Modular Theory: How and Why Non-equilibrium quantum statistical mechanics perspective

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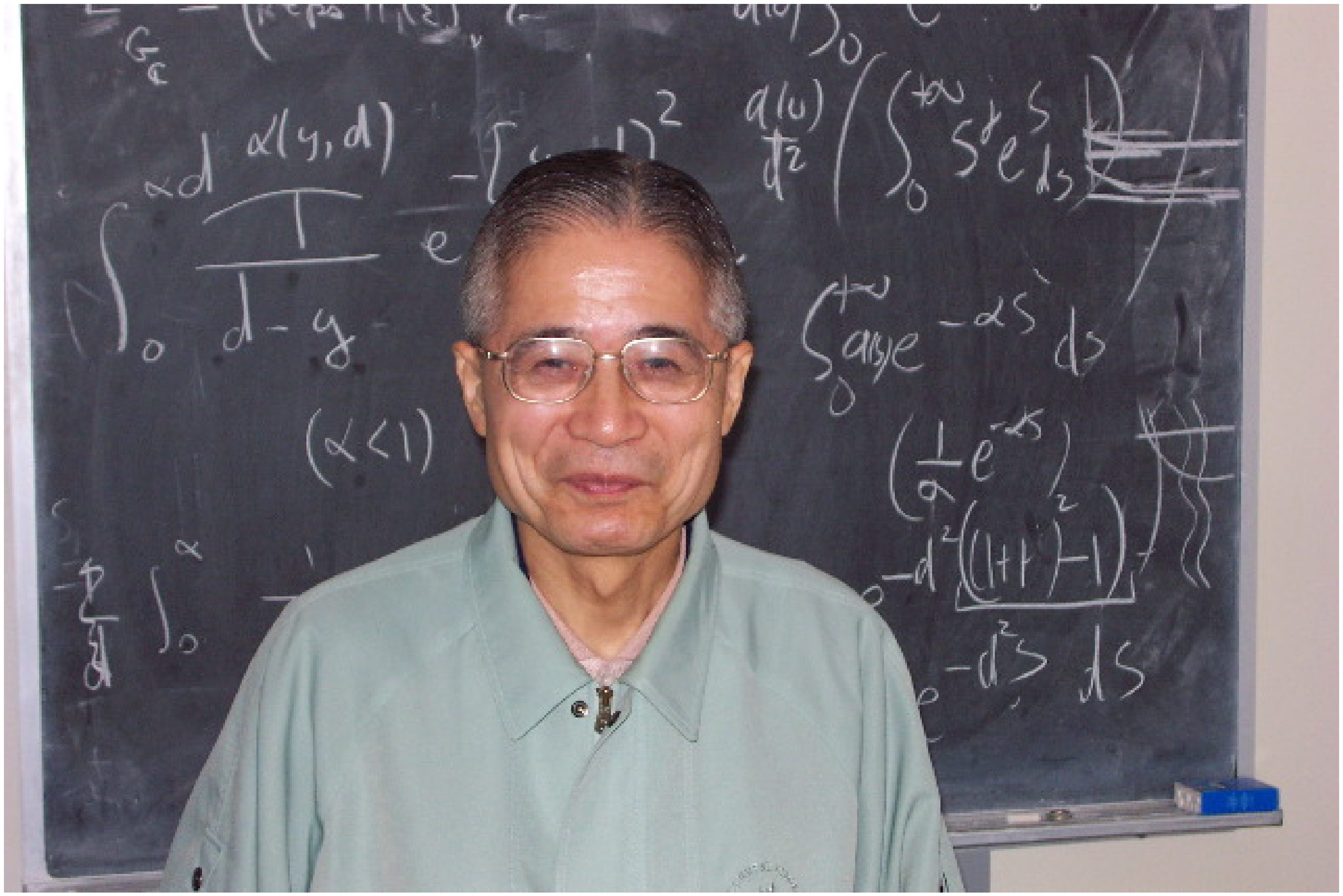
Dedicated to the memory of Huzihiro Araki 1932-2022

- Tomita's talk, 1967

- Haag-Hugenholtz-Winnink: On the equilibrium states in quantum statistical mechanics, CMP 1967.
  Building on Araki-Woods 1963, Araki-Wyss 1964.

- Takesaki book: Tomita's Theory of Modular Hilbert Algebras and Its Applications, 1970

- 70's - 80's Araki, Connes, Haagerup...



Huzihiro Araki 1932-2022

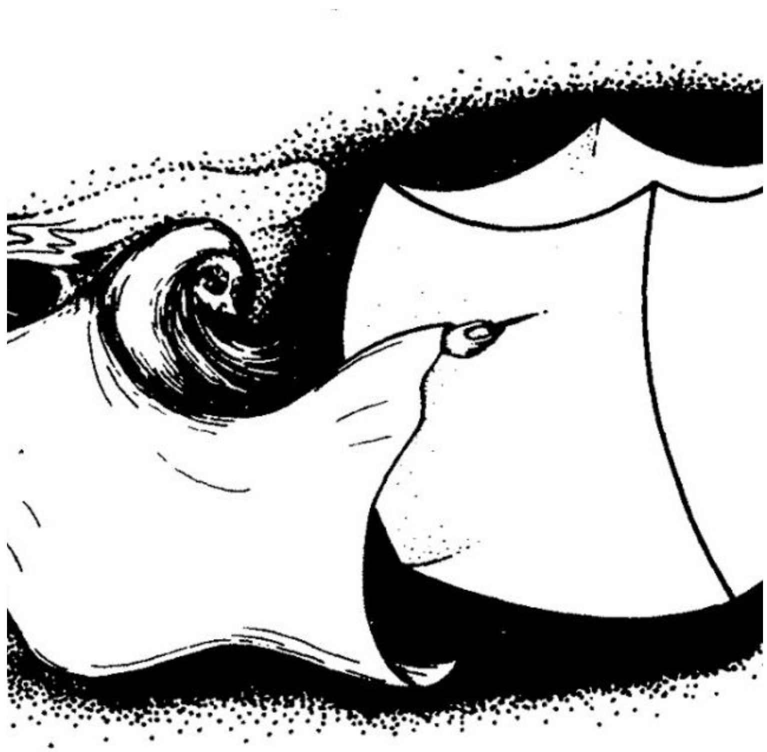
- The theory is multifaceted and can be described from many different starting points.

- We will choose an unusual one, the **entropic** starting point.

- Historically, it emerged as one of the conclusions:
  Araki, H: Relative entropy of states of von Neumann algebras I, II, 1976/77.

- The entropic perspective on modern non-equilibrium quantum statistical mechanics is the main theme of these lectures.

IN THE BEGINNING THERE WAS ENTROPY



God picking out the special (low-entropy) initial conditions of our universe. Penrose (1999).

$\mathcal{A}$ finite alphabet, P probability on $\mathcal{A}$,

$$S(P) = -\sum P(a) \log P(a).$$

$0 \le S(P) \le \log|\mathcal{A}|$, $S(P) = \log|\mathcal{A}|$ iff $P = P_{\mathsf{u}}$, $P_{\mathsf{u}}(a) = 1/|\mathcal{A}|$.

$$\begin{aligned} S(P|P_{\mathsf{u}}) &= \log|\mathcal{A}| - S(P) \\ &= \sum P(a) \log \frac{P(a)}{P_{\mathsf{u}}(a)} \ge 0. \end{aligned}$$

RELATIVE ENTROPY

$$S(P|Q) = \sum P(a) \log \frac{P(a)}{Q(a)}.$$

$S(P|Q) \geq 0$ and $S(P|Q) = 0$ iff $P = Q$.

Relative Renyi α-entropy

$$S_\alpha(P|Q) = \sum P(a) \left[\frac{P(a)}{Q(a)}\right]^{-\alpha}$$

$$\partial_\alpha S_\alpha(P|Q)|_{\alpha=0} = -S(P|Q)$$

$$\partial_\alpha S_\alpha(P|Q)|_{\alpha=1} = S(Q|P).$$

Radon-Nikodym derivative $\frac{\mathrm{d}P}{\mathrm{d}Q}(a) = P(a)/Q(a)$,

$$S(P|Q) = \int_{\mathcal{A}} \log \frac{\mathrm{d}P}{\mathrm{d}Q} \mathrm{d}P$$

$$S_\alpha(P|Q) = \int_{\mathcal{A}} \left[\frac{\mathrm{d}P}{\mathrm{d}Q}\right]^{-\alpha} \mathrm{d}P = \int_{\mathcal{A}} \mathrm{e}^{-\alpha \log \frac{\mathrm{d}P}{\mathrm{d}Q}} \mathrm{d}P$$

In this formulation relative entropies generalize to any measurable space $\mathcal{A}$ and any two equivalent probability measures P, Q on $\mathcal{A}$.

The key: Radon-Nikodym derivative that leads to the entropy function $\log \frac{\mathrm{d}P}{\mathrm{d}Q}$.

NON-COMMUTATIVE SETTING

Finite dim Hilbert space $\mathcal{H}$, states = density matrices ρ, ν.

Entropy: $S(\rho) = -\mathrm{tr}(\rho \log \rho)$.

Relative entropy: $S(\rho|\nu) = \mathrm{tr}(\rho(\log \rho - \log \nu))$.

Relative Renyi entropy: $S_\alpha(\rho|\nu) = \mathrm{tr}(\rho^{1-\alpha}\nu^\alpha)$.

But what is the Radon-Nikodym derivative now? How to extend these formula to the general non-commutative setting of von Neumann algebras?

Modular structure enters here!

$\mathcal{O} = \mathcal{B}(\mathcal{H})$ is Hilbert space with inner product $\langle X, Y \rangle = \mathtt{tr}(X^* Y)$. Superoperators $\mathcal{B}(\mathcal{O})$.

GNS representation: $\mathcal{O}$ is identified with the left multiplication map in $\mathcal{B}(\mathcal{O})$,

$$\mathcal{O} \ni X \mapsto AX \in \mathcal{O}.$$

$\pi(A)(X) = AX$,

$$\mathcal{O} \ni A \mapsto \pi(A) \in \mathcal{B}(\mathcal{O}).$$

$\pi(A)^* = \pi(A^*)$, $\pi(AB) = \pi(A)\pi(B)$, $\|A\| = \|\pi(A)\|$.

$\pi'(A)X = XA$. Commutant of $\pi(\mathcal{O})$ in $\mathcal{O}$ is $\pi'(\mathcal{O})$.

$\pi(\mathcal{O}) \vee \pi(\mathcal{O})' = \mathcal{B}(\mathcal{O})$, $\pi(\mathcal{O}) \cap \pi(\mathcal{O})' = \mathbb{C}\mathbf{1}$.

Relative modular operator $\Delta_{\rho|\nu} : \mathcal{O} \to \mathcal{O}$,

$$\Delta_{\rho|\nu} X = \rho X \nu^{-1}.$$

This is the non-commutative RN-derivative. It is not in $\pi(\mathcal{O})$!

$$\Delta_{\rho|\rho} = \Delta_\rho$$

is the modular operator of the state ρ. It is non-trivial, and this non-triviality is central to the richness of quantum statistical mechanics.

Connes's cocycle

$$[D\rho : D\nu](X) = \Delta_{\rho|\nu} \Delta_\nu^{-1}(X) = \rho\nu^{-1} X.$$

is in $\pi(\mathcal{O})$. Chain rule

$$[D\rho_1 : D\rho_2][D\rho_2 : D\rho_3] = [D\rho_1 : D\rho_3].$$

Hilbert space $\mathcal{O}$ comes with:

(a) Natural cone: $\mathcal{P} = \{X \in \mathcal{O} \,|\, X \geq 0\}$.

(b) Modular conjugation $J : \mathcal{O} \to \mathcal{O}$, $J(X) = X^*$.

$$J\pi(\mathcal{O})J = \pi'(\mathcal{O})$$

$$\mathcal{P} = \{XJ(X) \,|\, X \in \mathcal{O}\}$$

To any state ρ one associates $\Omega_\rho = \rho^{1/2} \in \mathcal{P}$, the so-called vector representative of ρ in the natural cone.

$$\rho(A) = \mathrm{tr}(\rho A) = \mathrm{tr}(\rho^{1/2} A \rho^{1/2}) = \langle \Omega_\rho, \pi(A)\Omega_\rho \rangle$$

$(\mathcal{O}, \pi, \Omega_\rho) =$ GNS representation of $\mathcal{O}$ induced by $\rho(> 0)$.

Define anti-linear map $S : \mathcal{O} \to \mathcal{O}$ by

$$S\pi(A)\Omega_\rho = \pi(A)^* \Omega_\rho.$$

Its polar decomposition is

$$S = J \Delta_\rho^{1/2}.$$

ENTROPIES

$$\log \Delta_{\rho|\nu}(X) = \log \rho X - X \log \nu.$$

$$S(\rho|\nu) = \mathrm{tr}(\rho(\log \rho - \log \nu)) = \langle \Omega_\rho, \log \Delta_{\rho|\nu} \Omega_\rho \rangle.$$

$S(\rho|\nu) \geq 0$ with equality iff $\rho = \nu$.

$$S_\alpha(\rho|\nu) = \mathrm{tr}(\rho^{1-\alpha} \nu^\alpha) = \langle \Omega_\rho, \Delta_{\rho|\nu}^{-\alpha} \Omega_\rho \rangle.$$

We have achieved our goal—the non-commutative Radon-Nikodym structure that allows to define directly relative entropies in the general setting (to which we will come at the end of these lectures).

And we got much more.

EQUILIBRIUM STATISTICAL MECHANICS

Dynamics: generated by Hamiltonian H on $\mathcal{H}$, Heisenberg flow

$$\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}.$$

$$\pi(\tau^t(A)) = \mathrm{e}^{\mathrm{i}t\mathcal{L}} \pi(A) \mathrm{e}^{-\mathrm{i}t\mathcal{L}},$$

$$\mathcal{L}(X) = HX - XH.$$

$\mathcal{L}$-the standard Liouvillean of τ^t. $\mathrm{e}^{\mathrm{i}t\mathcal{L}}\mathcal{P} = \mathcal{P}$.

A state of thermal equilibrium at inverse temperature β is

$$\rho_\beta = \mathrm{e}^{-\beta H}/Z(\beta),$$

where

$$Z(\beta) = \mathrm{tr}(\mathrm{e}^{-\beta H}).$$

Pressure $P(\beta) = \log Z(\beta)$. Gibbs variational principle:

$$P(\beta) = \max_\rho (S(\rho) - \beta \text{tr}(\rho H))$$

with unique maximizer $\rho = \rho_\beta$.

Proof:

$$\begin{aligned} S(\rho|\rho_\beta) &= \text{tr}(\rho(\log \rho - \log \rho_\beta)) \\ &= -S(\rho) + \beta \text{tr}(\rho H) + P(\beta). \end{aligned}$$

GVP follows from $S(\rho|\rho_\beta) \geq 0$ with equality iff $\rho = \rho_\beta$.

β-KMS-characterization: ρ_β is unique state satisfying β-KMS boundary condition

$$\text{tr}(\rho B_t A) = \text{tr}(\rho A B_{t+\text{i}\beta}),$$

$B_t = \tau^t(B)$. ρ is β-KMS state.

To any ρ one associates modular dynamics

$$\sigma_\rho^t(A) = \mathrm{e}^{\mathrm{i}t\log\rho} A \mathrm{e}^{-\mathrm{i}t\log\rho}$$

For Hamiltonian $\log\rho$, ρ is (-1)-KMS state. The corresponding standard Liouviellan is

$$\mathcal{L}_\rho = \log\Delta_\rho.$$

ρ is β-KMS for dynamics generated by H iff

$$\mathcal{L}_\rho = -\beta\mathcal{L}.$$

In general setting of von Neumann algebras this is known as *Takesaki theorem.*

NON EQUILIBRIUM QUANTUM STATISTICAL MECHANICS

Dynamics generated by H. Shrödinger flow $\rho_t = \mathrm{e}^{-\mathrm{i}tH}\rho\mathrm{e}^{\mathrm{i}tH}$.

Fix initial state ρ, $\rho_t \neq \rho$.

Chain rule:

$$[D\rho_{t+s} : D\rho] = \tau^{-t}([D\rho_s : D\rho])[D\rho_t : D\rho].$$

$$\ell_{\rho_t|\rho} = \log \Delta_{\rho_t|\rho} - \log \Delta_\rho.$$

$\ell_{\rho_t|\rho} \in \pi(\mathcal{O})$, $\ell_{\rho_t|\rho}(X) = (\log \rho_t - \log \rho)X$.

$$\ell_{\rho_{t+s}|\rho} = \tau^{-t}(\ell_{\rho_s|\rho}) + \ell_{\rho_t|\rho}.$$

Entropic cocycle $c^t = \tau^t(\ell_{\rho_t|\rho}) = \log\rho - \log\rho_{-t}$,

$$c^{t+s} = c^s + \tau^s(c^t)$$

$S = -\log\rho$ entropy observable. Heisenberg picture $\Rightarrow$

$$c^t = S_t - S.$$

Entropy production observable = quantum phase space contraction rate =

$$\sigma = \frac{\mathrm{d}}{\mathrm{d}t}c^t\Big|_{t=0} = \mathrm{i}[\log\rho, H].$$

Entropy production along the trajectory

$$c^t = \int_0^t \sigma_s \mathrm{d}s.$$

It has positive and negative eigenvalues ($\mathrm{tr}(c^t) = 0$).

Entropy balance equation–genesis of the second law

$$S(\rho_t|\rho) = \rho(c^t) = \mathrm{tr}(\rho c^t) = \int_0^t \rho(\sigma_s)\mathrm{d}s \geq 0.$$

If the system is time-reversal invariant (TRI) with time reversal ϑ (complex conjugation wrt which H and ρ are real), then

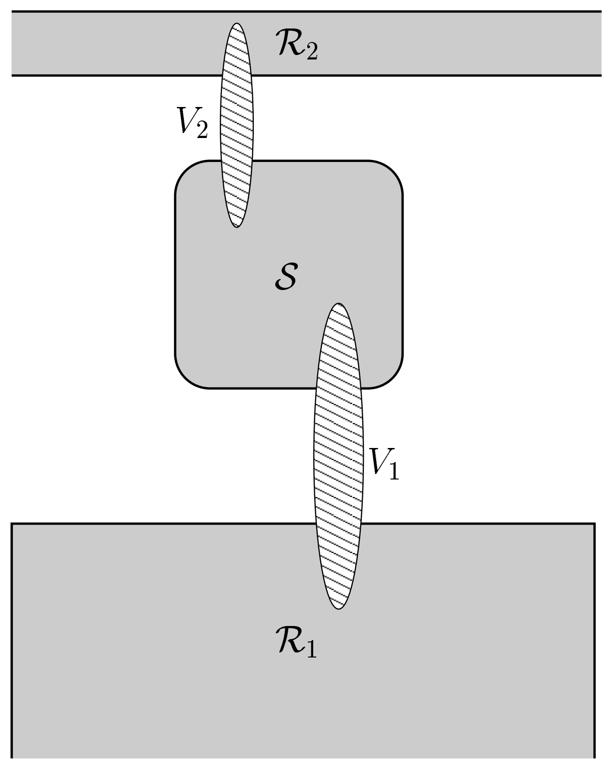
$$\vartheta(c^t) = c^{-t}, \qquad \vartheta(\sigma) = -\sigma,$$

and so the eigenvalues of c^t are symmetric wrt 0!

FROM NOW ON WE ASSUME TRI

EXAMPLE: OPEN QUANTUM SYSTEMS

Small Hamiltonian system S coupled to two thermal reservoirs.



Hilbert space $\mathcal{H}_{R_1} \otimes \mathcal{H}_S \otimes \mathcal{H}_{R_2}$.

Hamiltonians: $H_0 = H_S + H_{R_1} + H_{R_2}$,

$$H = H_0 + V.$$

Initial state:

$$\rho = \frac{1}{Z} \mathrm{e}^{-\beta(H_S+V)-\beta_1 H_{R_1}-\beta_2 H_{R_2}}.$$

$X_j = \beta - \beta_j$ (thermodynamical force).

$\Phi_j = \mathrm{i}[H_j, H]$ the energy flux out of the j-th reservoir.

Entropy production observable is

$$\sigma = X_1\Phi_1 + X_2\Phi_2.$$

$$\int_0^t \rho(\sigma_s)\mathrm{d}s = X_1 \underbrace{\int_0^t \rho(\tau^s(\Phi_1))\mathrm{d}s}_{\text{Energy change of } R_1} + X_2 \underbrace{\int_0^t \rho(\tau^s(\Phi_2))\mathrm{d}s}_{\text{Energy change of } R_2}$$

$\geq 0 \iff$ heat flows from hot to cold

(QUANTUM) OBJECTIONS

The exposed theory parallels the classical one, with modular structure replacing classical measure theory/probability. We will refer to it as the **direct modular quantization.**

There are however several objections from the physical perspective.

(a) Finite time fluctuation relation fails.

(b) The observational status of $\int_0^t \sigma_s \mathrm{d}s$ and of the fluctuations of entropy production along the state trajectory is questionable.

(c) Ruelle's counterproposal how should one define entropy production of open quantum systems.

FLUCTUATION RELATION FAILS

Spectral decomposition

$$c^t = \sum_{s \in \mathsf{sp}(c^t)} s P_s$$

The spectral measure for ρ and c^t is

$$Q_t(s) = \rho(P_s), \qquad s \in \mathsf{sp}(c^t).$$

We have

$$\begin{aligned} S(\rho_t|\rho) = \rho(c^t) &= \int s \mathsf{d} Q_t(s) \\ &= \sum_{s \in \mathsf{sp}(c^t)} s \rho(P_s) \geq 0. \end{aligned}$$

Time reversal $\Rightarrow$ sp(c^t) is symmetric wrt to zero. ρ favours positive eigenvalues (second law, direction of time).

However, the fluctuation relation (the fine form of the second law)

$$\frac{Q_t(-s)}{Q_t(s)} = \mathrm{e}^{-s}$$

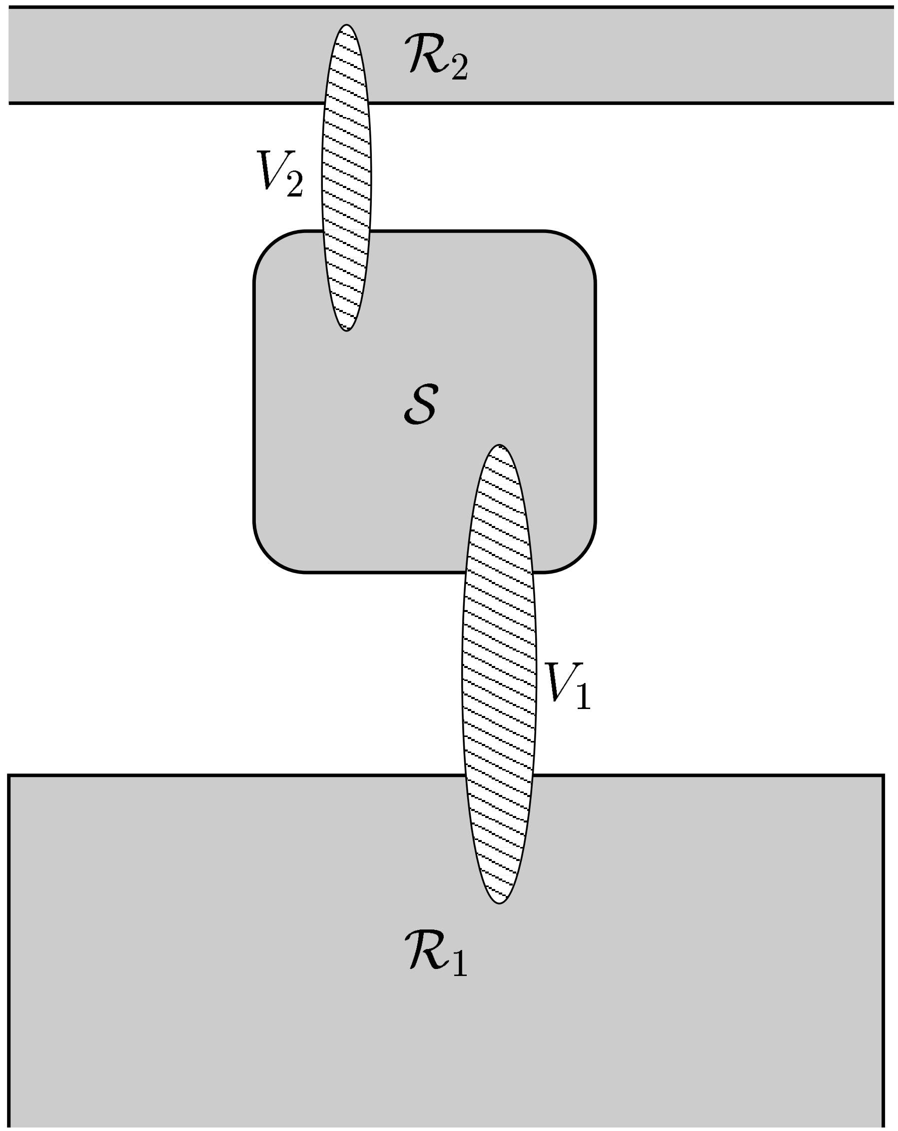
fails except in trivial cases.

Break with classical theory.

RUELLE'S PROPOSAL

”How should one define entropy production for nonequilibrium quantum spin systems?” Rev. Math. Phys. 14,701-707(2002).

Back to open quantum systems – small Hamiltonian system S coupled to two thermal reservoirs.


$\mathcal{R}_2$
V_2
$\mathcal{S}$
V_1
$\mathcal{R}_1$

Hilbert space $\mathcal{H}_{R_1} \otimes \mathcal{H}_S \otimes \mathcal{H}_{R_2}$.

Hamiltonian generating flow: $H_0 = H_S + H_{R_1} + H_{R_2}$,

$$H = H_0 + V.$$

For convenience we take the initial state to be

$$\rho = \frac{1}{Z} \mathrm{e}^{-\beta_1 H_{R_1} - \beta_2 H_{R_2}}$$

where $\mathcal{S}$ is in the infinite temperature state $\mathbf{1}/\mathrm{dim}(\mathcal{H}_S)$. This choice has no effect on the thermodynamics of the system (after the thermodynamic limit in which reservoirs became infinitely extended and the large time limit).

MUTUAL INFORMATION

$$\rho(t) = \mathrm{e}^{-\mathrm{i}tH}\rho\mathrm{e}^{\mathrm{i}tH},$$

$$\rho_S(t) = \mathrm{tr}_{\mathcal{H}_{R_1}\otimes\mathcal{H}_{R_2}}\rho(t),$$

$$\rho_{R_1}(t) = \mathrm{tr}_{\mathcal{H}_S\otimes\mathcal{H}_{R_2}}\rho(t),$$

$$\rho_{R_2}(t) = \mathrm{tr}_{\mathcal{H}_{R_1}\otimes\mathcal{H}_S}\rho(t).$$

The open quantum system mutual information is

$$I(t) = S(\rho(t)|\rho_{R_1}(t)\otimes\rho_S(t)\otimes\rho_{R_2}(t))$$

$$= -S(\rho(t)) + S(\rho_{R_1}(t)) + S(\rho_S(t)) + S(\rho_{R_2}(t)).$$

Note that $S(\rho(t))$ does not depend on t and that $I(0) = 0$. Ruelle is interested in $\frac{\mathrm{d}}{\mathrm{d}t}I(t)$.

Note first that ($\# \in \{R_1, S, R_2\}$)

$$\mathrm{tr}_{\mathcal{H}_\#}\left(\rho_\#(t)\frac{\mathrm{d}}{\mathrm{d}t}\log\rho_\#(t)\right) = \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{tr}_{\mathcal{H}_\#}(\rho_\#(t)) = 0.$$

This gives that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}S(\rho_\#(t)) &= -\mathrm{tr}_{\mathcal{H}_\#}\left(\log\rho_\#(t)\left[\frac{\mathrm{d}}{\mathrm{d}t}\rho_\#(t)\right]\right)\\ &= \mathrm{i}\mathrm{tr}_{\mathcal{H}}\left(\rho(t)[H, \log\rho_\#(t)\otimes \mathbf{1}]\right),\end{aligned}$$

and we arrive at the Ruelle's formula

$$\frac{\mathrm{d}}{\mathrm{d}t}I(t) = -\mathrm{i}\mathrm{tr}_{\mathcal{H}}\left(\rho(t)[H, \log\rho_{R_1}(t)\otimes\rho_S(t)\otimes\rho_{R_2}(t)]\right),$$

or equivalently to the Ruelle's mutual information balance equation

$$I(t) = -\mathrm{i} \int_0^t \rho(s) \left([H, \log \rho_{R_1}(s) \otimes \rho_S(s) \otimes \rho_{R_2}(s)] \right) \mathrm{d}s.$$

Since

$$\mathrm{tr}_{\mathcal{H}_\#}(\rho_\#(t)[H_\#, \log \rho_\#(t)]) = 0,$$

we also have

$$\frac{\mathrm{d}}{\mathrm{d}t} I(t) = -\mathrm{i}\,\mathrm{tr}_{\mathcal{H}} \left(\rho(t)[V, \log \rho_{R_1}(t) \otimes \rho_S(t) \otimes \rho_{R_2}(t)] \right)$$

and

$$I(t) = -\mathrm{i} \int_0^t \rho(s) \left([V, \log \rho_{R_1}(s) \otimes \rho_S(s) \otimes \rho_{R_2}(s)] \right) \mathrm{d}s.$$

This should be compared with the previous formula for the average entropy production over the time-interval $[0, t]$ (the entropy balance equation)

$$
\begin{aligned}
S(\rho(t)|\rho) &= -\mathrm{i}\int_0^t \rho(s)\left([H, \log \rho_{R_1}(0) \otimes \rho_S(0) \otimes \rho_{R_2}(0)]\right) \mathrm{d}s \\
&= -\mathrm{i}\int_0^t \rho(s)\left([V, \log \rho_{R_1}(0) \otimes \rho_S(0) \otimes \rho_{R_2}(0)]\right) \mathrm{d}s.
\end{aligned}
$$

Note the identity

$$
S(\rho(t)|\rho) = I(t) + \sum_{\#=R_1,S,R_2} S(\rho_{\#}(t)|\rho_{\#}).
$$

This gives the inequality $S(\rho(t)|\rho) \geq I(t)$.

The Ruelle's proposal has not been systematically studied and is a part of our current research program. An important open question is when this proposal is equivalent to the direct modular quantization of the entropy production. Ruelle made a suggestion:

> *In any case we are interested in a double limit where first the reservoirs are allowed to be infinite and then, perhaps, the boundaries between the small system and the reservoirs are allowed to move to infinity. This double limit is more or less imposed by physics, but seems hard to analyze mathematically.*

TWO-TIME MEASUREMENT AND MODULAR THEORY

Radically different proposal for quantum mechanical entropy production based on the two-time measurement of the entropy observable $S = -\log \rho$.

$$\rho = \sum \lambda P_\lambda.$$

First measurement at $t = 0$, $-\log \lambda$ is observed with probability $\mathrm{tr}(\rho P_\lambda)$. State reduction

$$\rho \mapsto \rho P_\lambda / \mathrm{tr}(\rho P_\lambda).$$

Reduced state evolves to

$$\mathrm{e}^{-\mathrm{i}tH} \left[\rho P_\lambda / \mathrm{tr}(\rho P_\lambda)\right] \mathrm{e}^{\mathrm{i}tH}.$$

The second measurement at time t gives $-\log \mu$ with probability

$$\mathrm{tr}\left(\mathrm{e}^{-\mathrm{i}tH} \left[\rho P_\lambda / \mathrm{tr}(\rho P_\lambda)\right] \mathrm{e}^{\mathrm{i}tH} P_\mu\right).$$

The probability that the pair $(-\log\lambda, -\log\mu)$ is observed is

$$p_t(\lambda,\mu) = \mathrm{tr}\left(\mathrm{e}^{-\mathrm{i}tH}\rho P_\lambda \mathrm{e}^{\mathrm{i}tH} P_\mu\right).$$

The entropy production random variable is

$$\mathcal{E}(\lambda,\mu) = -\log\mu - (-\log\lambda).$$

The distribution $\mathcal{Q}_t$ of $\mathcal{E}$ wrt p_t is

$$\mathcal{Q}_t(s) = \sum_{\mathcal{E}(\lambda,\mu)=s} p_t(\lambda,\mu).$$

$\mathcal{Q}_t$ is physically natural and experimentally accessible (in principle).

Basic fact

$$\int_{\mathbb{R}} \mathrm{e}^{-\alpha s} \mathrm{d}\mathcal{Q}_t(s) = \langle \Omega_\rho, \Delta^{\alpha}_{\rho_{-t}|\rho} \Omega_\rho. \rangle$$
$$= S_\alpha(\rho_t|\rho)$$
$$= S_{1-\alpha}(\rho_t|\rho).$$

$\mathcal{Q}_t$ = spectral measure of $-\log \Delta_{\rho_{-t}|\rho}$ for Ω_ρ.

The characteristic function of $\mathcal{Q}_t$ is the Renyi's relative entropy of the pair (ρ_t, ρ). Observational status of the modular structure!

TRI gives $\mathcal{Q}_t(s) \neq 0 \Leftrightarrow \mathcal{Q}_t(-s) \neq 0$.

Comparison with the direct modular quantization (Q_t spectral measure for ρ and c^t) under TRI.

$$\int_{\mathbb{R}} s \mathrm{d}\mathcal{Q}_t(s) = \int_0^t \rho(\sigma_s)\mathrm{d}s = S(\rho_t|\rho) = \int_{\mathbb{R}} s \mathrm{d}Q_t(s),$$

$$\int_{\mathbb{R}} s^2 \mathrm{d}\mathcal{Q}_t(s) = \int_{\mathbb{R}} s^2 \mathrm{d}Q_t(s).$$

However, the third moments of $\mathcal{Q}_t$ and Q_t are typically different.

$\mathcal{Q}_t = Q_t$ only in trivial cases.

Crucial observation (Kurchan, Tasaki, Tasaki-Matsui): the fluctuation relation hold for $\mathcal{Q}_t$. Under TRI,

$$\frac{\mathcal{Q}_t(-s)}{\mathcal{Q}_t(s)} = \mathrm{e}^{-s}.$$

$\mathcal{Q}_t$ - two times measurement entropy production (2TMEP) - is mathematically beautiful and physically natural proposal for the quantization of the entropy production.

But there are objections.

(a) The experiments are done only on the models with small $\dim\mathcal{H}$. The 2TMEP is obviously only a thought experiment if $\dim\mathcal{H}$ is large. But in the thermodynamic limit $\dim\mathcal{H} \to \infty$!

(b) The conceptual difficulty regarding the role of quantum measurements in development of quantum statistical mechanics.

We will discuss recently proposed solution to (a). We will not discuss the point (b) for which we refer to

Recent series by Benoist, Bruneau, J, Panati, Pillet:

A note on two-times measurement entropy production and modular theory, Lett. Math. Phys. 2024.

On the thermodynamic limit of two-times measurement entropy production, to appear in Rev. Math. Phys.

Entropic fluctuations in statistical mechanics II. Quantum dynamical systems, preprint

Entropic fluctuation theorems for spin-fermion model, preprint.

ENTROPIC ANCILLA STATE TOMOGRAPHY

The ancilla's Hilbert space is $\mathbb{C}^2$ and its initial state is a density matrix

$$\rho_{\mathrm{a}} = \begin{bmatrix} \rho_{++} & \rho_{+-} \\ \rho_{-+} & \rho_{--} \end{bmatrix},$$

with $\rho_{+-} \neq 0$.

The Hilbert space of the coupled system is $\widehat{\mathcal{H}} = \mathcal{H} \otimes \mathbb{C}^2$ and its initial state is $\widehat{\rho} = \rho \otimes \rho_{\mathrm{a}}$.

The coupling between the system and the ancilla is given by the Hamiltonian

$$\widehat{H}_\alpha = \mathrm{e}^{\frac{\alpha}{2}\log\rho\otimes\sigma_z}\,(H\otimes\mathbf{1})\,\mathrm{e}^{-\frac{\alpha}{2}\log\rho\otimes\sigma_z},$$

parametrized by $\alpha \in \mathrm{i}\mathbb{R}$.

If $H = H_0 + V$ with $[H_0, \rho] = 0$, then

$$\widehat{H}_\alpha = H\otimes\mathbf{1} + \widehat{W}_\alpha,$$

$$\widehat{W}_\alpha = \frac{1}{2}W_\alpha\otimes(\mathbf{1}+\sigma_z) + \frac{1}{2}W_\alpha\otimes(\mathbf{1}-\sigma_z),$$

$$W_\alpha = \rho^\alpha(V) - V.$$

The ancilla's state at time t is given by

$$\rho_{\mathrm{a}}(t) = \mathrm{tr}_{\mathcal{H}}(\mathrm{e}^{-\mathrm{i}t\widehat{H}_\alpha}\widehat{\rho}\mathrm{e}^{\mathrm{i}t\widehat{H}_\alpha}) = \begin{bmatrix} \rho_{++} & \mathcal{F}_t(\alpha)\rho_{+-} \\ \overline{\mathcal{F}_t(\alpha)}\rho_{-+} & \rho_{--} \end{bmatrix}.$$

where

$$\mathcal{F}_t(\alpha) = \int_{\mathbb{R}} \mathrm{e}^{-\alpha s}\mathrm{d}\mathcal{Q}_t(s).$$

Ancilla state tomography (projective measurements on $\mathbb{C}^2$) gives the access to $\rho_{\mathrm{a}}(t)$!

This is of fundamental theoretical and experimental importance and resolves objection (a).

BMV ENTROPY PRODUCTION

Direct quantization:

$$c^t = \int_0^t \sigma_s \mathrm{d}s = S_t - S,$$

$S = -\log \rho$, $S_t = \mathrm{e}^{\mathrm{i}tH} S \mathrm{e}^{-\mathrm{i}tH}$. Q_t- spectral measure for ρ and c^t,

$$\begin{aligned} \mathcal{F}_t^{\text{direct}}(\alpha) &= \int_{\mathbb{R}} \mathrm{e}^{-\alpha s} \mathrm{d}Q_t(s) \\ &= \mathrm{tr}(\rho \mathrm{e}^{-\alpha(S_t - S)}) \\ &= \mathrm{tr}(\mathrm{e}^{-S} \mathrm{e}^{-\alpha(S_t - S)}) \end{aligned}$$

Fluctuation relation fails (TRI assumed) $\Leftrightarrow$ the relation

$$\mathcal{F}_t^{\text{direct}}(\alpha) = \mathcal{F}_t^{\text{direct}}(1-\alpha)$$

cannot hold for all α.

Two-time measurement of $S = -\log\rho$ gives statistics $\mathcal{Q}_t^{\mathtt{ttm}}$,

$$\mathcal{F}_t^{\mathtt{ttm}}(\alpha) = \int_{\mathbb{R}} \mathrm{e}^{-\alpha s}\mathrm{d}\mathcal{Q}_t^{\mathtt{ttm}}(s)$$
$$= \mathrm{tr}(\rho\mathrm{e}^{-\alpha S_t}\mathrm{e}^{\alpha S}).$$

Fluctuation relation holds $\Leftrightarrow$ the relation

$$\mathcal{F}_t^{\mathtt{ttm}}(\alpha) = \mathcal{F}_t^{\mathtt{ttm}}(1-\alpha)$$

holds for all α.

$\mathtt{direct} \ \rightarrow \ \mathtt{ttm}$ amounts to

$$\mathrm{e}^{-\alpha(S_t - S)} \rightarrow \mathrm{e}^{-\alpha S_t}\mathrm{e}^{\alpha S}.$$

Playing the game further, one can replace

$$\rho \mathrm{e}^{-\alpha(S_t - S)} = \mathrm{e}^{-S}\mathrm{e}^{-\alpha(S_t - S)} \to \mathrm{e}^{-S-\alpha(S_t - S)}$$
$$= \mathrm{e}^{-(1-\alpha)S - \alpha S_t}$$

and introduce

$$\mathcal{F}_t^{\mathrm{BMV}}(\alpha) = \mathrm{tr}(\mathrm{e}^{-(1-\alpha)S-\alpha S_t}).$$

TRI $\Rightarrow$

$$\mathcal{F}_t^{\mathrm{BMV}}(\alpha) = \mathcal{F}_t^{\mathrm{BMV}}(1-\alpha).$$

This brings us to **B**essis-**M**oussa-**V**illani1975 conjecture, resolved by Stahl in 2011.

A, B self-adjoint matrices. Then there exists Borel measure $\mu_{A,B}$ on $\mathbb{R}$ such that for $\alpha \in \mathbb{R}$,

$$\mathrm{tr}(\mathrm{e}^{A-\alpha B}) = \int_{\mathbb{R}} \mathrm{e}^{-\alpha s} \mathrm{d}\mu_{A,B}(s).$$

Except in trivial cases, $\mu_{A,B}$ has a continuous component.

Hence, there exists $\mathcal{Q}_t^{\mathrm{BMV}}$ such that

$$\mathcal{F}_t^{\mathrm{BMV}}(\alpha) = \int_{\mathbb{R}} \mathrm{e}^{-\alpha s} \mathrm{d}\mathcal{Q}_t^{\mathrm{BMV}}(s),$$

and

$$\frac{\mathrm{d}\mathcal{Q}_t^{\mathrm{BMV}}(-s)}{\mathrm{d}\mathcal{Q}_t^{\mathrm{BMV}}(s)} = \mathrm{e}^{-s}.$$

$\mathcal{F}_t^{\mathsf{BMV}}$ has been useful in study of the structure of non-equilibrium quantum statistical mechanics.

Important open question: direct physical interpretation of $\mathcal{Q}_t^{\mathsf{BMV}}$. Is this measure experimentally accessible?

But there is more to this story. Golden-Thompson inequality gives that for $\alpha \in \mathbb{R}$,

$$\mathcal{F}_t^{\mathsf{BMV}}(\alpha) \leq \mathcal{F}_t^{\mathsf{ttm}}(\alpha).$$

Can $\mathcal{F}_t^{\mathsf{BMV}}$ be connected naturally to $\mathcal{F}_t^{\mathsf{ttm}}$?

ENTROPIC INTERPOLATION

For $p \in [1, \infty)$,

$$\mathcal{F}_t^{(p)}(\alpha) = \mathrm{tr}\left(\mathrm{e}^{-\frac{1-\alpha}{p}S}\mathrm{e}^{-\frac{2\alpha}{p}S_t}\mathrm{e}^{-\frac{1-\alpha}{p}S}\right)^{p/2}$$

$$= \mathrm{tr}\left(\rho^{\frac{1-\alpha}{p}}\rho_t^{\frac{2\alpha}{p}}\rho^{\frac{1-\alpha}{p}}\right)^{p/2}.$$

- $\mathcal{F}_t^{(2)}(\alpha) = \mathcal{F}_t^{\mathrm{ttm}}(\alpha)$.
- $\mathcal{F}_t^{(\infty)}(\alpha) = \lim_{p\to\infty} \mathcal{F}_t^{(p)}(\alpha) = \mathcal{F}_t^{\mathrm{BMV}}(\alpha)$.

- $\mathcal{F}_t^{(p)}(\alpha) = \mathcal{F}_t^{(p)}(1-\alpha)$

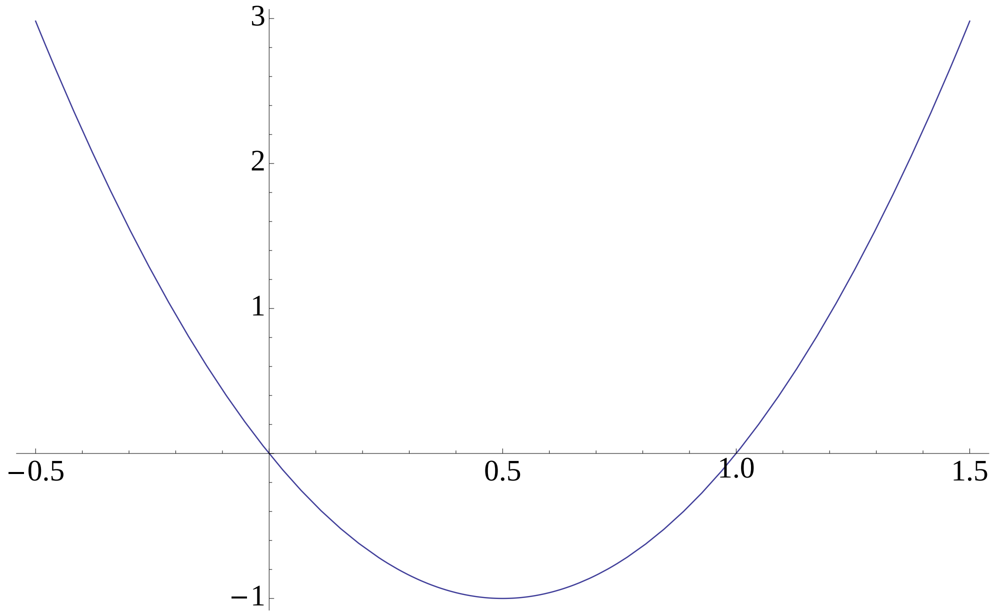
- $\mathcal{F}_t^{(p)}(0) = \mathcal{F}_t^{(p)}(1) = 1.$

- $\alpha \mapsto \mathcal{F}_t^{(p)}(\alpha)$ is convex.

-
$$\partial_\alpha \mathcal{F}_t^{(p)}(\alpha)|_{\alpha=0} = -S(\rho_t|\rho)$$
$$\partial_\alpha \mathcal{F}_t^{(p)}(\alpha)|_{\alpha=1} = S(\rho_t|\rho).$$

No p-dependence! The second derivatives are p-dependent.

- $[1, \infty] \ni p \mapsto \mathcal{F}_t^{(p)}(\alpha)$ is decreasing (strictly): (Araki)-Lieb-Thirring.



- Interpolating functionals motivated works in quantum information: Audenaert-Datta: α-z-relative Renyi entropies.

$$S_{p,\alpha}(\nu,\zeta) = \log \operatorname{tr}\left(\nu^{\frac{1-\alpha}{p}}\zeta^{\frac{2\alpha}{p}}\nu^{\frac{1-\alpha}{p}}\right)^{p/2}.$$

Obtaining a single quantum generalization of the classical relative Renyi entropy, which would cover all possible operational scenarios in quantum information theory, is a challenging (and perhaps impossible) task. However, we believe $S_{p,\alpha}$ is thus far the best candidate for such a quantity, since it unifies all known quantum relative entropies in the literature.

Lots of works on the convexity/concavity properties of the map

$$(\nu,\zeta) \mapsto S_{p,\alpha}(\nu,\zeta).$$

- Quantum transfer operators. Act on $\mathcal{B}(\mathcal{H})$. Specific norm:

$$\|X\|_p = \left(\mathrm{tr}(|X\rho^{1/p}|^p)\right)^{1/p}.$$

$$U_p(t)X = \mathrm{e}^{-\mathrm{i}tH} X \mathrm{e}^{\mathrm{i}tH} \mathrm{e}^{\frac{1}{p}S_{-t}} \mathrm{e}^{-\frac{1}{p}S}.$$

Properties:

$$U_p(t_1+t_2) = U_p(t_1)U_p(t_2)$$
$$U_p(-t)\pi(A)U_p(t) = \pi(\mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}) \qquad (1)$$
$$\|U_p(t)X\|_p = \|X\|_p.$$

Basic fact:

$$\mathcal{F}_t^{(p)}(\alpha) = \|U_{p/\alpha}(t)\mathbf{1}\|_p^p.$$

- Non-commutative extensions of Ruelle's transfer operators in classical dynamical system theory based on Araki-Masuda non-commutative L^p-spaces and modular theory.

- If dynamics is generated by Hamiltonian H,

$$U_p(t) = \mathrm{e}^{-\mathrm{i}tL_p},$$

$$L_p(X) = HX - X\Delta_\rho^{\frac{1}{p}-\frac{1}{2}} H \Delta_\rho^{\frac{1}{2}-\frac{1}{p}}.$$

$L_2 = \mathcal{L}$, the standard Liouvillean that implements the dynamics and preserves the natural cone. In open quantum system with $H = H_0 + V$, $[H_0, \rho] = 0$,

$$L_p = \mathcal{L}_0 + \pi(V) - J\Delta_\rho^{\frac{1}{p}-\frac{1}{2}} \pi(V) \Delta_\rho^{\frac{1}{2}-\frac{1}{p}} J$$

- The p-th cone is

$$\mathcal{P}^{(p)} = \{A \in \mathcal{B}(\mathcal{H}) \,|\, A = X\rho^{\frac{1}{2}-\frac{1}{p}},\ X \geq 0\}.$$

$\mathcal{P}^{(2)} = \mathcal{P}$, the natural cone.

- $U_p(t)\mathcal{P}^{(p)} = \mathcal{P}^{(p)}$ and together with (1) this uniquely determines the group U_p.

- All p's are important!

$$\mathcal{F}_t^{\mathsf{ttm}}(\alpha) = \int_{\mathbb{R}} \mathrm{e}^{-\alpha s} \mathrm{d}\mathcal{Q}_t^{\mathsf{ttm}}(s) = \langle \Omega_\rho, \mathrm{e}^{-\mathrm{i}tL_p}\Omega_\rho \rangle$$

with $p = 1/\alpha$. This formula is of central computational and conceptual importance.

REMARKS

1. The entropic non-equilibrium algebraic quantum statistical mechanics remains only partially understood.

2. The results obtained so far hint at structure of great mathematical beauty centred around modular theory.

3. The equilibrium theory is also centred around the modular theory via KMS condition. The non-equilibrium theory can be viewed as the deformation of the equilibrium one (think about open quantum systems with $\beta_1 = \beta_2$ (equilibrium) and $\beta_1 \neq \beta_2$ (non-equilibrium)).

4. The role time plays in two theories is completely different.

The last two remarks cannot be fully understood in the current setting. To proceed one needs to pass from finite system setting to infinitely extend system setting.

This is already necessary in equilibrium to develop the theory of phase transitions and define phases, and to study dynamically ergodic properties of the system. Although the understanding of the dynamical theory of phases (approach to equilibrium, dynamical justification of the zeroth law of thermodynamics) remains in its infancy, the Gibbs variational principle and KMS-condition allow to bypass this fundamental problem.

In non-equilibrium case the idealization of infinitely extended system is necessary to have mathematically sharp definition of entropy production per unit time (constant in time heat flow from hot to cold requires idealization of infinite reservoirs energy). However, to achieve this one needs also to control the **large time** limit of entropy production and, on a deeper level, introduce **Non-Equilibrium Steady States** to which infinitely extended system relaxes in the large time limit and which sustain constant entropy production. The large time limit is needed to define the key objects of the theory and the fundamental **relaxation problem** cannot be bypassed like in equilibrium theory.

THERMODYNAMIC LIMIT

or passage to infinitely extended systems. Extensively studied in early days of rigorous statistical mechanics (1960's and 70's).

The physical considerations lead to a sequence of finite dimensional systems with Hilbert spaces $\mathcal{H}_\Lambda$ and Hamiltonians H_Λ. The size of the system is characterized by the parameter Λ. For lattice quantum spin systems Λ is a finite subset of an infinite countable set G (an example is $G = \mathbb{Z}^d$) describing possible spin sites.

That will be our concrete example: lattice quantum spin systems.

Let G be a countably infinite set. The collection of all finite subsets of G is denoted by $\mathfrak{G}_{\mathsf{fin}}$. Let $\mathfrak{h}$ be the finite dimensional Hilbert space of a single spin. To each $x \in G$ we associate a copy $\mathfrak{h}_x$ of $\mathfrak{h}$, and to each $\Lambda \in \mathfrak{G}_{\mathsf{fin}}$ the Hilbert space

$$\mathcal{H}_\Lambda = \bigotimes_{x \in \Lambda} \mathfrak{h}_x.$$

To any $\mathcal{X} \in \mathfrak{G}_{\mathsf{fin}}$ one associates self-adjoint $\Phi(\mathcal{X}) \in \mathcal{B}(\mathcal{H}_X)$. that describes the interaction of the spins located at the sites in $\mathcal{X}$. The local Hamiltonians are

$$H_\Lambda = \sum_{\mathcal{X} \subseteq \Lambda} \Phi(\mathcal{X}).$$

This defines the net $(\mathcal{H}_\Lambda, H_\Lambda)_{\Lambda \in \mathfrak{G}_{\mathsf{fin}}}$. One is interested in the finite systems quantum mechanical properties in the limit $\Lambda \uparrow G$.

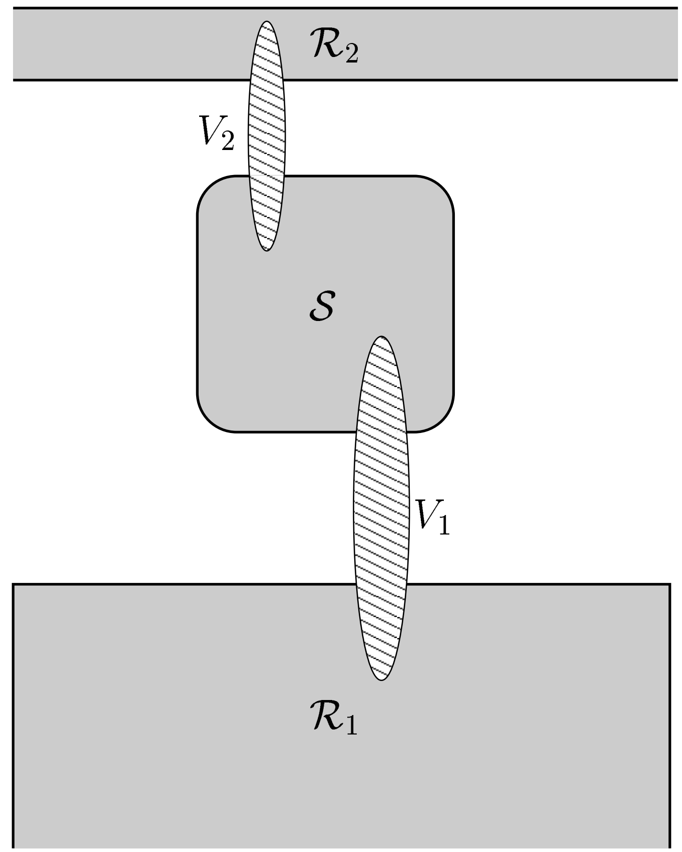
Examples (in equilibrium theory) are specific pressure and energy at inverse temperature β,

$$P(\beta) = \lim_{\Lambda \uparrow G} \frac{1}{|\Lambda|} \log \mathrm{tr}(\mathrm{e}^{-\beta H_\Lambda}),$$

$$E(\beta) = \lim_{\Lambda \uparrow G} \frac{1}{|\Lambda|} \frac{\mathrm{tr}(H_\Lambda \mathrm{e}^{-\beta H_\Lambda})}{\mathrm{tr}(\mathrm{e}^{-\beta H_\Lambda})}$$

Conditions on Φ are needed to ensure the existence of these limits and to develop thermodynamics. We will return to this latter.

David Ruelle in 2001 was first to consider open quantum lattice spin systems that correspond to



Disjoint decomposition

$$G = G_{\mathcal{R}_1} \cup G_{\mathcal{S}} + G_{\mathcal{R}_2}.$$

$G_{\mathcal{S}}$ finite, $G_{\mathcal{R}_j}$'s infinite. Φ is such that

$$\Phi(\mathcal{X}) = 0 \text{ if} \mathcal{X} \cap G_{\mathcal{R}_1} \neq \emptyset \text{ and } \mathcal{X} \cap G_{\mathcal{R}_2} \neq \emptyset.$$

One considers only Λ's such that $G_{\mathcal{S}} \subset \Lambda$,

$$\Lambda_1 = \Lambda \cap G_{\mathcal{R}_1} \neq \emptyset, \ \Lambda_2 = \Lambda \cap G_{\mathcal{R}_2} \neq \emptyset.$$

For fixed Λ, $H_{\mathcal{S}} = H_{G_{\mathcal{S}}}$, $H_{\mathcal{R}_1} = H_{\Lambda_1}$, $H_{\mathcal{R}_2} = H_{\Lambda_2}$.

The reservoirs are connected to the small system $\mathcal{S}$ by $V_{\Lambda,1}$ and $V_{\Lambda,2}$ given by

$$V_j = \sum_{\mathcal{X} \subset G_{\mathcal{S}} \cup \Lambda_j, \mathcal{X} \cap G_{\mathcal{S}} \neq \emptyset, \mathcal{X} \cap \Lambda_j \neq \emptyset} \Phi(\mathcal{X}).$$

Hence,

$$H_\Lambda = H_0 + V_\Lambda,$$

$$H_0 = H_{\mathcal{S}} + H_{\Lambda_1} + H_{\Lambda_2}, \; V = V_{\Lambda,1} + V_{\Lambda,2}.$$

Initial states:

$$\rho_\Lambda = \frac{1}{Z} \mathrm{e}^{-\beta(H_{\mathcal{S}}+V_\Lambda)-\beta_1 H_{\Lambda_1}-\beta_2 H_{\Lambda_2}}$$

or

$$\rho_\Lambda = \frac{1}{Z} \mathrm{e}^{-\beta_1 H_{\Lambda_1}-\beta_2 H_{\Lambda_2}},$$

and we are in the setting of open quantum systems.

Set

$$\mathrm{Ep}_\Lambda(t) = \mathrm{tr}(\rho_\Lambda c_\Lambda^t) = \int_0^t \mathrm{tr}(\rho_\Lambda \mathrm{e}^{\mathrm{i}sH_\Lambda} \sigma_\Lambda \mathrm{e}^{-\mathrm{i}sH_\Lambda}) \mathrm{d}s.$$

$\mathcal{Q}_\Lambda^{\mathrm{direct}}$, $\mathcal{Q}_\Lambda^{\mathrm{ttm}}$, $\mathcal{Q}_\Lambda^{\mathrm{BMV}}$, $\mathcal{F}_{t,\Lambda}^{(p)}(\alpha)$ are defined as before.

We are interested in the limit $\Lambda \uparrow G$.

Regularity assumption: For some $\lambda > 0$,

$$\sup_{x \in G} \sum_{\mathcal{X} \ni x} \|\Phi(\mathcal{X})\| \mathrm{e}^{\lambda |\mathcal{X}|} < \infty.$$

To avoid dealing with possible reservoirs phase transitions, we also assume that β_1, β_2 are sufficiently small (high temperature regime); otherwise one needs to take $\Lambda \uparrow \mathcal{G}$ along subnets and face some additional technical issues. Then

$$\mathrm{Ep}(t) = \lim_{\Lambda \uparrow G} \mathrm{E}_\Lambda(t),$$

$$\mathrm{w} - \lim_{\Lambda \uparrow G} \mathcal{Q}^{\#} = \mathcal{Q}^{\#},$$

$\# \in \{\text{direct, ttm, BMV}\}$, and for $\alpha \in \mathrm{i}\mathbb{R}$,

$$\lim_{\Lambda \uparrow G} \mathcal{F}_{t,\Lambda}^{(p)}(\alpha) = \mathcal{F}_t^{(p)}(\alpha).$$

Proof is relatively straightforward; see BBJPP On the thermodynamic limit of two-times measurement entropy production, to appear in Rev. Math. Phys.

The large time $t \to \infty$ is much more delicate, as expected. One would like to prove that

$$\mathsf{Ep}_+ = \lim_{t\to\infty} \frac{1}{t}\mathsf{Ep}(t) > 0,$$

followed by the weak convergence of the families $\mathcal{Q}_t^{\#}(t\cdot)$ to δ_{Ep_+}, then to establish Central Limit Theorem and the Large Deviation Principle, then to study the existence and regularity of the limits

$$\mathcal{F}_+^{(p)}(\alpha) = \lim_{t\to\infty} \frac{1}{t}\log \mathcal{F}_t^{(p)}(\alpha).$$

These are very hard problems in physically interesting models.

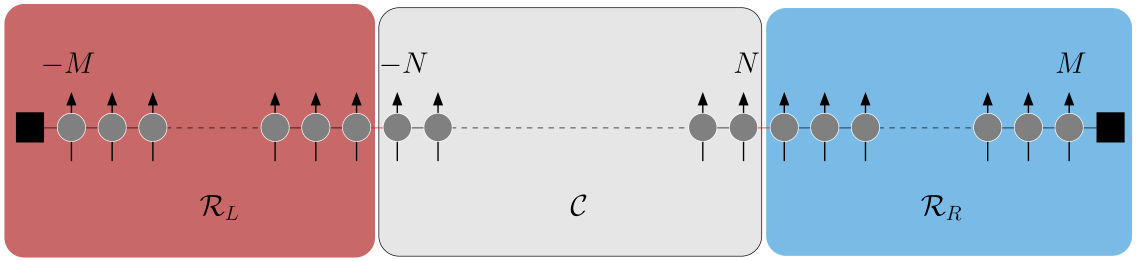
One important example, however, allows for direct computations and explicit formulas.

OPEN XY SPIN CHAIN

$\Lambda = [A, B] \subset \mathbb{Z}$, Hilbert space $\mathcal{H}_\Lambda = \bigotimes_{x\in\Lambda} \mathbb{C}^2$.
Hamiltonian

$$H_\Lambda = \frac{1}{2} \sum_{x\in[A,B[} J_x \left(\sigma_x^{(1)} \sigma_{x+1}^{(1)} + \sigma_x^{(2)} \sigma_{x+1}^{(2)} \right) + \frac{1}{2} \sum_{x\in[A,B]} \lambda_x \sigma_x^{(3)}.$$

$$\sigma_x^{(1)} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_x^{(2)} = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}, \quad \sigma_x^{(3)} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$



Central part $\mathcal{C}$ (small system $\mathcal{S}$): XY-chain on $\Lambda_{\mathcal{C}} = [-N, N]$.

Two reservoirs $\mathcal{R}_{L/R}$ $(L = 1, R = 2)$:
XY-chains on $\Lambda_L = [-M, -N - 1]$ and $\Lambda_R = [N + 1, M]$.

N fixed, thermodynamic limit $M \to \infty$.
Easily embedded in the spin system language (exercise).

Decoupled Hamiltonian $H_0 = H_{\Lambda_L} + H_{\Lambda_{\mathcal{C}}} + H_{\Lambda_R}$.

The full Hamiltonian is

$$H = H_{\Lambda_L \cup \Lambda_{\mathcal{C}} \cup \Lambda_R} = H_0 + V_L + V_R,$$

$$V_L = \frac{J_{-N-1}}{2} \left(\sigma^{(1)}_{-N-1} \sigma^{(1)}_{-N} + \sigma^{(2)}_{-N-1} \sigma^{(2)}_{-N} \right), \text{ etc.}$$

Initial state:

$$\rho = \mathrm{e}^{-\beta_L H_{\Lambda_L}} \otimes \rho_0 \otimes \mathrm{e}^{-\beta_R H_{\Lambda_R}} \Big/ Z,$$

$$\rho_0 = \mathbf{1} / \dim \mathcal{H}_{\Lambda_{\mathcal{C}}}.$$

Fluxes and entropy production:

$$\Phi_{L/R} = \mathrm{i}[H_{L/R}, H],$$

$$\sigma = -\beta_L \Phi_L - \beta_R \Phi_R.$$

First the thermodynamic limit $M \to \infty$, and then $t \uparrow \infty$ limit.

Araki-Ho, Ashbacher-Pillet $\sim$ 2000, J-Landon-Pillet 2012:

$$\mathrm{Ep}_+ = \frac{\Delta\beta}{4\pi} \int_{\mathbb{R}} |T(E)|^2 \frac{E \sinh(\Delta\beta E)}{\cosh \frac{\beta_L E}{2} \cosh \frac{\beta_R E}{2}} \mathrm{d}E > 0.$$

$\Delta\beta = \beta_L - \beta_R$. Landauer-Büttiker formula.

Idea of the proof – Jordan-Wigner transformation reduces the study of $t \uparrow \infty$ limit to the scattering problem for the Jacobi matrix

$$hu_x = J_x u_{x+1} + J_{x-1} u_{x-1} + \lambda_x u_x, \qquad u \in \ell^2(\mathbb{Z}).$$

Decomposition

$$\ell^2(\mathbb{Z}) = \ell^2(]-\infty, -N-1]) \oplus \ell^2([-N, N]) \oplus \ell^2([N+1, \infty[),$$

$$h_0 = h_L + h_{\mathcal{C}} + h_R,$$

$$h = h_0 + v_L + v_R,$$

$$v_R = J_N(|\delta_{N+1}\rangle\langle\delta_N| + \text{h.c})$$

The wave operators

$$w^{\pm} = \mathsf{s} - \lim_{t \to \pm\infty} \mathrm{e}^{\mathrm{i}th} \mathrm{e}^{-\mathrm{i}th_0} \mathbf{1}_{\mathrm{ac}}(h_0)$$

exist and are complete.

The scattering matrix:

$$s = w_+^* w_- : \mathcal{H}_{\mathrm{ac}}(h_0) \to \mathcal{H}_{\mathrm{ac}}(h_0)$$

$$s(E) = \begin{bmatrix} A(E) & T(E) \\ T(E) & B(E) \end{bmatrix}.$$

$$T(E) = \frac{2\mathrm{i}}{\pi} J_{-N-1} J_N \langle \delta_N | (h - E - \mathrm{i}0)^{-1} \delta_{-N} \rangle \sqrt{F_L(E) F_R(E)}$$

$$F_{L/R}(E) = \mathrm{Im}\, \langle \delta_{L/R} | (h_{L/R} - E - \mathrm{i}0)^{-1} \delta_{L/R} \rangle,$$

$$\delta_L = \delta_{-N-1}, \ \delta_R = \delta_{N+1}.$$

$T(E)$ is non-vanishing on the set $\mathrm{sp}_{\mathrm{ac}}(h_L) \cap \mathrm{sp}_{\mathrm{ac}}(h_R)$.

If $J_x = const$,$\lambda_x = const$ (or periodic) them $|T(E)| = 1$ for $E \in \mathrm{sp}(h)$.

Assumption: h has no singular continuous spectrum

Open question: What happens if h has some singular continuous spectra? Transport in quasi-periodic structures.

Beyond computing Ep_+, the following was was establised in JPL 2012.

$$\mathcal{F}_+^{\mathrm{direct}}(\alpha) = \lim_{t\to\infty} \frac{1}{t} \log \mathcal{F}_t(\alpha)$$
$$= \int_{\mathbb{R}} \log \left(\frac{\det(1 + K_\alpha(E))}{\det(1 + K_0(E))} \right) \frac{\mathrm{d}E}{2\pi},$$

$$K_\alpha(E) = \mathrm{e}^{k_0(E)/2} \mathrm{e}^{\alpha(s^*(E)k_0(E)s(E) - k_0(E))} \mathrm{e}^{k_0(E)/2},$$

$$k_0(E) = \begin{bmatrix} -\beta_L E & 0 \\ 0 & -\beta_R E \end{bmatrix}, \quad s(E) = \begin{bmatrix} A(E) & T(E) \\ T(E) & B(E) \end{bmatrix}$$

$$\mathcal{F}_+^{(p)}(\alpha) = \lim_{t\to\infty} \frac{1}{t} \log \mathcal{F}_t^{(p)}(\alpha)$$

$$= \int_{\mathbb{R}} \log\left(\frac{\det(1+K_{\alpha p}(E))}{\det(1+K_0(E))}\right) \frac{\mathrm{d}E}{2\pi},$$

where

$K_{\alpha p}(E)$

$$= \left(\mathrm{e}^{k_0(E)(1-\alpha)/p} s(E) \mathrm{e}^{k_0(E)2\alpha/p} s^*(E) \mathrm{e}^{k_0(E)(1-\alpha)/p}\right)^{p/2}.$$

The maps

$$\alpha \mapsto \mathcal{F}_+^{\mathsf{direct}}(\alpha), \qquad \alpha \mapsto \mathcal{F}_+^{(p)}(\alpha),$$

are real-analytic.

The map

$$[1, \infty] \ni p \mapsto \mathcal{F}_+^{(p)}(\alpha)$$

is continuous and decreasing. It is strictly decreasing unless h is reflectionless:

$$|T(E)| \in \{0, 1\} \qquad \forall E.$$

If h is reflectionless, then $\mathcal{F}^{(p)}(\alpha)$ does not depend on p and

$$\mathcal{F}_{+}^{(p)}(\alpha) = \mathcal{F}_{+}^{\text{direct}}(\alpha) =$$

$$\frac{1}{2\pi}\int_{\text{sp}(h)} \frac{\cosh((\beta_L(1-\alpha)+\beta_R\alpha)E/2)\times(L\to R)}{\cosh(\beta_L E/2)\cosh(\beta_R E/2)}\text{d}E.$$

Phenomenon: ”Entropic triviality.”

If h is not reflectionless,

$$\mathcal{F}_{+}^{\text{direct}}(1) > 0 = \mathcal{F}_{+}^{\text{direct}}(0).$$

The Law of Large Numbers, Central Limit Theorem and the Large Deviation Principle hold for measures $\mathcal{Q}_t^{\#}(t\cdot)$ in the limit $t\uparrow\infty$.

$$\mathcal{Q}_t^{\#}\to\delta_{\mathrm{Ep}_+},$$

Gärtner-Ellis theorem yields LDP

$$\mathcal{Q}_t^{\#}(tB)\simeq \mathrm{e}^{-t\inf_{\varsigma\in B}I^{\#}(\varsigma)}$$

$$I^{\#}(\varsigma)=-\inf_{\alpha\in\mathbb{R}}\Big(\alpha\varsigma+\mathcal{F}_+^{\#}(\alpha)\Big)$$

Fluctuation relation implies celebrated symmetries

$$I^{\#}(-\varsigma)=\varsigma+I^{\#}(\varsigma),$$

for $\# = \mathtt{ttm},\mathsf{BMV}$. The symmetry fails for $\# = \mathtt{direct}$ unless h is reflectionless.

HEISENBERG SPIN CHAIN

The Hamiltonian H of the open XY spin chain is changed to

$$H_P = H + P$$

where

$$P = K\frac{1}{2}\sum_{x\in[-N,N[}\sigma_x^{(3)}\sigma_{x+1}^{(3)}.$$

The central (system $\mathcal{S}$) part is now Heisenberg spin chain

$$\frac{1}{2}\sum_{x\in[-N,N[} J_x\sigma_x^{(1)}\sigma_{x+1}^{(1)} + J_x\sigma_x^{(2)}\sigma_{x+1}^{(2)} + K\sigma_x^{(3)}\sigma_{x+1}^{(3)}$$

$$+\frac{1}{2}\sum_{x\in[-N,N]}\lambda_x\sigma_x^{(3)}.$$

The thermodynamic limit $M \to \infty$ is not difficult.

Assumption For all $x, y \in \mathbb{Z}$,

$$\int_0^\infty |\langle \delta_x, \mathrm{e}^{\mathrm{i}th}\delta_y\rangle| \mathrm{d}t < \infty.$$

Denote

$$\ell_N = \int_0^\infty \sup_{x,y\in[-N,N[} |\langle \delta_x, \mathrm{e}^{\mathrm{i}th}\delta_y\rangle| \mathrm{d}t,$$

$$\bar{K} = \frac{6^6}{7^6}\frac{1}{24N}\frac{1}{\ell_N}.$$

If $|K| < \bar{K}$, then Ep_+ exists and is analytic function of K. In particular, $\mathrm{Ep}_+ > 0$ apart from possibly discrete set of K's.

The $t \uparrow \infty$ limit of $\mathcal{Q}_t^{\#}$ and $\mathcal{F}_t^{(p)}$ has not been studied and remains an important open problem. Technical suggestion: cluster expansion.

For the Pauli-Fierz systems, the $t \uparrow \infty$ limit of $\mathcal{Q}_t^{\mathtt{ttm}}$ and $\mathcal{F}_t^{\mathtt{ttm}}$, including the Large Deviation Principle, was analyzed in

de Roeck, W: Large deviation generating function for currents in the Pauli-Fierz model. Rev.Math. Phys. 21, 2009.

BBJPP: Entropic fluctuation theorems for spin-fermion model, preprint.

The quantum transfer operators played a key role in these works.

FULL DESCRIPTION OF QUANTUM SPIN SYSTEMS

Full quantum mechanical passage to $\Lambda \uparrow G$ limit.

Local pairs $(\mathcal{H}_\Lambda, H_\Lambda)$ lead to $(\mathcal{O}_\Lambda, \tau_\Lambda)$, where

$$\mathcal{O}_\Lambda = \mathcal{B}(\mathcal{H}_\Lambda), \qquad \tau_\Lambda^t(A) = \mathrm{e}^{\mathrm{i}tH_\Lambda} A \mathrm{e}^{-\mathrm{i}tH_\Lambda}.$$

Since $\mathcal{H}_\Lambda = \bigotimes_{x\in\Lambda} \mathfrak{h}_x$, if $\Lambda \subset \Lambda'$ we have natural inclusion $\mathcal{O}_\Lambda \subset \mathcal{O}_{\Lambda'}$ which gives that

$$\mathcal{O}_{\mathrm{loc}} = \bigcup_{\Lambda \in \mathfrak{G}_{\mathrm{fin}}} \mathcal{O}_\Lambda$$

is a normed $*$-algebra with the C^*-property $\|A^* A\| = \|A\|^2$.

$\mathcal{O}_{\mathrm{loc}}$ is the algebra of local observables of the quantum spin system with set of sites G and single spin Hilbert space $\mathfrak{h}$.

Its completion, $\mathcal{O}$, is the C^*-algebra of observables of extended quantum spin system. The algebra $\mathcal{O}$ is unital, simple and separable.

We now turn to the description of the full dynamics assuming that for some $\lambda > 0$,

$$\sup_{x\in G} \sum_{\mathcal{X}\ni x} \|\Phi(\mathcal{X})\| \mathrm{e}^{\lambda|\mathcal{X}|} < \infty.$$

For $A \in \mathcal{O}_{\mathrm{loc}}$ set

$$\tau_\Lambda^t(A) = \mathrm{e}^{\mathrm{i}tH_\Lambda} A \mathrm{e}^{-\mathrm{i}tH_\Lambda}$$

and

$$\tau^t(A) = \lim_{\Lambda \uparrow G} \tau_\Lambda^t(A).$$

The limit exist uniformly for t in compacts. τ^t is a norm-continuous group of $*$-automorphisms of $\mathcal{O}_{\mathrm{loc}}$ and as such uniquely extends to $\mathcal{O}$. τ^t defines Heisenberg time evolution on $\mathcal{O}$. The pair $(\mathcal{O}, \tau^t)$ is a C^*-dynamical system.

We now turn to the description of the states.

$\mathcal{O}^*$ - dual of $\mathcal{O}$. By the Banach-Alaoglu theorem, the unit ball in $\mathcal{O}^*$ is weak compact.

Physical states of our quantum spin system are described by mathematical states on $\mathcal{O}$, that is, positive normalized linear functionals in $\mathcal{O}^*$. A state ω evolves in time as $\omega_t = \omega \circ \tau^t$.

The number $\omega(A)$ is the expectation value of the observable A if the system is in the state ω.

$\beta > 0$ inverse temperature. Thermal equilibrium states are characterized by the β-KMS condition: for all $A, B \in \mathcal{O}$, the map

$$\mathbb{R} \ni t \mapsto F_{A,B}(t) = \omega(A\tau^t(B))$$

has analytic continuation to the strip $0 < \mathrm{Im}\, z < \beta$ that is bounded and continuous on its closure and satisfies

$$F_{A,B}(t + \mathrm{i}\beta) = \omega(\tau^t(B)A).$$

KMS states are stationary.

This definition extends to $\beta < 0$.

If ω is β-KMS, the quantum spin system described by $(G, \mathfrak{h}, \Phi)$ in thermal equilibrium at inverse temperature β is described by the quantum dynamical system $(\mathcal{O}, \tau^t, \omega)$.

Any weak limit point of the net of states

$$\omega_{\beta,\Lambda}(A) = \frac{\mathrm{tr}(A\mathrm{e}^{-\beta H_\Lambda})}{\mathrm{tr}(\mathrm{e}^{-\beta H_\Lambda})}$$

is β-KMS. These specific states are called thermodynamic limit point β-KMS states.

EQUILIBRIUM STAT MECH OF SPIN SYSTEMS

In equilibrium statistical mechanics one commonly consider the case $G = \mathbb{Z}^d$ where the translational invariance plays a role. The translational invariance connects Λ and $\Lambda + x$ and leads to a group of $*$-automorphisms φ^x of $\mathcal{O}$. The interaction is translation invariant if $\varphi^x(\Phi(X)) = \Phi(X + c)$, and a state ν is translationally invariant if $\nu \circ \varphi^x = \nu$. If ν is translationally invariant, its specific entropy

$$s(\nu) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} - \mathrm{tr}(\nu_\Lambda \log \nu_\Lambda),$$

$\nu_\Lambda = \nu \restriction \mathcal{O}_\Lambda$, exists by sub-additivity and takes values in $[0, \log \dim \mathfrak{h}]$.

We consider translationally invariant interaction Φ satisfying our regularity assumption. The pressure

$$P(\beta) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log \mathrm{tr}(\mathrm{e}^{-\beta H_\Lambda})$$

exists and is finite.

The specific energy observable is defined by

$$E = \sum_{0 \in X} \frac{1}{|X|} \Phi(X).$$

It is a self-adjoint element of $\mathcal{O}$ satisfying

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \left\| H_\Lambda - \sum_{x \in \Lambda} \varphi^x(E) \right\| = 0.$$

In particular, for any translationally invariant state ν,

$$\lim_{\Lambda\uparrow\mathbb{Z}^d} \frac{1}{|\Lambda|}\nu(H_\Lambda) = \nu(E).$$

Energy, pressure, and entropy are connected by the **cornerstone** of the equilibrium statistical mechanics: the **Gibbs variational principle**

$$P(\beta) = \sup_\nu \left(s(\nu) - \beta\nu(E)\right).$$

The set of maximizers is a non-empty convex compact subsets of the set of all states. The maximizers are *equilibrium states* or *phases* of interaction Φ at inverse temperature β.

Another fundamental result: the set of phases is precisely the set of translationally invariant β-KMS states! (Modular theory enters crucially here).

BEYOND SPIN SYSTEM

At this point, the setting can be abstracted. The C^*-dynamical system is a pair $(\mathcal{O}, \tau^t)$, where $\mathcal{O}$ is a unital C^*-algebra. The states and β-KMS states are defined as before. The triple $(\mathcal{O}, \tau, \omega)$, where ω is a β-KMS state is called a thermal system. The set of KMS-states is denoted $\mathcal{S}_\beta$.

The two basic questions of quantum equilibrium statistical mechanics are:

QI Describe properties of KMS-states and structure of the sets $\mathcal{S}_\beta$.

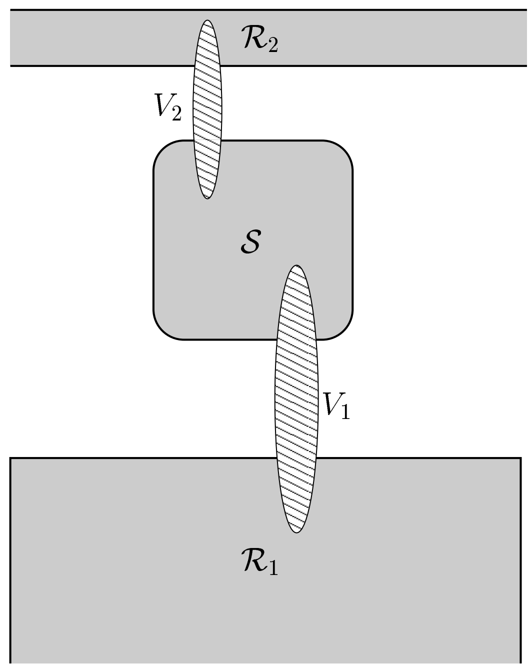
QII Elucidate dynamical and in particular ergodic properties of thermal quantum dynamical systems.

QI and **QII** have trivial answer in the finite setting: The set of phases is a singleton and no thermal system is ergodic. It is this triviality that forces consideration of infinitely extended systems from the outset in study of **QI** and **QII**.

From the general perspective, a great deal of progress has been made on **QI** and **QII** in 1970's. **The general link between KMS-condition and Tomita-Takesaki modular theory, which we yet have to describe, has played a central role in these developments.** From the perspective of concrete physically relevant quantum spin systems, the progress has been much slower and comparatively little is known on mathematically rigorous level.

NON-EQUILIBRIUM STAT MECH OF SPIN SYSTEMS

Back to Ruelle's 2001 open quantum lattice spin systems describing



with $G = G_{\mathcal{S}} \cup G_{\mathcal{R}_1} \cup G_{\mathcal{R}_2}$.

We take

$$\rho_\Lambda = \frac{1}{Z} \mathrm{e}^{-\beta_1 H_{\Lambda_1} - \beta_2 H_{\Lambda_2}}$$

and the corresponding local entropy production observable σ_Λ. The entropy production observable of the extended is system

$$\sigma = \lim_{\Lambda \uparrow G} \sigma_\Lambda = \sum_{j=1}^{2} \sum_{Y \subset \mathcal{R}_j} \sum_{X \cap \mathcal{S} \cap \mathcal{R}_j \neq \emptyset} -\mathrm{i}\beta_j [\Phi(Y), \Phi(X)].$$

The initial state of the extended system is any weak-limit point of the net ρ_Λ. Note that the extended system C^*-algebra has the structure

$$\mathcal{O} = \mathcal{O}_{\mathcal{S}} \otimes \mathcal{O}_{\mathcal{R}_1} \otimes \mathcal{O}_{\mathcal{R}_2},$$

where $\mathcal{O}_{\mathcal{S}} = \mathcal{B}(\mathcal{H}_{G_{\mathcal{S}}})$, and $\mathcal{O}_{\mathcal{R}_j}$ is the quantum spin system C^*-algebra over $G_{\mathcal{R}_j}$.

The individual dynamics τ_j^t of $\mathcal{R}_j$ is generated by the restricted interaction $\Phi_j = \Phi \restriction \mathfrak{G}_{\mathsf{fin},j}$ where $\mathfrak{G}_{\mathsf{fin},j}$ is the collection of all finite subsets of $G_{\mathcal{R}_j}$. Any weak-point of the net ρ_Λ has the form

$$\omega = \omega_{\mathcal{S}} \otimes \omega_{\mathcal{R}_1} \otimes \omega_{\mathcal{R}_2},$$

where $\omega_{\mathcal{R}_j}$ is β_j-KMS state of $(\mathcal{O}_{\mathcal{R}_j}, \tau_j^t)$.

Ruelle also introduced the key concept of Non-Equilibrium Steady States (NESS). They are weak-limit points of the net

$$\left\{ \frac{1}{T} \int_0^T \omega_t \mathrm{d}t \right\}_{T>0}$$

as $T \uparrow \infty$. The set of NESS is non-empty and any NESS is stationary.

The NESS are non-trivial only for extended quantum spin systems.

The key result of Ruelle is that for any NESS ω_+,

$$\omega_+(\sigma) \geq 0.$$

The argument goes by proving directly (without using relative entropy but repeating the argument that leads to its non-negativity) that

$$\mathrm{Ep}_\Lambda(t) = \int_0^t \mathrm{tr}(\rho_\Lambda \mathrm{e}^{\mathrm{i}sH_\Lambda} \sigma_\Lambda \mathrm{e}^{-\mathrm{i}sH_\Lambda}) \mathrm{d}s \geq 0,$$

which yields the results by taking the first the limit $\Lambda \uparrow G$ and then $T \uparrow \infty$ along suitable subnets.

Ruelle also develops the structural theory of NESS. He does not make use of modular theory.

In the same year 2001, J-Pillet have developed the non-equilibrium statistical mechanics in the general C^*-algebraic setting beyond quantum spin systems. They rely heavily on the modular theory. The original 2001 setting is the following.

Let $(\mathcal{O}, \tau, \omega)$ be a C^*-quantum dynamical system whose reference state ω is not τ-invariant. The NESS of $(\mathcal{O}, \tau, \omega)$ are the limit points of the net

$$\left\{\frac{1}{T}\int_0^T \omega \circ \tau^t \mathrm{d}t\right\}_{T>0}$$

as $T \uparrow \infty$. The set $\mathcal{S}_+(\omega)$ of NESS is non-empty and its elements are stationary.

To introduce entropy production observable, one assumes that ω is (-1)-KMS state for some C^*-dynamics ς_ω^t (such states and dynamics are called modular). Let δ_ω be the generator ς_ω, $\varsigma_\omega^t = \mathrm{e}^{t\delta_\omega}$. We further assume that the generator δ of τ^t has the form

$$\delta = \delta_{\mathsf{fr}} + \mathrm{i}[V, \cdot\,]$$

where V is a self-adjoint element of $\mathcal{O}$ and δ_{fr} generates a "free" C^*-dynamics τ_{fr}^t such that $\omega \circ \tau_{\mathsf{fr}}^t = \omega$.

If $V \in \mathsf{Dom}(\delta_\omega)$, the entropy production observable of LP system is defined by

$$\sigma := \delta_\omega(V).$$

The starting point of the 2001 JP theory is the entropy balance equation

$$S(\omega_t|\omega) = \int_0^t \omega_s(\sigma)\mathrm{d}s \tag{2}$$

where $S(\cdot|\cdot)$ is the Araki's relative entropy of two states on $\mathcal{O}$. The proof relies heavily on the modular theory. This cannot be proven by ”naive” thermodynamic limit arguments since the entropy map is not continuous (it is lower-semicontinuous).

The sign of relative entropy then gives that

$$\omega_+(\sigma) \geq 0$$

for any NESS $\omega_+ \in \mathcal{S}_+$.

The Ruelle's results are deduced by restricting to open quantum spin system setting. We already have defined V,

$$\tau_{\mathrm{fr}}^t = \tau_{\mathcal{S}}^t \otimes \tau_1^t \otimes \tau_2^t.$$

and

$$\delta_\omega = -\beta_1\delta_1 - \beta_2\delta_2.$$

The thermodynamic limit $\Lambda \uparrow G$ leading connecting the finite-dimensional entropy balance equation to (2) is essential for physical foundation of the extended systems theory (but can be proven only once we have the limiting balance equation established separately!)

JP obviously applies to abstract open quantum systems.

A more general approach to JP theory is based on Araki-Connes cocycles (recall finite setting) and will be described latter.

The above discussion leads to the two basic questions of non-equilibrium quantum statistical mechanics:

> **QIII** Describe properties of NESS and structure of the set $\mathcal{S}_+$.

> **QIV** Elucidate the dynamical mechanisms that ensure the strict positivity $\omega_+(\sigma) > 0$ of the entropy production of NESS ω_+ and apply them to concrete physically relevant models.

Much work has ben done since 2001 with theory going far beyond the basic questions **QIII** and **QIV** and the entropy production observable. The emerging non-equilibrium theory exhibits richness far beyond its equilibrium counterpart (and the classical non-equilibrium counterpart).

We have described some of these developments in the finite dimensional setting, emphasizing the fundamental role the modular role plays.

To proceed, one needs to have the the full description of modular theory!

FULL DESCRIPTION OF MODULAR THEORY
sketch of a sketch

$\mathfrak{M}$ von Neumann algebra on a Hilbert space $\mathcal{H}$. $\mathfrak{M} \subset \mathcal{B}(\mathcal{H})$ and $\mathfrak{M} = \mathfrak{M}''$.

$\Omega \in \mathcal{H}$ reference unit vector. Cyclic ($\overline{\mathfrak{M}\Omega} = \mathcal{H}$) and separating $\overline{\mathfrak{M}'\Omega} = \mathcal{H}$ for $\mathfrak{M}$. Reference state

$$\rho_0(A) = \langle \Omega, A\Omega \rangle.$$

ρ_0-normal states = states represented by density matrices on $\mathcal{H}$. $\mathcal{N}_{\rho_0}$.

The map

$$SA\Omega = A^*\Omega, \qquad A \in \mathfrak{M},$$

extends to a closed antilinear operator on $\mathcal{H}$ with polar decomposition

$$S = J\Delta^{\frac{1}{2}}$$

where $\Delta \geq 0$ and J is antilinear involution.

Δ-modular operator of ρ_0/Ω. J is the modular conjugation. Basic facts:

(1) $J\mathfrak{M}J = \mathfrak{M}'$.

(2) Natural cone $\mathcal{P}$: Closure of $\{AJAJ\Omega \,|\, A \in \mathfrak{M}\}$.

(3) For any normal $\rho \in \mathcal{N}_{\rho_0}$ there exists unique $\Omega_\rho \in \mathcal{P}$ such that

$$\rho(A) = \langle \Omega_\rho, A\Omega_\rho \rangle.$$

Ω_ρ is cyclic iff it is separating.

(4)

$$\|\Omega_{\rho_1} - \Omega_{\rho_2}\|^2 \leq \|\rho_1 - \rho_2\| \leq \|\Omega_{\rho_1} - \Omega_{\rho_2}\| \|\Omega_{\rho_1} + \Omega_{\rho_2}\|.$$

(5) The map

$$SA\Omega_{\rho_1} = A^*\Omega_{\rho_2}, \qquad A \in \mathfrak{M}$$

extends to a anti-linear closed operator on $\mathcal{H}$ with polar decomposition

$$S = J\Delta^{\frac{1}{2}}_{\rho_2|\rho_1}.$$

$\Delta_{\rho_2|\rho_1}$ is the relative modular operator of the pair (ρ_1, ρ_2).
$\Delta_\rho = \Delta_{\rho|\rho}$ the modular operator of ρ.

(6) $\sigma_\rho^t = \Delta_\rho^{\mathrm{i}t} \cdot \Delta_\rho^{-\mathrm{i}t}$ preserves $\mathfrak{M}$. Modular dynamics

(7) ρ is (-1)-KMS state for its modular dynamics.

(8) Connes cocycle:

$$[D\rho_1 : D\rho_2]_\alpha = \Delta_{\rho_1|\rho_2}^{\mathrm{i}\alpha} \Delta_{\rho_2}^{-\mathrm{i}\alpha}$$

is a family of unitaries in $\mathfrak{M}$ satisfying

$$[D\rho_1 : D\rho_2]_\alpha [D\rho_2 : D\rho_3]_\alpha = [D\rho_1 : D\rho_3]_\alpha.$$

(9) Araki's relative entropy:

$$S(\nu_1|\nu_2) = \langle \Omega_{\nu_1} | \log \Delta_{\nu_1|\nu_2} \Omega_{\nu_1} \rangle.$$

(10) Renyi's relative entropy

$$S_\alpha(\nu_1|\nu_2) = \langle \Omega_{\nu_1}, \Delta_{\nu_1|\nu_2}^{-\alpha} \Omega_{\nu_1} \rangle.$$

(11) For any W^*-dynamics τ^t on $\mathfrak{M}$ there exists unique self-adjoint $\mathcal{L}$, called standard Liouvillean of τ^t, such that

$$\tau^t(A) = \mathrm{e}^{\mathrm{i}t\mathcal{L}} A \mathrm{e}^{\mathrm{i}t\mathcal{L}}, \qquad \mathrm{e}^{-\mathrm{i}t\mathcal{L}} \mathcal{P} \subset \mathcal{P}.$$

(11) Koopmanism: $\nu \circ \tau = \nu$ iff $\mathcal{L}\Omega_\nu = 0$. $(\mathfrak{M}, \tau, \nu)$ is ergodic, i.e.

$$\lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \nu(B^* \tau^t(A) B) \mathrm{d}t = \nu(B^* B) \nu(A)$$

iff 0 is a simple eigenvalue of $\mathcal{L}$.

(12) ν is a β-KMS state,

$$\nu(\tau^t(B)A) = \nu(A\tau^{t+\mathrm{i}\beta}(B)),$$

iff

$$\mathcal{L}_\nu = -\beta\mathcal{L}$$

where $\mathcal{L}_\nu$ is the standard Liouvillean of σ_ν.

(13) and much much more: $\mathcal{P}_\alpha$-cones, $0 \leq \alpha \leq 1/2$ (natural cone is $\alpha = 1/4$), non-commutative L^p-spaces, $p = 1/2\alpha \in [1, \infty)$, etc....**and we need all of it!**

EQUILIBRIUM STATISTICAL MECHANICS

Quantum spin systems on lattice $\mathbb{Z}^d$. Equivalence of:

(1) β-KMS condition

(2) Gibbs variational principle

(3) Araki-Gibbs condition (quantum analog of Dobrushin-Lanford-Ruelle theory, Araki theory of perturbation of KMS structure).

Modular theory (and Araki's perturbation theory of it) play a key role.

NON-EQUILIBRIUM STATISTICAL MECHANICS

More general starting point then JP 2001 – Araki-Connes cocycle.

One starts with quantum dynamical system $(\mathcal{O}, \tau^t, \rho)$.
$(\mathcal{H}_\rho, \pi_\rho, \Omega_\rho)$ – the GNS representation of $\mathcal{O}$ induced by ρ with Ω separating for $\mathfrak{M} = \pi(\mathcal{O})''$.
The dynamics and the states ρ_t extended to $\mathfrak{M}$.

One further assumes that

$$[D\rho_t : D\rho]_\alpha \in \pi(\mathcal{O}).$$

Chain rule:

$$[D\rho_{t+s} : D\rho]_\alpha = \tau^{-t}([D\rho_s : D\rho]_\alpha)[D\rho_t : D\rho]_\alpha.$$

Leads to:

$$\ell_{\rho_t|\rho} = \log \Delta_{\rho_t|\rho} - \log \Delta_\rho$$

$$\ell_{\rho_{t+s}|\rho} = \tau^{-t}(\ell_{\rho_s|\rho}) + \ell_{\rho_t|\rho}$$

$$c^t = \tau^t(\ell_{\omega_t|\omega}).$$

$$c^{t+s} = c^s + \tau^s(c^t)$$

$$\sigma = \frac{\mathrm{d}}{\mathrm{d}t} c^t \Big|_{t=0}$$

$$c^t = \int_0^t \sigma_s \mathrm{d}s$$

$$S(\rho_t|\rho) = \rho(c^t) = \int_0^t \rho(\sigma_s)\mathrm{d}s \geq 0$$

One continues with NESS and development of non-equilibrium qsm. Direct quantization of the classical theory.

Two-times measurement entropy production: spectral measure $\mathcal{Q}_t$ for $-\log \Delta_{\rho|\rho_{-t}}$ and Ω.

$$\int_{\mathbb{R}} s \mathrm{d}\mathcal{Q}_t(s)\mathrm{d}s = \int_0^t \rho(\sigma_s)\mathrm{d}s = S(\rho_t|\rho) \geq 0$$

$\mathfrak{r}(s) = -s$, $\bar{\mathcal{Q}}_t = \mathcal{Q}_t \circ \mathfrak{r}$,

$$\frac{\mathrm{d}\bar{\mathcal{Q}}_t}{\mathrm{d}\mathcal{Q}_t}(s) = \mathrm{e}^{-s}.$$

One then proceeds with structural study of the statistics of the family $\mathcal{Q}_t$ in view of applications to concrete models.

Ancilla state tomography: see

BBJPP Entropic fluctuations in statistical mechanics II. Quantum dynamical systems, preprint.

The structural theory of p-functionals $\mathcal{F}_t^{(p)}$ and associated quantum transfer operators relies heavily on Araki-Masuda theory of L^p-spaces, $p \in [1, \infty]$,

Araki-Masuda: Positive Cones and L^p-Spaces for von Neumann Algebras, 1982.

J-Pillet-Ogata: unpublished.

Regarding $\mathcal{F}_t^{(\infty)}$, the algebraic BMV conjecture is open!

ALGEBRAIC BMV CONJECTURE

The setting is:

Pair $(\mathfrak{M}, \Omega)$ on a Hilbert space $\mathcal{H}$. Dynamics

$$\tau^t(A) = \mathrm{e}^{\mathrm{i}tL} A \mathrm{e}^{-\mathrm{i}tL}$$

where L is the standard Liouvillean. The vector state

$$\rho(A) = \langle \Omega, A\Omega \rangle$$

is β-KMS.

$V \in \mathfrak{M}$ self-adjoint, perturbed dynamics

$$\tau_V^t(A) = \mathrm{e}^{\mathrm{i}t(L+V)} A \mathrm{e}^{-\mathrm{i}t(L+V)}$$

Perturbed β-KMS vector

$$\Omega_V = \mathrm{e}^{-\frac{\beta}{2}(L+V)}\Omega.$$

$$\rho_V(A) = \langle \Omega, A\Omega_V \rangle / \|\Omega_V\|^2$$

β-KMS state for τ_V.

The Pierls-Bogoluibov and Golden-Thompson inequality hold:

$$\mathrm{e}^{-\beta\langle\Omega, V\Omega\rangle/2} \leq \|\Omega_V\| \leq \|\mathrm{e}^{-\beta V/2}\Omega\|.$$

All these results are part of Araki's theory of perturbation of the KMS/modular structure.

Conjecture: There exists measure $\mathcal{Q}$ on $\mathbb{R}$ such that for $\alpha \in \mathbb{R}$,

$$\|\Omega_{\alpha V}\|^2 = \int_{\mathbb{R}} \mathrm{e}^{-\alpha s} \mathrm{d}\mathcal{Q}(s).$$

Finite systems:

$$\|\Omega_{\alpha V}\|^2 = \mathrm{tr}(\mathrm{e}^{-\beta(H+\alpha V)})/\mathrm{tr}(\mathrm{e}^{-\beta H}),$$

and we are in the BMV-Stahl setting.

Finite dimensional result implies the algebraic one in the thermodynamic limit setting. Is the algebraic one consequence of the modular theory?

NON-EQUILIBRIUM TAKE HOME MESSAGE (AGAIN)

To remember.

Finite t theory provides only the setting/language.

The non-equilibrium structure emerges only in the limit $t \to \infty$!

Equilibrium parallel: Phase transitions via Gibbs variational principle and thermodynamic limit.

TOPICS NOT DISCUSSED

(1) Weak coupling limit in open quantum systems (Davies 1974, Lebowitz-Spohn 1978, J-Pillet-Westrich 2014)

(2) TTM entropy production and hypothesis testing of arrow time. Foundational topic shared by the classical theory.

J-Ogata-Pillet-Seiringer: Hypothesis testing and non-equilibrium statistical mechanics.

(3) Stability of TTM entropy production wrt initial state, full Fluctuation Theorems via resonances of quantum transfer operators: recent BBJPP series.

(4) Adiabatic (time-dependent) thermodynamics of open quantum systems. Realization of quasi-static processes in qsm. Related discussion of the Landauer principle: the energy cost of erasing quantum bit of information by action of a thermal reservoir at temperature T is $\geq kT \log 2$ with the equality for quasi-static processes.

J- Pillet C-A: A note on the Landauer principle in quantum statistical mechanics, 2014.

Benoist-Fraas-J-Pillet C-A: Full statistics of erasure processes: Isothermal adiabatic theory and a statistical Landauer principle, 2017

Benoist-Fraas-J-Pillet C-A: Adiabatic theorem in quantum statistical mechanics, in preparation

Related works: Abou Salem – Frohlich.

(5) Non-equilibrium statistical mechanics of repeated quantum measurement processes.

Benoist-J-Pautrat-Pillet: On entropy production of repeated quantum measurements I. General theory, 2018.

Cuneo- Benoist-J- Pillet: On entropy production of repeated quantum measurements II. Examples, 2021

(6) Work in progress on following topics:

Ruelle's mutual information in open quantum systems, parameter estimation, role of Fisher entropy, entropic/information geometry...

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