Modular Theory: How and Why

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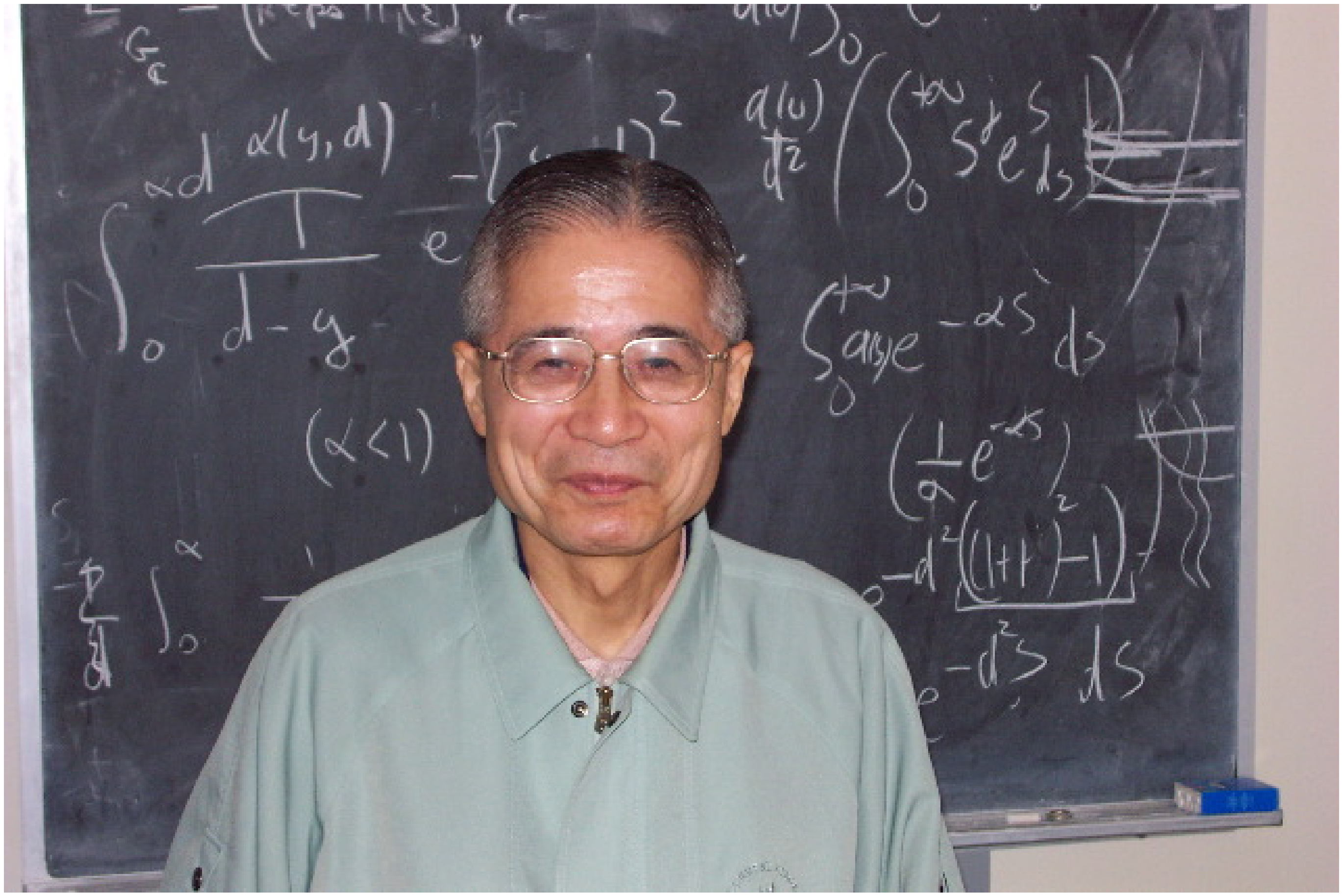
Dedicated to the memory of Huzihiro Araki 1932-2022

- Tomita's talk, 1967
- Haag-Hugenholtz-Winnink: On the equilibrium states in quantum statistical mechanics, CMP 1967.
- Takesaki book: Tomita's Theory of Modular Hilbert Algebras and Its Applications, 1970
- 70's - 80's Araki, Connes, Haagerup...



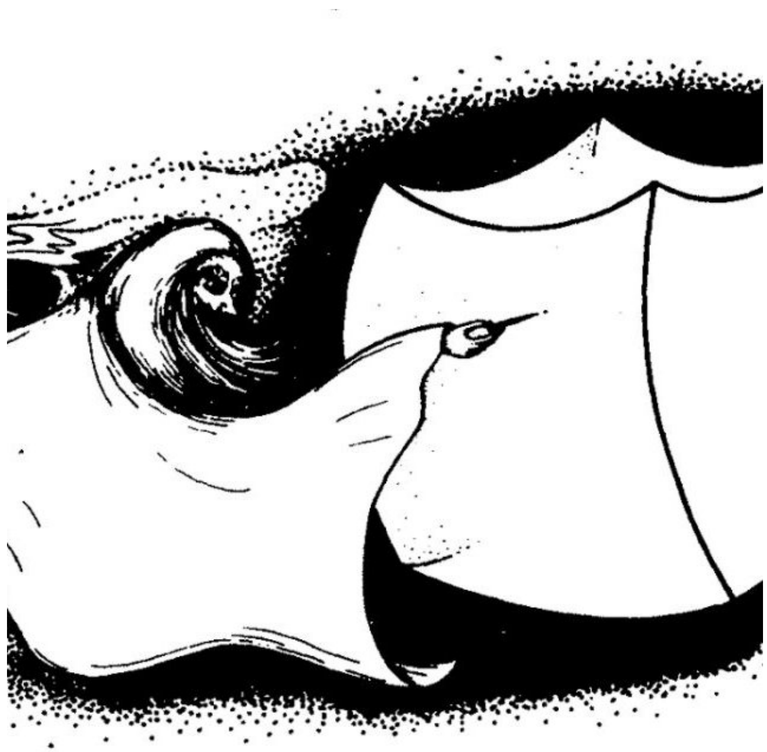
Huzihiro Araki 1932-2022

- 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.

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 $P = P_{\mathrm{u}}$, $P_{\mathrm{u}}(a) = 1/|\mathcal{A}|$.

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

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 $\frac{\mathrm{d}P}{\mathrm{d}Q}(a) = P(a)/Q(a)$,

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

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

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 $\mathcal{B}(\mathcal{O})$,

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

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

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

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

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

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

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

To any state ρ one associates $\Omega_\rho = \rho^{1/2} \in \mathcal{P}$:

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

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

$$J \Delta_\rho^{1/2} \pi(A) \Omega_\rho = \pi(A)^* \Omega_\rho.$$

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 $\rho = \mu$.

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

We have achieved our goal—the non-commutative Radon-Nikodym structure that allows to define directly relative entropies in the general setting.

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.

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:

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

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

Proof:

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

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

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

$B_t = \tau^t(B)$. 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 $\rho_t = \rho^{-\mathrm{i}tH}\rho\mathrm{e}^{\mathrm{i}tH}$.

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

Chain rule:

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

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

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

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

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

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

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 may have negative eigenvalues.

Entropy balance equation–genesis of the second law

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

If the system is time-reversal invariant with time reversal ϑ,

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

Eigenvalues of c^t are symmetric wrt 0!

Spectral decomposition

$$c_t = \sum sP_s$$

$$\rho(c_t) = \sum s\rho(P_s) \geq 0.$$

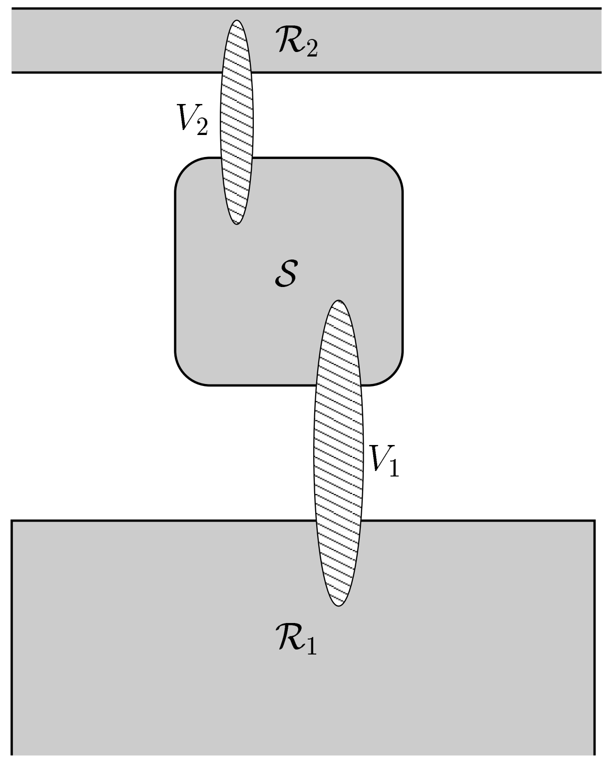
However, the fluctuation relation

$$\frac{\rho(P_{-s})}{\rho(P_s)} = \mathrm{e}^{-s}$$

fails. To restore it, we need new new players. But first an example.

OPEN QUANTUM SYSTEMS

Small Hamiltonian system S coupled to two thermal reservoirs.



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

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

$$H = H_0 + V.$$

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

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

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

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

Two-times measurement and modular theory

Two-times quantum measurement of the entropy observable $-\log\rho$.

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

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

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

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

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

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

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

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

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

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

The characteristic function is Renyi's relative entropy of the pair (ρ, ρ_{-t}). Observational status of the modular structure!

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

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

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

GENERAL SETTING

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

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

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 $\tau = \{\tau^t \mid t \in \mathbb{R}\}$ on $\mathfrak{M}$ there exists unique self-adjoint $\mathcal{L}$, called standard Liouvillean of τ, 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 (τ, 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 generator 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....

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).

NON-EQUILIBRIUM STATISTICAL MECHANICS

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:

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

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

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

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

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

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

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

Two-times measurement entropy production: spectral measure Q_t for $-\log \Delta_{\nu|\nu_{-t}}$ and Ω_ν.

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

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

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

IMPORTANT REMARK ABOUT NON-EQUILIBRIUM

Finite t theory provides only the setting.

The non-trivial results emerge only in the limit $t \to \infty$!

Equilibrium parallel: Phase transitions and thermodynamic limit.

REFERENCES

Recent works:

Benoist, Bruneau, J, Panati, Pillet: A note on two times measurement entropy production and modular theory, LMP (2024)

BBJPPb : On the thermodynamic limit of the two times measurement entropy production, submitted.

BBJPPc: Entropic fluctuations in statistical mechanics II. Quantum dynamical systems, in preparation.

BBJPPd: Entropic fluctuation theorems for Spin-Fermion model, in preparation.

For modular theory, classical monographs Bratelli-Robinson, Haag.

For quantum entropies: monograph of Ohya-Petz

Pedagogical introduction: J-Ogata-Pautrat-Pillet.: Entropic fluctuations in quantum statistical mechanics. An Introduction, 2010.

Classical non-equilibrium theory:

Reviews:

Ruelle: Smooth dynamics and new theoretical ideas in nonequilibrium statistical mechanics, 1999

J-Pillet-Rey-Bellet : Entropic fluctuations in statistical mechanics I. Classical dynamical system, 2011.