Port-Hamiltonian formulations of open quantum systems

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Introduction

Introduction

A port-Hamiltonian perspective on open quantum systems

- ERC Q_feedback project : one main subject is contribution of Control Theory to Quantum systems' stabilization and control
- Thanks to Pierre Rouchon for his persistent invitation to events on Quantum Systems and Control : 2018 Trimester at the Insitut Henri Poincaré, the school at CIRM, etc ... and to Nina Amini, John Gough, Arjan van der Schaft for the numerous discussions and invitations ..
- This talk pressents very recent results on port-Hamiltonian formulation of dissipative quantum systems
  based on Ph.D. of Jonas Kirchhoff (Dec. 2025) on the geometric structure of irreversible port-Hamiltonian systems .

Motivation

The parallel circuit realization of a dissipative LC circuit

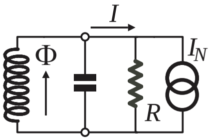

Figure – Dissipative LC circuit (Vool and Devoret, Les Houches Notes)

- linear capacitor, linear/nonlinear inductor,
- linear resistor (Ohm's law)
- noise (current) source: ignored in the sequel.

Dissipative quantum systems and ports ?

Open quantum systems interconnected with thermal bath

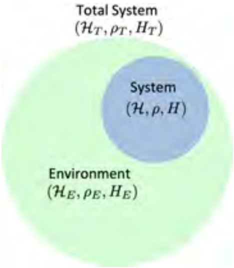

Figure – (Manzano, 2020)

Aim : suggest a Irreversible port-Hamiltonian formulation of the single jump Lindblad equation.

Structure of the talk

1. Introduction to Irreversible port-Hamiltonian systems on an LC-circuit coupled to a resistor as extending the Hamiltonian model of the circuit with an entropy balance equation
2. Formal definition of irreversible port-Hamiltonian systems on the base of a 4-tensor
3. Irreversible port-Hamiltonian representation of the single jump Lindblad equation

Irreversible port-Hamiltonian systems for dissipative classical systems

Irreversible port-Hamiltonian Systems for dissipative classical systems

Canonical example : the dissipative LC-circuit

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The dissipative LC-circuit

Consider the an LC cell connected to a resistor

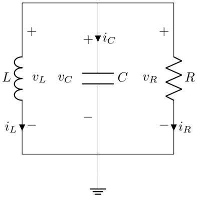

Figure – Dissipative LC circuit

The dissipative LC-circuit : topological relations

Let us first write Gustav Kirchhoff's relations

$$\begin{pmatrix} i_C \\ v_L \\ v_R \end{pmatrix} = \begin{pmatrix} 0 & -1 & -1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} v_C \\ i_L \\ i_R \end{pmatrix}$$

where

- the first line corresponds to the co-cycle (node rule) formed by the branches C, L and R
- the second and third lines correspond to the cycles (L, C) and (R, C) (loop rule)

associated with the capacitor's spanning tree.

Skew-symmetry of Kirchhoff's relations !

Implicit dissipative Hamiltonian system

The Hamiltonian formulation is obtained by defining

- state variables: the charge of the capacitor $Q(t)$ and the total magnetic flux of the inductor $\varphi(t)$
- circuit variables: $i_C = \frac{dQ}{dt}$, $v_L = \frac{d\varphi}{dt}$, $v_C = \frac{\partial H}{\partial Q}$, $i_L = \frac{\partial H}{\partial \varphi}$,
- the electro-magnetic energy:
$H(Q,\varphi) = \frac{1}{2C}(Q - Q_{\text{offset}})^2 + \frac{\varphi_0^2}{L_J}\left(1 - \cos\left(\frac{(\varphi - \varphi_{\text{offset}})}{\varphi_0}\right)\right)$
- and the dissipative Ohm relation $v_R = R\, i_R$, $R > 0$.

$$\begin{pmatrix} \frac{dQ}{dt} \\ \frac{d\varphi}{dt} \\ v_R \end{pmatrix} = \begin{pmatrix} 0 & -1 & -1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial H}{\partial Q} \\ \frac{\partial H}{\partial \varphi} \\ i_R \end{pmatrix}$$

which is an implicit dissipative Hamiltonian system defined on a Dirac structure (graph of the Poisson tensor).

Side remark on LC circuit dynamics

The dynamics of the LC-circuit is a Hamiltonian system:

- generated by the Hamiltonian: $H_0(Q, \phi)$, the total electromagnetic energy
- with respect to the Kirchhoff Dirac structure

$$\left(\begin{pmatrix} \frac{dQ_C}{dt} \\ \frac{\partial H_{mg}}{\partial \phi_L} \end{pmatrix}, \begin{pmatrix} \frac{\partial H_{el}}{\partial Q_C} \\ \frac{d\phi_L}{dt} \end{pmatrix} \right) \in B_K(\mathscr{G}) = \ker \partial \times \operatorname{im} d \subset \Lambda_1 \times \Lambda^1 \tag{1}$$

where $\partial$is the boundary operator and d is the co-boundary operator of the network graph $\mathscr{G}$
and writing G. Kirchhoff's laws $\partial I = 0$ and $V \in \operatorname{im} d$.

A systems' and control perspective : open systems

The systems' and control perspective, the port-Hamiltonian formulation, introduces two conjuguated port-variables $(f, e) \in P \times P^*$

$$\begin{pmatrix} \frac{dQ}{dt} \\ \frac{d\varphi}{dt} \\ f \end{pmatrix} = \begin{pmatrix} 0 & -1 & -1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial H}{\partial Q} \\ \frac{\partial H}{\partial \varphi} \\ e \end{pmatrix}$$

Ports allow the interaction with the environment of open systems , for instance for the dissipative Ohm relation

$$e = \frac{1}{R} f$$

or more complex systems.

Port Hamiltonian systems are closed with respect to interconnection through Dirac structures !

Explicit dissipative Hamiltonian system

Decompose the topological (skew-symmetric) structure matrix

$$\begin{pmatrix} 0 & -1 & -1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} J & g \\ -g^\top & 0 \end{pmatrix}$$

into symplectic matrix $J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ and port-map $g = \begin{pmatrix} -1 \\ 0 \end{pmatrix}$ to the resistor

Eliminate the pair of variables associated with the inductor (i_R, v_R), and obtain the explicit dissipative Hamiltonian system

$$\frac{d}{dt}\begin{pmatrix} Q \\ \varphi \end{pmatrix} = \left[J - g^\top \frac{1}{R} g \right] \begin{pmatrix} \frac{\partial H}{\partial Q} \\ \frac{\partial H}{\partial \varphi} \end{pmatrix} = \begin{pmatrix} -\frac{1}{R} & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial H}{\partial Q} \\ \frac{\partial H}{\partial \varphi} \end{pmatrix}$$

where $\left[J - g^\top \frac{1}{R} g \right]$ is neither symmetric nor skew-symmetric and defines a Leibniz bracket.

The dissipative LC-circuit connected to a thermostat (1)

The dissipative system may be rendered conservative by considering an thermal reservoir (e.g.a thermostat at temperature $T_0 > 0$) and complete the dissipative system

$$\frac{d}{dt}\begin{pmatrix} Q \\ \varphi \end{pmatrix} = \left[J - g^\top \frac{1}{R} g\right]\begin{pmatrix} \frac{\partial H}{\partial Q} \\ \frac{\partial H}{\partial \varphi} \end{pmatrix} = \begin{pmatrix} -\frac{1}{R} & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \frac{\partial H}{\partial Q} \\ \frac{\partial H}{\partial \varphi} \end{pmatrix}$$

with the entropy balance equation

$$\frac{dS}{dt} = \frac{1}{T_0}\frac{v_R^2}{R} \doteq f_S$$

where $f_S \geq 0$ is the *entropy creation* due to the Ohmic dissipation relation.

The dissipative LC-circuit connected to a thermostat (2)

Considering the total energy

$$H_{\text{tot}}(Q,\varphi,S) = H(Q,\varphi) + U(S)$$

being the sum of the electromagnetic energy and the internal energy of the thermostat $U(S) = T_0 S$
and using Kirchhoff's relation $v_R = v_C$, the extended system becomes a quasi-Hamiltonian system,

$$\frac{d}{dt}\begin{pmatrix} Q \\ \varphi \\ S \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & -1 & -\frac{1}{R}\frac{v_C}{T_0} \\ 1 & 0 & 0 \\ \frac{1}{R}\frac{v_C}{T_0} & 0 & 0 \end{pmatrix}}_{=J_{\text{tot}}} \begin{pmatrix} v_C \\ i_L \\ T_0 \end{pmatrix} = \begin{pmatrix} -i_L - \frac{v_C}{R} \\ v_C \\ f_S \end{pmatrix}$$

however the structure matrix depends on the co-state $v_C = \frac{\partial H}{\partial Q}$!!

The dissipative LC-circuit connected to a thermostat (3)

Decompose the system into a reversible and irreversible part

$$\frac{d}{dt}\begin{pmatrix} Q \\ \varphi \\ S \end{pmatrix} = \left[\underbrace{\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{=J_{\mathrm{rev}}} + \frac{1}{R\,T_0} v_C \underbrace{\begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}}_{=J_{\mathrm{irr}}} \right] \left(\begin{pmatrix} \frac{\partial H_{\mathrm{tot}}}{\partial Q} \\ \frac{\partial H_{\mathrm{tot}}}{\partial \varphi} \\ \frac{\partial H_{\mathrm{tot}}}{\partial S} \end{pmatrix} \right)$$

- with respect to the two Poisson brackets defined by the decomposed Kirchhoff's relations J_{rev} and J_{irr}

where

- the dissipative part is characterized by
  - its driving force $v_C = \{S, H_{\mathrm{tot}}\}_{J_{\mathrm{irr}}}$ and
  - its constitutive relation $\frac{1}{R\,T_0} > 0$.

Irreversible Hamiltonian systems

Irreversible Hamiltonian systems: reminder

Irreversible port-Hamiltonian system

$$\dot{x} = \gamma\left(x, \frac{\partial U}{\partial x}\right) \underbrace{\frac{\partial S}{\partial x}(x)^T J \frac{\partial H}{\partial x}(x)}_{=\{S,H\}_J} J \frac{\partial H}{\partial x}(x)$$

with

1. the state vector $x \in \mathbb{R}^n$, the Hamiltonian function $H(x) : \mathscr{C}^\infty(\mathbb{R}^n) \to \mathbb{R}$ and the entropy function $S(x) : \mathscr{C}^\infty(\mathbb{R}^n) \to \mathbb{R}$.
2. the constant skew-symmetric structure matrix $J \in \mathbb{R}^n \times \mathbb{R}^n$, defining the Poisson bracket $\{S, H\}_J = \frac{\partial S}{\partial x}(x)^T J \frac{\partial H}{\partial x}(x)$
3. a positive definite function: $\gamma(x, \frac{\partial H}{\partial x}) = \hat{\gamma}(x) > 0$.

Irreversible Port Hamiltonian arize naturally for heat exchangers, Chemical reactors, etc..:

- the bracket $\{S, H\}_J$ is the thermodynamic force
- the function $\gamma\left(x, \frac{\partial H}{\partial x}\right)$ the constitutive relation

Energy and entropy balance equations

The conservation equation of the internal energy,

$$\frac{dH}{dt} = \gamma\left(x, \frac{\partial H}{\partial x}\right)\{S, H\}_J \{H, H\}_J = 0, \tag{2}$$

follows from the skew-symmetry of the structure matrix J.

The entropy balance equation with the irreversible entropy production

$$\frac{dS}{dt} = \gamma\left(x, \frac{\partial H}{\partial x}\right)\{S, H\}_J^2 \geq 0$$

Geometric structure of Irreversible Hamiltonian systems

Geometric structure of irreversible Hamiltonian systems: reminder

3-function associated with irreversible Hamiltonian system

The evolution of any observable $f \in \mathscr{C}^\infty(\mathbb{R}^n)$

$$\frac{\mathrm{d}}{\mathrm{d}t} f \circ x = \gamma(x, \mathrm{d}H(x)) \{S, H\}_J(x) \{f, H\}_J(x).$$

leads to consider the 3-argument function

$$E : \mathscr{C}^\infty(\mathbb{R}^n)^3 \to \mathscr{C}^\infty(\mathbb{R}^n), \qquad E(f, S, H) = \gamma \{S, H\}_J \{f, H\}_J.$$

and symmetrize to a 4-argument function.

Conservative-irreversible function

A IPHS function is a function

$$E : \mathscr{C}^\infty(\mathbb{R}^n)^3 \to \mathscr{C}^\infty(\mathbb{R}^n)$$

so that there is a 4-bracket

$$\varepsilon : \mathscr{C}^\infty(\mathbb{R}^n)^4 \to \mathscr{C}^\infty(\mathbb{R}^n)$$

with the properties

1. $\varepsilon(f,s,g,h)$ is a derivation (i.e. linearity and Leibniz's rule) in each argument,
2. $\forall f,s,h \in \mathscr{C}^\infty(\mathbb{R}^n) : \varepsilon(f,s,h,h) = \varepsilon(s,f,h,h)$: symmetry
3. $\forall s,h \in \mathscr{C}^\infty(\mathbb{R}^n)\ \forall x \in \mathbb{R}^n : \varepsilon(s,s,h,h)(x) \geq 0 = \varepsilon(h,s,h,h)$ positivity,

which induces E as

$$\forall f,s,h \in \mathscr{C}^\infty(\mathbb{R}^n) : E(f,s,h) = \varepsilon(f,s,h,h).$$

Tensor representation of the 4-bracket

A function $\varepsilon : \mathscr{C}^\infty(\mathbb{R}^n)^4 \to \mathscr{C}^\infty(\mathbb{R}^n)$ is a IPHS function if, and only if, ε has a 4-tensor representation $e \in \mathscr{C}^\infty(\mathbb{R}^n, \mathbb{R}^{n\times n\times n\times n})$ with

$$\forall f, s, g, h \in \mathscr{C}^\infty(\mathbb{R}^n) : \varepsilon(f, s, g, h) = \sum_{i,j,k,\ell=1}^{n} e_{i,j,k,\ell} \mathrm{d}_i f \mathrm{d}_j s \mathrm{d}_k g \mathrm{d}_\ell h$$

so that, for all $i, j, k, \ell \in \underline{n}$,

1. $e_{i,j,k,\ell} = e_{i,j,\ell,k}$,
2. $e_{i,j,k,\ell} + e_{k,j,\ell,i} + e_{\ell,j,i,k} = 0$,
3. $\forall h \in \mathscr{C}^\infty(\mathbb{R}^n)\ \forall x \in \mathbb{R}^n : \left[\sum_{k,\ell=1}^{n} e_{i,j,k,\ell}(x) \mathrm{d}_k h(x) \mathrm{d}_\ell h(x)\right]_{i,j=1}^{n}$ symmetric and positive semi-definite.

Reversible-irreversible Hamiltonian systems

Let M be a smooth manifold with

- Poisson bracket $\{\cdot,\cdot\}$ and
- conservative-irreversible function E.

An *irreversible Hamiltonian system* with generating functions $(s,h) \in \mathscr{C}^\infty(M) \times \mathscr{C}^\infty(M)$ is the dynamical system

$$\frac{\mathrm{d}}{\mathrm{d}t} f \circ x = \{f,h\} + E(f,s,h) \qquad \text{for all } f \in \mathscr{C}^\infty(M), \tag{3}$$

with the *noninteraction condition* $\{s,h\} = 0$.

Often one requires the stronger condition:
the entropy function s is a Casimir function of the Poisson bracket, i.e.

$$\{s,g\} = 0 \quad \text{for all } g \in \mathscr{C}^\infty(M)$$

Irreversible port-Hamiltonian systems for disssipative quantum systems

Irreversible port-Hamiltonian Systems for dissipative quantum systems: on the example of the Lindblad model

Paradigmic system : the Linblad model

Paradigmic system: the Lindblad model

State variable : density operator

A density operator on a separable Hilbert space $\mathscr{H}$ is bounded operator $\rho \in \mathscr{B}(\mathscr{H})$ with the properties

- ρ is Hermitian, i.e. $\rho = \rho^\dagger$
- $\rho \geq 0$, i.e. $\langle \psi, \rho \psi \rangle \geq 0$ for all $\psi \in \mathscr{H}$
- $\mathrm{tr}\rho = 1$, where $\rho = \sum_{i=1}^{\infty} \langle \psi_i, \rho \psi_i \rangle$ for any orthonormal basis $(\psi_i)_{i \in \mathbb{N}}$ where tr denotes the trace of ρ.

The set of density operators is denoted by $\mathfrak{D}(\mathfrak{H})$

The Lindblad model

The Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) quantum master equation is the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = -\frac{i}{\hbar}[H,\rho] + \sum_{j=1}^{\ell}\left(L_j\rho L_j^{\dagger} - \frac{1}{2}\{L_j^{\dagger}L_j,\rho\}\right) \tag{4}$$

where

- $\rho \in \mathscr{B}(\mathscr{H})$ is the *density operator*
- $H \in \mathscr{B}(\mathscr{H})$ is the *Hamiltonian operator*
- $L_j \in \mathscr{B}(\mathscr{H})$, $j \in 1,\ldots,\ell$are *jump operators*
  [in the sequel $l = 1$ and L is Hermitian !]

where $[\cdot,\cdot]$ and $\{\cdot,\cdot\}$ denote the commutator and anticommutator of bounded operators, respectively.

Double bracket structure of dissipation

For Hermitian jump operators, the dissipative term in the GKSL equation has the structure of a double commutator.
Let $\mathscr{H}$ be a Hilbert space, and let $\rho, L \in \mathscr{B}(\mathscr{H})$ be Hermitian operators. Then

$$L\rho L - \frac{1}{2}\{LL, \rho\} = -\frac{1}{2}[L,[L,\rho]]$$

Proof:

$$[L,[L,\rho]] = L(L\rho - \rho L) - (L\rho - \rho L)L = -2L\rho L + \{LL, \rho\}$$

Hamiltonian formulation

Hamiltonian formulation

The functional space

Consider a Hermitian operator $H \in \mathscr{B}(\mathscr{H})$ on a a finite-dimensional Hilbert space $\mathscr{H}$, the induced functional F_H is defined as

$$\begin{aligned} F_H : \mathfrak{D}(\mathfrak{H}) &\to \mathbb{R} \\ \rho &\mapsto \mathrm{tr}(H\rho) = \langle H, \rho \rangle_{\mathrm{HS}}. \end{aligned}$$

The variational derivative $\frac{\delta F_H}{\delta \rho}(\rho_0)$ exists for all $\rho_0 \in \mathfrak{D}(\mathfrak{H})$, and is

$$\frac{\delta F_H}{\delta \rho}(\rho_0)v = \langle H, v \rangle_{\mathrm{HS}} = \langle H - \mathrm{tr}H, v \rangle_{\mathrm{HS}}$$

for all Hermitian trace-less operators v.

The Liouville- von Neumann equation

The Liouville-von Neumann equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = -\frac{i}{\hbar}[H,\rho] \tag{5}$$

is (formally) Poisson-Hamiltonian system

$$\frac{\mathrm{d}}{\mathrm{d}t}F\circ\rho = \{F, F_H\}_{\mathrm{LvN}}\circ\rho.$$

with Hamiltonian function $F_H = \langle H, \cdot\rangle_{\mathrm{HS}}$ and Poisson bracket $\{\cdot,\cdot\}_{\mathrm{LvN}}$ defined by

$$\{F,G\}_{\mathrm{LvN}} := \frac{1}{\hbar}\left\langle \cdot, i\left[\frac{\delta F}{\delta\rho}, \frac{\delta G}{\delta\rho}\right]\right\rangle_{\mathrm{HS}} \forall F, G : \mathfrak{D}(\mathfrak{H}) \to \mathbb{R}$$

where $\langle\,,\,\rangle_{\mathrm{HS}}$denotes the Hilbert-Schmidt inner product.

The Lindblad model

The (single jump) Lindblad equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = -\frac{i}{\hbar}[H,\rho] - \frac{1}{2}[L,[L,\rho]] \tag{6}$$

may be represented as an irreversible port-Hamiltonian system

$$\frac{\mathrm{d}}{\mathrm{d}t} F \circ \rho = \{F, F_H\}_{\mathrm{LvN}} + ((F, F_S, L, L))_{\mathrm{port}}$$

with Liouville - von Neuman Poisson bracket $\{\,,\,;\}_{\mathrm{LvN}}$
and the IPHS 4-bracket

$$((F,G,L_1,L_2))_{\mathrm{port}} := \frac{1}{8}\left(\langle i[L_1, \frac{\delta F}{\delta\rho}], i[L_2, \frac{\delta G}{\delta\rho}]\rangle_{\mathrm{HS}} + \langle i[L_2, \frac{\delta F}{\delta\rho}], i[L_1, \frac{\delta G}{\delta\rho}]\rangle_{\mathrm{HS}}\right),$$

generated by the expected value of the energy as Hamiltonian function $F_H := \langle H, \cdot\rangle_{\mathrm{HS}}$,
and (minus) purity of the system as entropy function$F_S(\rho) := -\mathrm{tr}(\rho^2)$.

The IPHS 4-bracket generates the interaction term

Consider ρ an integral curve of $[L,[L,\rho]]$ and the entropy functional which satisfies $\frac{\delta F_S}{\delta\rho} = 2\rho$, one obtains

$$\frac{\mathrm{d}}{\mathrm{d}t} F \circ \rho = \left\langle \frac{\delta F}{\delta \rho}, [L,[L,\rho]] \right\rangle_{HS} = 2 \left\langle \left[L, \frac{\delta F}{\delta \rho} \right], \left[L, \frac{\delta F_S}{\delta \rho} \right] \right\rangle_{\mathrm{HS}}$$
$$= \left(\left(\frac{\delta F}{\delta \rho}, \frac{\delta F_S}{\delta \rho}, L, L \right) \right)_{\mathrm{port}}.$$

The entropy F_S is in the kernel of the LvN-Poisson bracket hence satisfies the non-interaction condition.

Indeed ρ being Hermitian gives $(\rho H \rho) = (\rho^2 H)$ and hence

$$\langle \rho, i[H,\rho] \rangle_{\mathrm{HS}} = (\rho H \rho) - (\rho^2 H) = 0.$$

Balance equations

Linbladian dynamics:

$$\frac{\mathrm{d}}{\mathrm{d}t} F \circ \rho = \{F, F_H\}_{\mathrm{LvN}} + ((F, F_S, L, L))_{\mathrm{port}}$$

Energy balance equation

$$\frac{\mathrm{d}}{\mathrm{d}t} F_H \circ \rho = \{((F_H, F_S, L, L))_{\mathrm{port}} = tr\left([L, H]\,[L, \rho]\right)$$

Entropy balance equation

$$\frac{\mathrm{d}}{\mathrm{d}t} F_S \circ \rho = ((F_S, F_S, L, L))_{\mathrm{port}} = 2tr\left([L, \rho]^2\right) \geq 0$$

Conclusion

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We have shown that the 1-jump Lindblad equations may be written as an Irreversible Hamiltonian system :

- with geometric structure defined by
  - Liouville - von Neuman Poisson bracket $\{,;\}_{\mathrm{LvN}}$ and
  - the Linblad IPHS 4-bracket
- generated by the
  - the Hamiltonian function $F_H := \langle H, \cdot \rangle_{\mathrm{HS}}$,and
  - the entropy function$F_S(\rho) := \mathrm{tr}(\rho^2)$.

Open questions :

- define port variable for driven quantum circuits !
- use the IPHS structure to derive stabilizing controllers

Some references on the metriplectic formulation of the Lindblad equation

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