Dynamics of Open Quantum Systems

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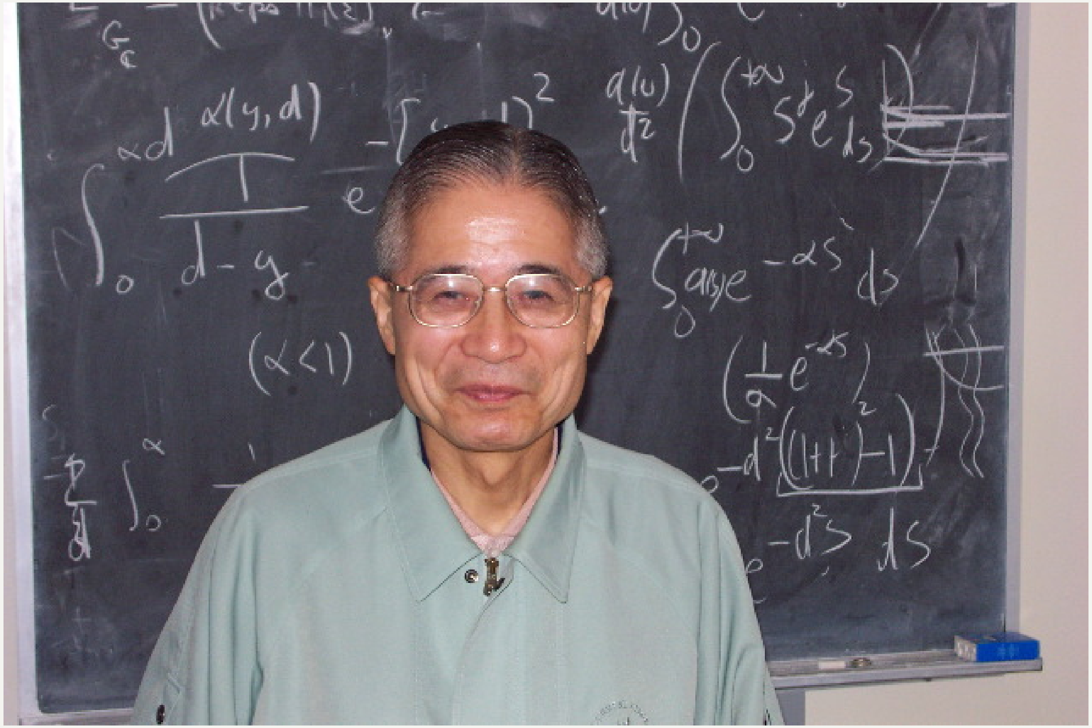
Plan

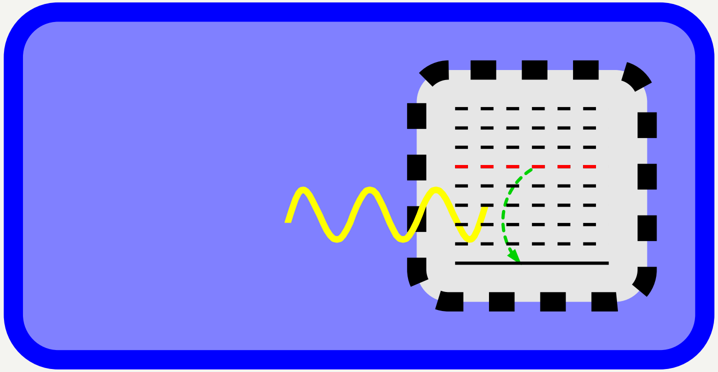
- Introduction: What and why ?
- The two approaches to open systems
- Mathematical framework
- Return to equilibrium
- Non-equilibrium steady states
- Further developments



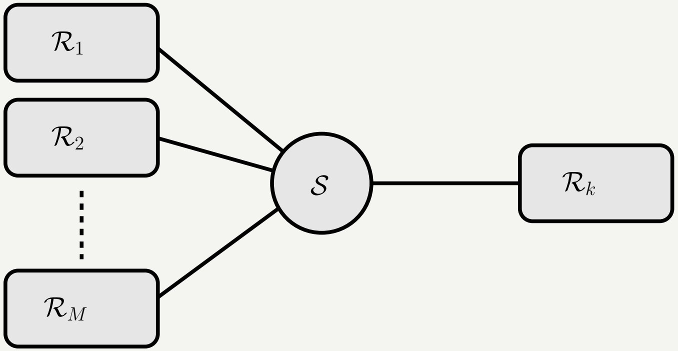
In Memory of Professor Huzihiro Araki 1932-2022

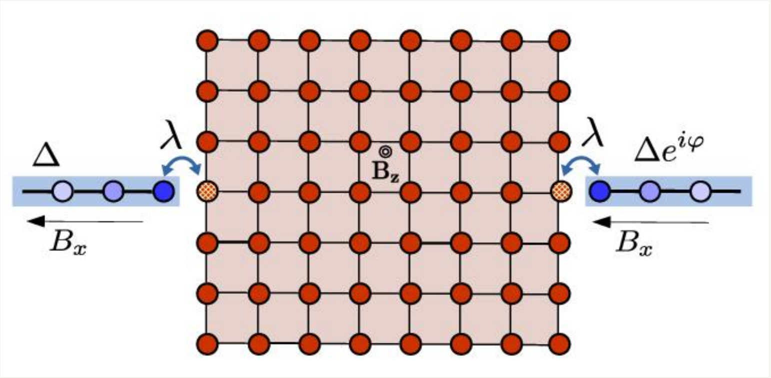
What are Open Systems and why are they useful ?

- Physical systems (think of an atom or molecule) are simplest when isolated from external influences $\Longrightarrow$ closed system.
- In reality, they are rarely isolated, but interact with their environment, and these interactions have important consequences on their properties $\Longrightarrow$ open systems.



- Open systems are paradigmatic models in non-equilibrium statistical mechanics.
- They allow to implement friction/dissipation in a conservative framework.
- They also provide good models of condensed matter devices .





Gavensky, Usaj, Balseiro PRR (2020)

The two approaches to open systems

- In the Markovian (phenomenological) approach

$\longrightarrow$ the small system $\mathcal{S}$ is acted upon by

  – a **quantum noise**,

  – a **dissipative** force (fluctuation–dissipation).

$\longrightarrow$ $\mathcal{S}$ evolves as a quantum Markov process.

$\longrightarrow$ "Integrating" the noise yields a **semigroup** of **completely positive** maps.

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- Long history
  - $\longrightarrow$ Einstein '17: AB-law of atomic radiation.
  - $\longrightarrow$ Pauli '28: Quantum master equation.
  - $\longrightarrow$ van Hove '55: $\lambda^2 t$-limit.
  - $\longrightarrow$ Pullé, Davies '74: Mathematical derivation of master equation from $\lambda^2 t$-limit.
  - $\longrightarrow$ Lebowitz-Spohn '78: Irreversible thermodynamics of weakly coupled systems.
  - $\longrightarrow$ Dereziński-De Roeck '08: Extended weak coupling limit.

- In the Hamiltonian (fundamental) approach, the model consists in:
  - $\longrightarrow$ Small **confined** system $\mathcal{S}$, **few degrees of freedom**,
  - $\longrightarrow$ coupled to $M \geqslant 1$ **large** reservoirs $\mathcal{R}_1, \ldots \mathcal{R}_M$.
  - $\longrightarrow$ **Closed** joint system $\mathcal{S} + \mathcal{R}_1 + \cdots + \mathcal{R}_M$ evolves with **conservative group** $t \mapsto \tau^t$.
  - $\longrightarrow$ **Not** the the subsystem $\mathcal{S}$ (memory, Nakajima–Zwanzig).

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> Reservoirs should be inexhaustible sources/bottomless sinks of energy
> with good ergodic properties !

$\longrightarrow$ Idealization: reservoirs are **infinitely extended** systems at **positive density**.

- Mathematical description of extended quantum systems at positive density was developed in the 60'-80'.

Mathematical Framework

- Basic QM: von Neumann theorem $i[p,x]=1 \Longrightarrow$ Schrödinger $\mathcal{H}=L^2(\mathbb{R})$.
- QFT or QSM: $a(k)a^*(k') \pm a^*(k')a(k) = \delta(k-k')$ have uncountably many inequivalent representations

  → A system of fermions/bosons is described by C^*/W^*-algebra $\mathcal{O}$ encoding these (anti)-commutation relations.

  → **Observables** are elements of $\mathcal{O}$.

  → A QM **state** is a positive normalized linear functional $\omega\colon \mathcal{O} \to \mathbb{C}$.

  → The Heisenberg **dynamics** is a group of $*$-automorphisms $t \mapsto \tau^t = e^{t\delta}$ of $\mathcal{O}$.

  → A **Quantum Dynamical System** (QDS) is a triple $(\mathcal{O}, \tau, \omega)$.

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  - $\longrightarrow$ A **Quantum Dynamical System** (QDS) is a triple $(\mathcal{O},\tau,\omega)$.
- The GNS construction puts $(\mathcal{O},\tau,\omega)$ in a Hilbertian context $(\mathcal{H}_\omega,\pi_\omega,\Omega_\omega,L)$

$$\omega(A)=\langle\Omega_\omega,\pi_\omega(A)\Omega_\omega\rangle,\qquad \pi_\omega(\tau^t(A))=e^{itL}\pi_\omega(A)e^{-itL},\qquad L\Omega_\omega=0.$$

  L is the **Liouvillean**, $\mathcal{N}_\omega$= set of states given by density matrices on $\mathcal{H}_\omega$ the **folium**.
- **β–Thermal** QDS: ω is equilibrium states for τ at inverse temperature β (characterized by the KMS condition).

The Modular structure

- The GNS representation of thermal QDS carries a rich mathematical structure which is the object of modular theory.

- First appeared in the QDS describing ideal Bose and Fermi gases in thermal equilibrium. GNS constructed in '63 by Araki and Woods, and Araki and Wyss.

- In a '67 paper, Haag, Hugenholtz and Winnink realized that this structure was more generally associated to the KMS condition.

- In a '67 unpublished note, Tomita introduced the modular operator and proved the main theorems of what is now known as Modular Theory or **Tomita-Takesaki Theory**. The first published account on it is Takesaki's LNM of '70.

The Modular structure

- Modular Theory is a main tool in the classification of type III factors by Connes in '73 (Fields Medal '82).
- It played an essential role in the major developments of equilibrium quantum statistical mechanics in the 70', 2 volumes monograph by Bratteli and Robinson.
- It plays a fundamenal role in Algebraic QFT.
- It is also central to more recent developments in non-equilibrium statistical mechanics...
- ... and very recent advances on entanglement in quantum field theory: Witten '18, Hollands-Sanders '18.

Return to Equilibrium: Robinson 1973

- $\mathcal{S}$ small system $(\mathcal{O}_{\mathcal{S}}, \tau_{\mathcal{S}}, \omega_{\mathcal{S}})$.
- $\mathcal{R}$ large reservoir in a β-thermal state $(\mathcal{O}_{\mathcal{R}}, \tau_{\mathcal{R}}, \omega_{\mathcal{R}})$.
- Joint but decoupled system $\mathcal{S}+\mathcal{R}$ described by $(\mathcal{O}, \tau, \omega)$ where

$$\mathcal{O} = \mathcal{O}_{\mathcal{S}} \otimes \mathcal{O}_{\mathcal{R}}, \qquad \tau^t = \tau^t_{\mathcal{S}} \otimes \tau^t_{\mathcal{R}} = e^{t(\delta_{\mathcal{S}}+\delta_{\mathcal{R}})}, \qquad \omega = \omega_{\mathcal{S}} \otimes \omega_{\mathcal{R}}.$$

- Coupled system described by locally perturbed QDS $(\mathcal{O}, \tau_V, \omega)$ where

$$\tau^t_V = e^{t(\delta_{\mathcal{S}}+\delta_{\mathcal{R}}+i[V,\,\cdot\,])}, \qquad V \,\tilde{\in}\, \mathcal{O}.$$

- Araki's perturbation theory (and extension by Dereziński-J-P '03)
  - $\longrightarrow$ τ_V has a unique β-thermal state $\omega_V \in \mathcal{N}_\omega$.
  - $\longrightarrow$ $(\mathcal{O}, \tau_V, \omega_V) \rightsquigarrow (\mathcal{H}_\omega, \pi_\omega, \Omega_{\omega_V}, L_V)$ with $\Omega_{\omega_V} \propto e^{-\beta(L+V)/2}\Omega_\omega$, $L_V = L + V - JVJ$

Return to Equilibrium: Robinson 1973

The Problem: Does the QDS $(\mathcal{O}, \tau_V, \omega)$ return to equilibrium

$$\lim_{t \to \infty} \nu \circ \tau_V^t(A) = \omega_V(A),$$

for all $\nu \in \mathcal{N}_\omega$ and all $A \in \mathcal{O}$?

- $\neq$ Approach to equilibrium (0th Law).
- Robinson '73: under strong asymptotic abelianness condition (scattering approach).
- Spohn '77: algebraic condition for Markovian dynamics (weak coupling limit).
- Maassen '84: Return to equilibrium for quantum Langevin equation.

- J-P '96: $\mathcal{S}$ coupled to scalar boson field, based on the following circle of ideas from classical dynamical systems:

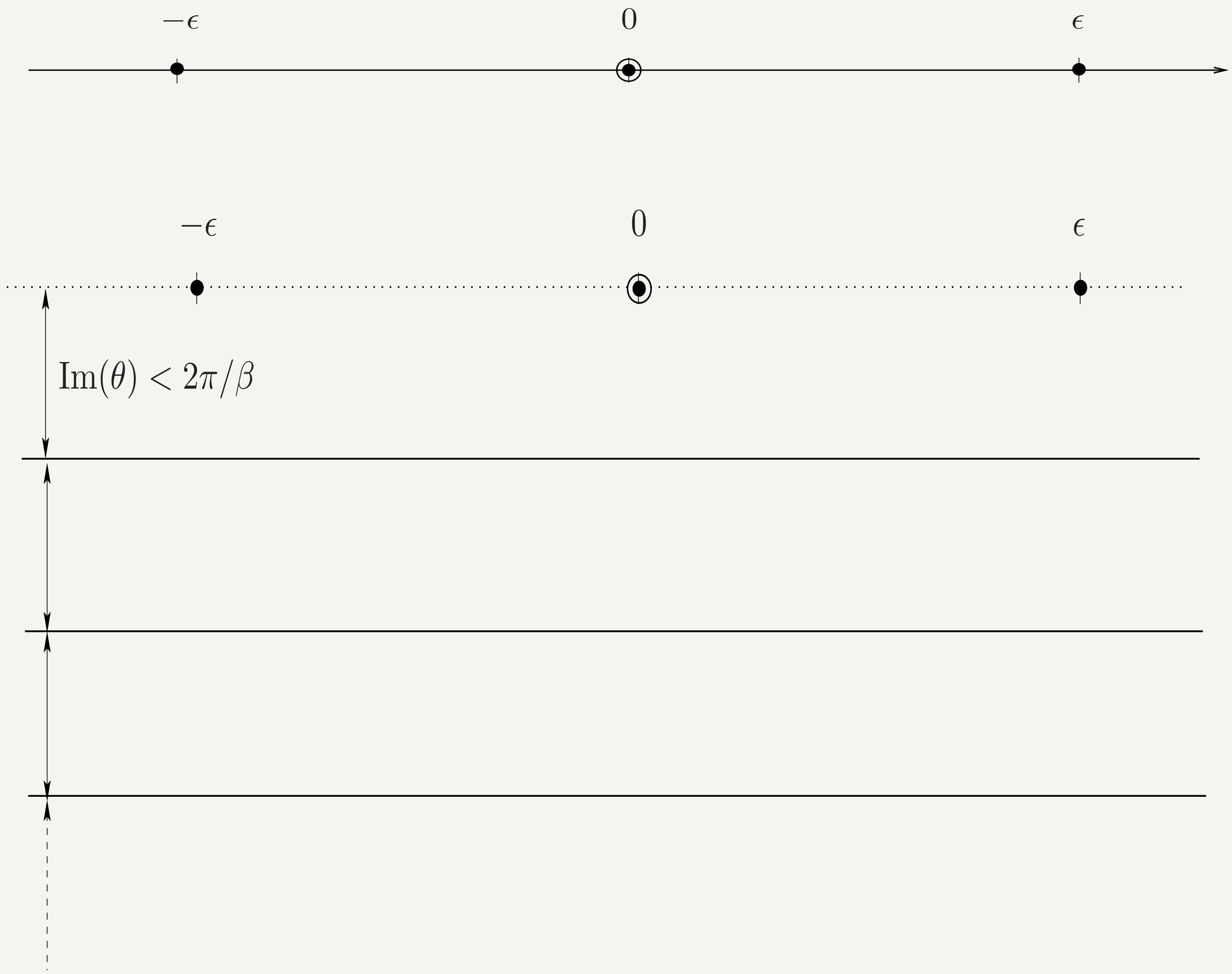
  (a) **Koopmanism.** We proved the following consequence of modular structure:

  Return to equilibrium holds if the locally perturbed Liouvillean L_V has purely a.c. spectrum, except for a simple eigenvalue 0.

  (b) **Spectral deformation.** Introduced in QM by Aguilar-Combes '71 using the dilation group in $\mathbb{R}^d$.

  From a dynamical perspective similar to analysis of Ruelle-Perron-Frobenius transfer operator: essential spectrum depends on the function space on which it acts. Proper choice of this space reveals Ruelle resonances which govern the decay of correlations.

J-P '96: Spectral picture of the Liouvillean for 2-level atom coupled to a β-thermal field



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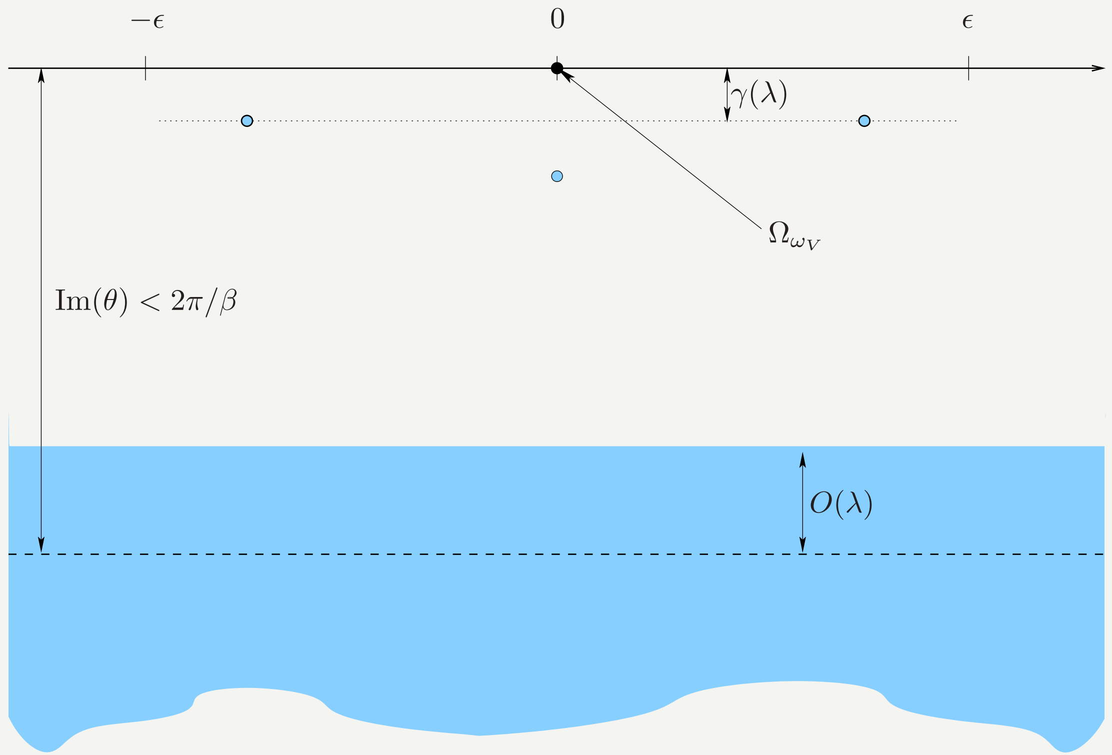


Inverse Laplace transform $\Longrightarrow$ return to equilibrium at exponential rate $\gamma(\lambda) = O(\lambda^2)$ for $0 < \lambda < \ell(\beta)$

- Dümcke-Spohn '79, J-P '97, Dereziński-Früboes '05, Dereziński-J '12: To 2nd order perturbation theory, resonances lead to the Davies generator.

- Bach-Fröhlich-Sigal '99: Related approaches using dilation analyticity and iteration of Feshbach map, λ small uniformly in temperature.

- Fidaleo-Liverani '99: Ergodic properties for a quantum nonlinear dynamics.

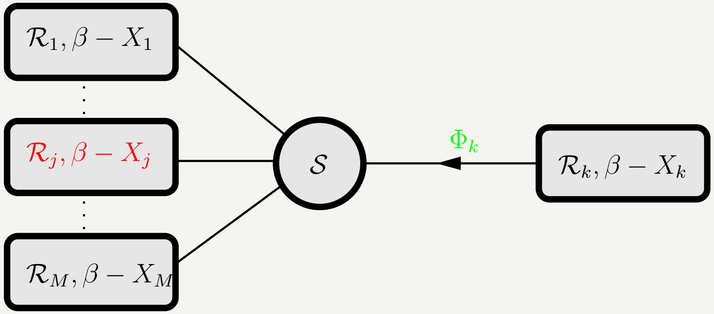
- Merkli '01: Virial theorem approach.

- Dereziński-J '03: Mourre theory approach, λ small uniformly in temperature.

- De Roeck-Kupiainen '11: Powerful result using cluster expansion.

Non-equilibrium Steady States

A physically different picture arises when the environment consists in several parts $\mathcal{R}_1, \ldots, \mathcal{R}_M$ (reservoirs or heat baths) with different intensive thermodynamic parameters.



It is then expected that the joint system relaxes to a Non-Equilibrium Steady State (NESS) ω_+ carrying energy currents Φ_k.

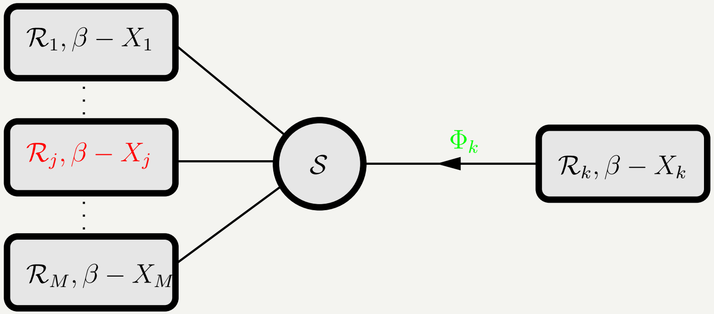
From the mathematical perspective the main difficulty is the fact that, unlike the thermal state, this NESS is unknown! Moreover, one expects that $\omega_+ \notin \mathcal{N}_\omega$.

The 1st Law

- Let $\tau^t_{\mathcal{R}_k} = e^{t\delta_k}$

- Heat flux out the reservoir $\mathcal{R}_k$ (=injected power)

$$\Phi_k = \delta_k(V)$$



- The first Law: for any τ_V-invariant state ν

$$\sum_{k=1}^{M} \nu(\Phi_k) = 0.$$

Ruelle's definition (Rutgers lecture notes 1999-2000)

A NESS is any w*-limit point of

$$\frac{1}{T}\int_0^T \omega \circ \tau_V^t dt$$

as $T \to +\infty$.

The set $\tau_V^+(\omega)$ of NESSs is non-empty, and consists of τ_V-invariant states.

Entropy production and the 2nd Law

- Relative entropy of 2 density matrices $\mathrm{Ent}(\mu|\nu) = \mathrm{tr}(\mu(\log\nu - \log\mu)) \leqslant 0$.
- Generalized by Araki to states $\mu, \nu \in \mathcal{N}_\omega$, using modular theory.
- $\mathrm{Ent}(\mu|\nu) = 0$ iff $\mu = \nu$.
- Entropy balance relation J-P '01 (consequence of Araki's perturbation theory)

$$\mathrm{Ent}(\nu\circ\tau_V^t|\omega) = \mathrm{Ent}(\nu|\omega) - \int_0^t \nu\circ\tau_V^s(\sigma)ds, \qquad \sigma = \sum_{k=1}^M \beta_k\Phi_k.$$

- Assuming $\omega_+ \in \tau_V^+(\nu)$, one has, for a sequence $T_n \to \infty$

$$\omega_+(\sigma) = -\lim_{n\to\infty}\frac{1}{T_n}\mathrm{Ent}(\nu\circ\tau_V^{T_n}|\omega) \geqslant 0.$$

which expresses the 2nd Law (phenomenologic non-equilibrium thermodynamics)

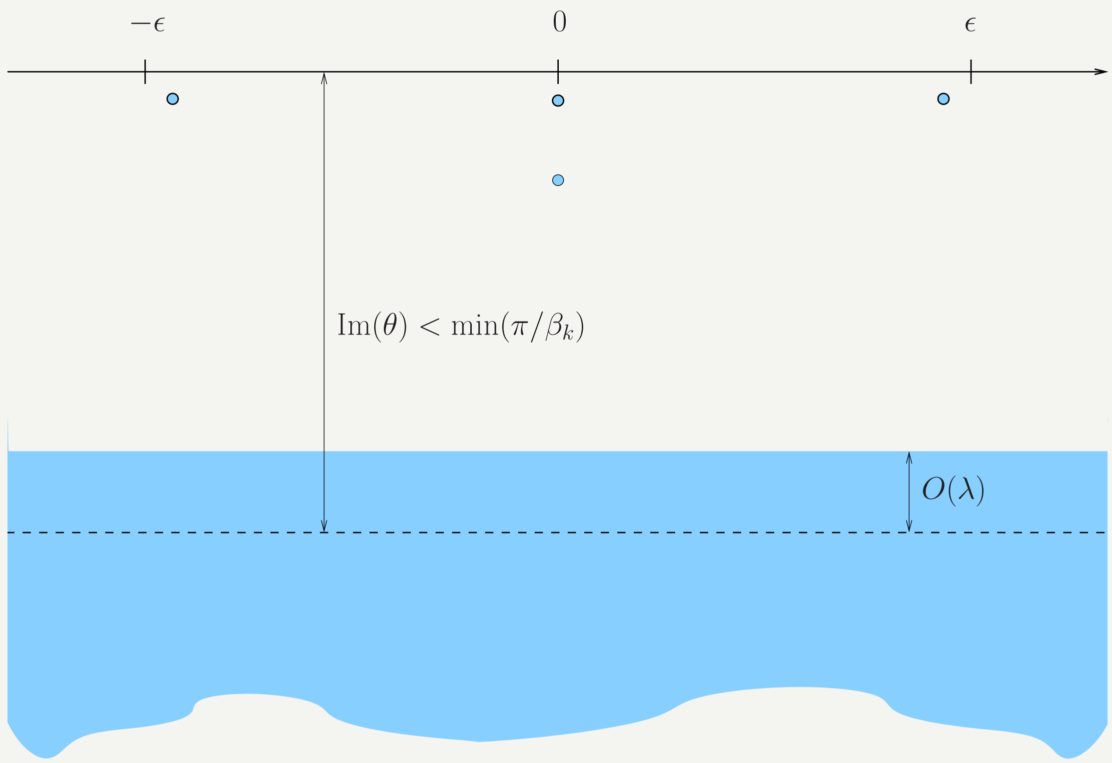
$$\sum_{k=1}^M X_k\,\omega_+(\Phi_k) \geqslant 0, \qquad X_k = \beta - \beta_k.$$

- Related results by Ojima-Hasegawa-Ichiyanagi '88 and Ruelle '01.

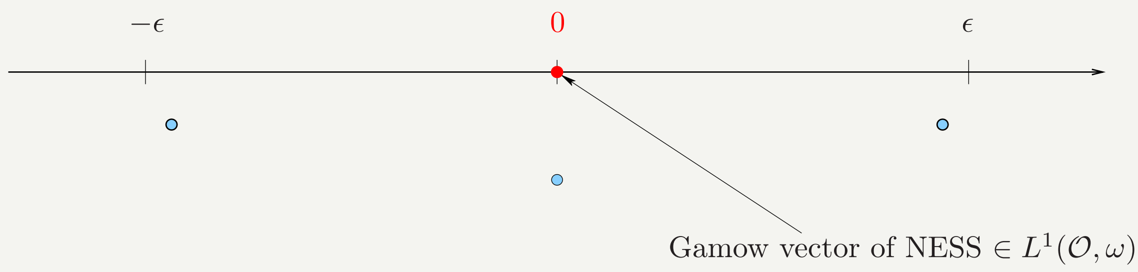
- On physical ground, we expect strict inequality $\omega_+(\sigma) > 0$ to be the signature of non-equilibrium. Structural theory then implies $\omega_+ \notin \mathcal{N}_\omega$.

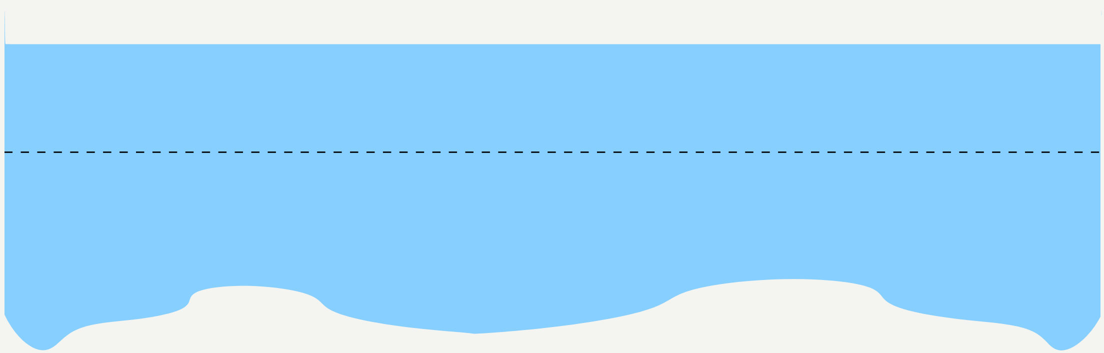
Spectral theory of NESS (J-P '02)

Spectral structure of Liouvillean L_V of the non-equilibrium spin-fermion model

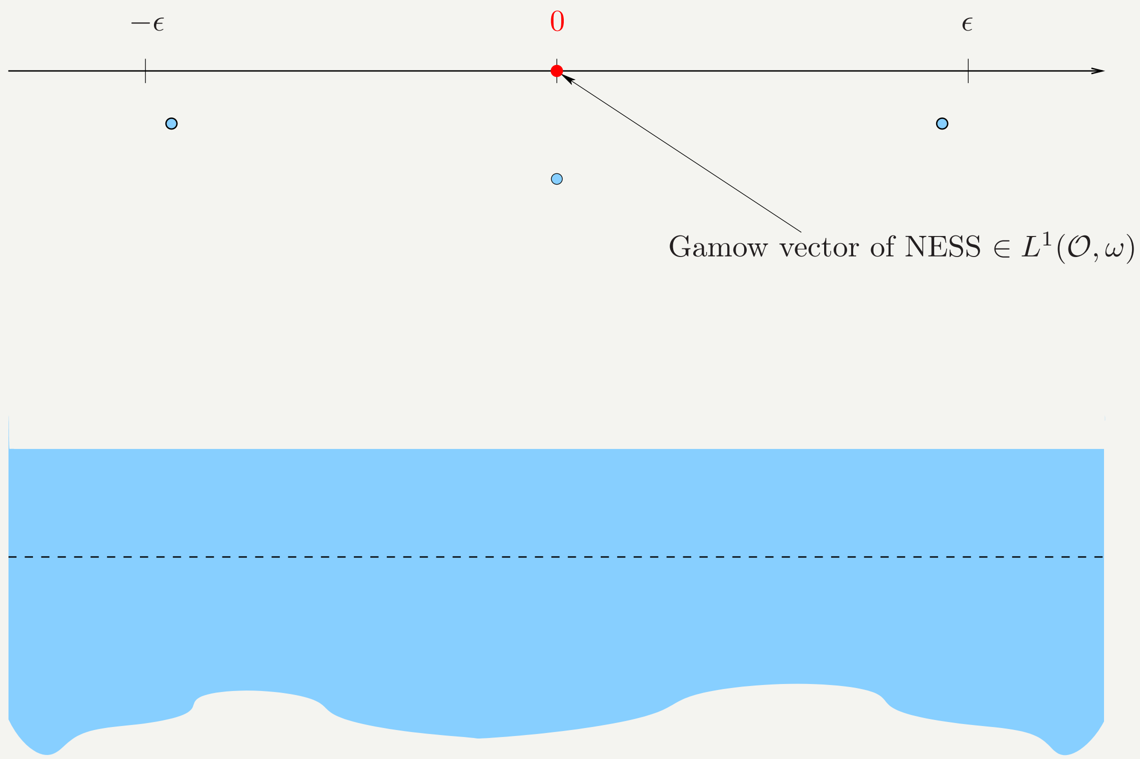


- The Liouvillean L_V acts on the Hilbert space $\mathcal{H}_\omega$.
- Araki-Masuda defined a family of Banach space $L^p(\mathcal{O},\omega)$,$p\in[1,\infty]$, $L^2(\mathcal{O},\omega)=\mathcal{H}_\omega$.
- J-P '02, dynamics is implemented isometrically on $L^p(\mathcal{O},\omega)$ by L^p-Liouvilleans.
- Spectral structure of L^1-Liouvillean of the non-equilibrium spin-fermion model





Spectral structure of L^1-Liouvillean of the non-equilibrium spin-fermion model



- Alternative scattering approach: (Hepp '72, Robinson '73, Botvich-Malyshev '83) Araki-Ho '00, Fröhlich-Merkli-Ueltschi '03, Aschbacher-P '03.
- Merkli-Mück-Sigal '07: bosonic reservoirs.

Some Further Developments

- J-Ogata-P '06-07: Linear response, Green-Kubo formula and Onsager reciprocity relations.
- Aschbacher-J-Pautrat-P '07: Landauer-Büttiker formalism.
- J-P '07: Strict positivity of entropy production
- J-Ogata-P-Seiringer '12: Entropy production and quantum hypothesis testing of the Arrow of Time.
- J-P '14: Quantum Landauer principle.
- Bruneau-J-Last-P '16: Schrödinger conjecture, Landauer-Büttiker and Thouless conductances and entropy production.
- Benoist-Cuneo-J-Pautrat-P '18-21: Entropy production of repeated quantum measurements.
- Benoist-Bruneau-J-Panati-P '24: Entropic fluctuations in quantum statistical mechanics.

Reviews

- J-P '97: Spectral theory of thermal relaxation
- J-P '02: Mathematical theory of non-equilibrium quantum statistical mechanics
- Aschbacher-J-Pautrat-P '06: Topics in non-equilibrium quantum statistical mechanics
- J-Kritchevski-P '06: Mathematical theory of the Wigner-Weisskopf atom
- J-Ogata-Pautrat-P '10: Entropic fluctuations in quantum statistical mechanics. An introduction
- J-P-Westrich '14: Entropic fluctuations of quantum dynamical semigroups