}^i} - \dfrac{\partial \mathcal{L}}{\partial x^i}(t, x, \dot{x}) = \displaystyle\sum_{r=1}^{m} \lambda_r A_i^r(t, x, \dot{x}), \quad i = 1, ..., n, \\ \displaystyle\sum_{i=1}^{n} A_i^r(t, x, \dot{x})\dot{x}^i + B^r(t, x, \dot{x}) = 0, \quad r = 1, ..., m, \end{cases}$$

- The covariant generalized energy $\mathcal{E}(t, x, v, \mathsf{p}, p)$ is preserved along the solution curve $\mathrm{x}(t) = (t, x(t), v(t), \mathsf{p}(t), p(t)) \in \mathcal{P}$ of the Dirac dynamical system as

$$\frac{d}{dt}\mathcal{E}(t, x, v, \mathsf{p}, p) = 0.$$

- Note that $\mathcal{E}$ is not the total energy of the system, but the total energy is represented by the generalized energy E and it follows that the balance of energy for the Dirac system is given by

$$\frac{d}{dt}E(t, x, v, p) = -\frac{d}{dt}\mathsf{p} = -\frac{\partial L}{\partial t}(t, x, v) - \sum_{r=1}^{m} \lambda_r B^r(t, x, v),$$

where $\frac{d}{dt}\mathsf{p}$ can be interpreted as the power flowing into/out of the system.

Variational structures of time-dependent nonholonomic systems

- Consider the LADP principle for an "arbitrary" curve $\mathrm{x}(\tau) = (t(\tau), x(\tau), v(\tau), \mathsf{p}(\tau), p(\tau))$ on $\mathcal{P}$ as

$$\delta \int_{\tau_1}^{\tau_2} \Big[\big\langle \theta_{\mathcal{P}}(\mathrm{x}(\tau)), \mathrm{x}'(\tau) \big\rangle - \mathcal{E}(\mathrm{x}(\tau)) \Big] d\tau = \delta \int_{\tau_1}^{\tau_2} \Big[\big\langle p, x' \big\rangle + \mathsf{p}t' - \mathcal{E}\big(t, x, v, \mathsf{p}, p\big) \Big] d\tau = 0$$

subject to the kinematic and variational constraints

$$\mathrm{x}'(\tau) \in \Delta_{\mathcal{P}}(\mathrm{x}(\tau)) \quad \text{and} \quad \delta\mathrm{x}(\tau) \in \Delta_{\mathcal{P}}(\mathrm{x}(\tau)),$$

namely, in coordinates,

$$\sum_{i=1}^{n} A_i^r\big(t, x, v\big) x'^i + B^r\big(t, x, v\big) t' = 0, \quad \text{and} \quad \sum_{i=1}^{n} A_i^r\big(t, x, v\big) \delta x^i + B^r\big(t, x, v\big) \delta t = 0,$$

together with the endpoint conditions $T\pi_{(\mathcal{P},Y)}(\delta\mathrm{x}(\tau_1)) = T\pi_{(\mathcal{P},Y)}(\delta\mathrm{x}(\tau_2)) = 0$.

- From this variational principle, the Lagrange-d'Alembert-Pontryagin equations can be recovered:

$$\mathbf{i}_{\mathrm{x}'}\omega_{\mathcal{P}} - \mathbf{d}\mathcal{E}(\mathrm{x}) \in \Delta_{\mathcal{P}}(\mathrm{x})^{\circ}, \qquad \mathrm{x}' \in \Delta_{\mathcal{P}}(\mathrm{x}),$$

which are given, in coordinates, by

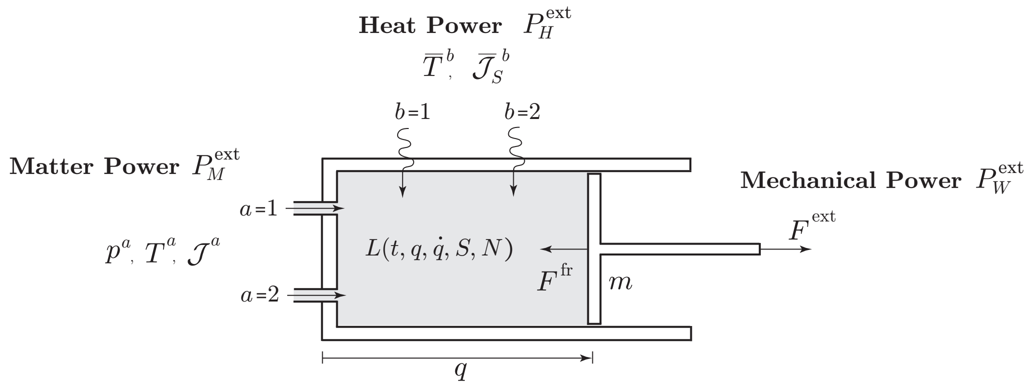
$$x' = v, \qquad t' = 1, \qquad p' - \frac{\partial \mathcal{L}}{\partial x} = \sum_{r=1}^{m} \lambda_r A^r(t, x, v), \qquad p = \frac{\partial L}{\partial v}, \qquad \mathsf{p}' = \frac{\partial \mathcal{L}}{\partial t} + \sum_{r=1}^{m} \lambda_r B^r(t, x, v),$$

together with

$$\sum_{i=1}^{n} A_i^r(t, x, v) x'^i + B^r(t, x, v) t' = 0.$$

Application to open thermodynamic systems

- Consider an illustrative example of open thermodynamic systems with a time-dependent Lagrangian $L(t, q, \dot{q}, S, N)$, namely, a forced piston with two ports through which matter flow into or out of the system and with two heat sources. So we have all the three kinds of external power flows from exterior into the system.



- Let $q \in Q$ be the mechanical coordinates and the thermodynamic configuration space is

$$\mathcal{Q} = Q \times \mathbb{R}^5 \ni x = (q, S, N, \Gamma, W, \Sigma),$$

where $(S, N, \Gamma, W, \Sigma) \in \mathbb{R}^5$ the thermodynamic configurations and where Γ, W are called thermodynamic displacements. Hence the extended configuration space is given by

$$\mathcal{Y} = \mathbb{R} \times \mathcal{Q} \ni (t, x)$$

- Assuming that the system has $2\,(= A)$ ports through which species can flow into or out of the system (matter exchange) and $2\,(= B)$ heat sources (heat exchange), define a Lagrangian $\mathcal{L} : J^1\mathcal{Y} \to \mathbb{R}$ by

$$\mathcal{L}(t, x, \dot{x}) = L(t, q, \dot{q}, S, N) + \underbrace{\dot{W}N\,(= \mu N)}_{\text{Giggs free energy}} + \underbrace{\dot{\Gamma}(S - \Sigma),}_{\text{entropy production}}$$

which can be regarded as a time-dependent augmented Lagrangian.

- By using the general definition of the variational constraint, we have

$$C_V = \Big\{(t,x,v,\delta t,\delta x) \in J^1\mathcal{Y} \times_{\mathcal{Y}} T\mathcal{Y} \;\Big|\; \frac{\partial L}{\partial S}\delta\Sigma = \left\langle F^{\rm fr}, \delta q\right\rangle + \sum_{a=1}^{A}\left[\mathcal{J}^a(\delta W - \mu^a\delta t) + \mathcal{J}_S^a(\delta\Gamma - T^a\delta t)\right] + \sum_{b=1}^{B}\bar{\mathcal{J}}_S^b(\delta\Gamma - \bar{T}^b\delta t)\Big\}.$$

- In the general context of time-dependent nonlinear nonholonomic constraints of thermodynamic type, the parts $A_i^r(t,x,\dot{x})\delta x^i$ and $B_i^r(t,x,\dot{x})\delta t$ in the constraints

$$A_i^r(t,x,\dot{x})\delta x^i + B_i^r(t,x,\dot{x})\delta t = 0$$

are such that

$$A_i^r(t,x,\dot{x})\delta x^i = -\frac{\partial L}{\partial S}\delta\Sigma + \left\langle F^{\rm fr}, \delta q\right\rangle + \sum_{a=1}^{A}\Big(\mathcal{J}^a\delta W + \mathcal{J}_S^a\delta\Gamma\Big) + \sum_{b=1}^{B}\bar{\mathcal{J}}_S^b\delta\Gamma,$$

$$B_i^r(t,x,\dot{x})\delta t = -\sum_{a=1}^{A}\Big(\mathcal{J}^a\mu^a + \mathcal{J}_S^a T^a\Big)\delta t - \sum_{b=1}^{B}\bar{\mathcal{J}}_S^b\bar{T}^b\delta t.$$

- Recall $\mathcal{P} = J^1\mathcal{Y} \times_{\mathcal{Y}} T^*\mathcal{Y}$ be the covariant Pontryagin bundle over $\mathcal{Y} = \mathbb{R} \times \mathcal{Q}$, with coordinates x $= (t,x,v,\mathsf{p},p) \in \mathcal{P}$. The distribution on $\mathcal{P}$ is induced by

$$\Delta_{\mathcal{P}}(t,x,v,\mathsf{p},p) := \left(T_{(t,x,v,\mathsf{p},p)}\pi_{(\mathcal{P},\mathcal{Y})}\right)^{-1}(C_V(t,x,v)) \subset T_{(t,x,v,\mathsf{p},p)}\mathcal{P}.$$

- From the canonical forms on $T^*\mathcal{Y}$, the presymplectic form $\omega_{\mathcal{P}} = \pi^*_{(\mathcal{P},T^*\mathcal{Y})}\Omega_{T^*\mathcal{Y}} = dx \wedge dp + dt \wedge d\mathsf{p}$ is

$$\omega_{\mathcal{P}} = dq \wedge dp_q + dS \wedge dp_S + dN \wedge dp_N + d\Gamma \wedge dp_\Gamma + dW \wedge dp_W + d\Sigma \wedge dp_\Sigma + dt \wedge d\mathsf{p}.$$

- From the distribution $\Delta_{\mathcal{P}}$ and the presymplectic form $\omega_{\mathcal{P}}$, define the induced Dirac structure on $\mathcal{P}$ as

$$D_{\Delta_{\mathcal{P}}} \subset T\mathcal{P} \oplus T^*\mathcal{P}$$

- The time-dependent Dirac dynamical system is given by

$$\big(\dot{\mathrm{x}}(t), \mathbf{d}\mathcal{E}(\mathrm{x}(t))\big) \in D_{\Delta_{\mathcal{P}}}(\mathrm{x}(t)),$$

  and it follows the Lagrange-d'Alembert-Pontryagin evolution equations:

$$\mathbf{i}_{\dot{\mathrm{x}}}\Omega_{\mathcal{P}} - \mathbf{d}\mathcal{E}(\mathrm{x}) \in \Delta_{\mathcal{P}}(\mathrm{x})^{\circ}, \ \ \dot{\mathrm{x}} \in \Delta_{\mathcal{P}}(\mathrm{x}).$$

- Thus the evolution equations of Dirac dynamical system include all the thermodynamic relations:

$$\begin{cases} p_q = \dfrac{\partial L}{\partial \dot{q}}, \qquad \dot{p}_q = \dfrac{\partial L}{\partial q} + F^{\mathrm{fr}} + F^{\mathrm{ext}}, & \text{Lagrange-d'Alembert-Pontryagin equations} \\[2ex] p_W = N, \qquad \dot{p}_W = \displaystyle\sum_{a=1}^{A} \mathcal{J}^a, & \textsf{Mass continuity equation} \\[2ex] p_\Gamma = S - \Sigma, \qquad \dot{p}_\Gamma = \displaystyle\sum_{a=1}^{A} \mathcal{J}_S^a + \sum_{b=1}^{B} \bar{\mathcal{J}}_S^b, & \textsf{Entropy balance equation} \\[2ex] \dot{\Gamma} = -\dfrac{\partial L}{\partial S}, \quad \dot{W} = -\dfrac{\partial L}{\partial N}, & \text{Temperature and chemical potential} \\[2ex] \dot{\Sigma} = \dfrac{1}{\frac{\partial L}{\partial S}} \left[\left\langle F^{\mathrm{fr}}, \dot{q} \right\rangle + \displaystyle\sum_{a=1}^{A} \left[\mathcal{J}^a (\dot{W} - \mu^a) + \mathcal{J}_S^a (\dot{\Gamma} - T^a) \right] + \sum_{b=1}^{B} \bar{\mathcal{J}}_S^b (\dot{\Gamma} - \bar{T}^b) \right], & \\ & \textsf{Internal entropy production (2nd law)} \\[2ex] \dot{\mathsf{p}} = \dfrac{\partial L}{\partial t} - \displaystyle\sum_{a=1}^{A} (\mathcal{J}^a \mu^a + \mathcal{J}_S^a T^a) - \sum_{b=1}^{B} \bar{\mathcal{J}}_S^b \bar{T}^b, & \textsf{Energy balance (1st law)} \end{cases}$$

(1) Mass continuity equation: The conjugate momentum $p_W = N$ associated to W is interpreted as the number of moles in the system, whose rate of change is indeed given by

$$\dot{p}_W = \sum_{a=1}^{A} \mathcal{J}^a.$$

(2) Entropy balance equation: Regarding the 3rd equation, the conjugate momentum

$$p_\Gamma = S - \Sigma$$

associated to Γ corresponds to the entropy of the system due to the exchange of entropy with exterior and its time derivative is equal to the sums of the external entropy flow rates through ports A and B:

$$\dot{p}_\Gamma = \dot{S} - \dot{\Sigma} = \sum_{a=1}^{A} \mathcal{J}_S^a + \sum_{b=1}^{B} \bar{\mathcal{J}}_S^b.$$

- From the 3rd and 5th equations, the rate of the total entropy change of the system can be rewritten as

$$\dot{S} = \dot{\Sigma} + \dot{p}_\Gamma = I + \sum_{a=1}^{A} \mathcal{J}_S^a + \sum_{b=1}^{B} \bar{\mathcal{J}}_S^b \quad \Longleftrightarrow \quad dS = d_i S + d_e S,$$

where the internal entropy production $\dot{\Sigma} = I$ is always positive by the second law of thermodynamics and

$$d_i S = \dot{\Sigma} dt \quad \text{and} \quad d_e S = \dot{p}_\Gamma dt.$$

- Note that the famous expression "$dS = d_i S + d_e S$" can be mathematically understood.

(3) Energy balance equation: The momentum p, which corresponds to the covariant Hamiltonian, represents minus the interaction power from the exterior through its ports, whose time rate is given by

$$\dot{\mathsf{p}} = \frac{\partial L}{\partial t} - \underbrace{\sum_{a=1}^{A} (\mathcal{J}^a \mu^a + \mathcal{J}_S^a T^a)}_{=P_M^{\mathrm{ext}}} - \underbrace{\sum_{b=1}^{B} \bar{\mathcal{J}}_S^b \, \bar{T}^b}_{=P_H^{\mathrm{ext}}} .$$

- Then, the rate of the covariant generalized energy is

$$\frac{d}{dt}\mathcal{E} = \frac{d}{dt}E_L + \frac{d}{dt}\mathsf{p} = \left\langle F^{\mathrm{ext}}, \dot{q} \right\rangle .$$

and hence the rate of the total energy induces the energy balance equation (1st law) is given by

$$\begin{aligned} \frac{d}{dt}E_L &= \left\langle F^{\mathrm{ext}}, \dot{q} \right\rangle - \dot{\mathsf{p}} \\ &= -\frac{\partial L}{\partial t} + \underbrace{\left\langle F^{\mathrm{ext}}, \dot{q} \right\rangle}_{=P_W^{\mathrm{ext}}} + \underbrace{\sum_{a} (\mathcal{J}^a \mu^a + \mathcal{J}_S^a T^a)}_{=P_M^{\mathrm{ext}}} + \underbrace{\sum_{b} \bar{\mathcal{J}}_S^b \bar{T}^b}_{=P_H^{\mathrm{ext}}} . \end{aligned}$$

- For the case in which the given Lagrangian L does not depend on time t explicitly, the usual expression of the first law for open systems is recovered as:

$$\frac{d}{dt}E_L = P_W^{\mathrm{ext}} + P_H^{\mathrm{ext}} + P_M^{\mathrm{ext}} .$$

Conclusions

- We have shown a general framework of the Dirac formulation for open thermodynamical systems, where a nonlinear constraint of the thermodynamic type associated to the entropy production in all the irreversible processes can be incorporated into the context of Dirac structures and the associated Dirac dynamical systems.

- In order to formulate the open systems in the context of time-dependent nonholonomic systems, we have used the specific feature between C_V and C_K, called the nonlinear constraints of thermodynamic type, in which we have also used the thermodynamic displacements to get the natural correspondences

$$A_i^r(t,x,\dot{x})\dot{x}^i + B_i^r(t,x,\dot{x})\dot{t} = 0 \quad \leftrightsquigarrow \quad A_i^r(t,x,\dot{x})\delta x^i + B_i^r(t,x,\dot{x})\delta t = 0$$

between C_K and C_V.

- In particular, using a framework of classical field theories, we have proposed a time-dependent Dirac dynamical systems on the covariant Pontryagin bundles $\mathcal{P} = J^1\mathcal{Y} \oplus J^1\mathcal{Y}^\star$,

$$\big(\dot{\mathrm{x}}(t), \mathbf{d}\mathcal{E}(\mathrm{x}(t))\big) \in D_{\Delta_{\mathcal{P}}}(\mathrm{x}(t)),$$

together with the generalized Lagrange-d'Alembert-Pontryagin principle.

- We have illustrated our theory of Dirac formulation for open systems by an illustrative example of a forced piston–cylinder system with friction, which includes matter and heat transfer.

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Thank you for your attention !