Some Remarks on Mathematical Theory of Non Equilibrium Quantum Statistical Mechanics

Vojkan Jaksic
McGill University

Venice 2022 - Quantissima in the Serenissima IV

Statistical mechanics away from equilibrium is in a formative stage, where general concepts slowly emerge.

David Ruelle (2008)

QUANTUM STATISTICAL MECHANICS

- Classical monographs (equilibrium theory):

  Ruelle: *Statistical Mechanics: Rigorous Results* (1969);
  Bratteli-Robinson: *Operator Algebras and Quantum Statistical Mechanics. I,II* (1979/81);
  Haag: *Local Quantum Physics* (1992);
  Israel: *Convexity in the Theory of Lattice Gases* (1979);
  Simon: *The Statistical Mechanics of Lattice Gases* (1993);
  Thirring: *Quantum Mathematical Physics: Atoms, Molecules and Large Systems* (1980);

These lectures deal with the second of two relatively ”recent” research directions in the theory of quantum dynamical systems.

- The problem of return to equilibrium (Robinson 1973); 1996–

- Development of non-equilibrium quantum statistical mechanics; 2001–

Reviews:

Ruelle: *Topics in quantum statistical mechanics and operator algebras* (2001);

J-Pillet: *Mathematical theory of non-equilibrium quantum statistical mechanics* (2002);

Pillet: *Quantum dynamical systems* (2006);

Aschbacher-J-Pautrat-Pillet: Introduction to non-equilibrium quantum statistical mechanics (2006);

J-Ogata-Pautrat-Pillet: *Entropic fluctuations in quantum statistical mechanics – an introduction* (2012).

Papers:

Ruelle: Natural nonequilibrium states in quantum statistical mechanics (2000);

Ruelle: Entropy production in quantum spin systems (2001);

J-Pillet: On entropy production in quantum statistical mechanics (2001);

Many others...

ROOTS

Quantum theory was much influenced by dynamical system approach to classical non-equilibrium statistical mechanics developed in 1990's (Chaotic hypothesis of Gallavotti-Cohen)

Reviews:

Ruelle: Smooth dynamics and new theoretical ideas in nonequilibrium statistical mechanics (1999);

Gallavotti: Thermostats and chaotic hypothesis (2006);

J-Pillet-Rey-Bellet: Entropic fluctuations in statistical mechanics I. Classical dynamical systems (2011);

ENTROPY PRODUCTION OBSERVABLE

Hilbert space $\mathcal{H}$, $\dim \mathcal{H} < \infty$. Hamiltonian H.

Observables: $\mathcal{O} = \mathcal{B}(\mathcal{H})$. $\langle A, B \rangle = \mathrm{tr}(A^* B)$.

State: density matrix $\rho > 0$. $\rho(A) = \mathrm{tr}(\rho A) = \langle A \rangle$.

Time-evolution:

$$\rho_t = \mathrm{e}^{-\mathrm{i}tH} \rho \mathrm{e}^{\mathrm{i}tH}$$

$$O_t = \mathrm{e}^{\mathrm{i}tH} O \mathrm{e}^{-\mathrm{i}tH}.$$

The expectation value of O at time t:

$$\langle O_t \rangle = \mathrm{tr}(\rho O_t) = \mathrm{tr}(\rho_t O) = \rho_t(A)$$

”Entropy observable” (information function):

$$S = -\log \rho.$$

Entropy:

$$S(\rho) = -\mathrm{tr}(\rho \log \rho) = \langle S \rangle.$$

Average entropy production over the time interval $[0, t]$:

$$\Delta\sigma(t) = \frac{1}{t}(S_t - S).$$

Entropy production observable

$$\sigma = \lim_{t \to 0} \Delta\sigma(t) = \mathrm{i}[H, S].$$

$$\Delta\sigma(t) = \frac{1}{t}\int_0^t \sigma_s \mathrm{d}s.$$

The entropy production observable = ”quantum phase space contraction rate”.

Radon-Nikodym derivative=relative modular operator

$$\Delta_{\rho_t|\rho}(A) = \rho_t A \rho^{-1}.$$

$\Delta_{\rho_t|\rho}$ is a self-adjoint operator on $\mathcal{O}$ and

$$\mathrm{tr}(\rho\Delta_{\rho_t|\rho}(A)) = \mathrm{tr}(\rho_t A)$$

$$
\begin{aligned}
\log \Delta_{\rho_t|\rho}(A) &= (\log \rho_t)A - A \log \rho \\
&= \log \Delta_{\rho|\rho}(A) + \left(\int_0^t \sigma_{-s} \mathrm{d}s \right) A.
\end{aligned}
$$

$$
\frac{\mathrm{d}}{\mathrm{d}t} \log \Delta_{\rho_t|\rho}(A) \Big|_{t=0} = \sigma A.
$$

BALANCE EQUATION

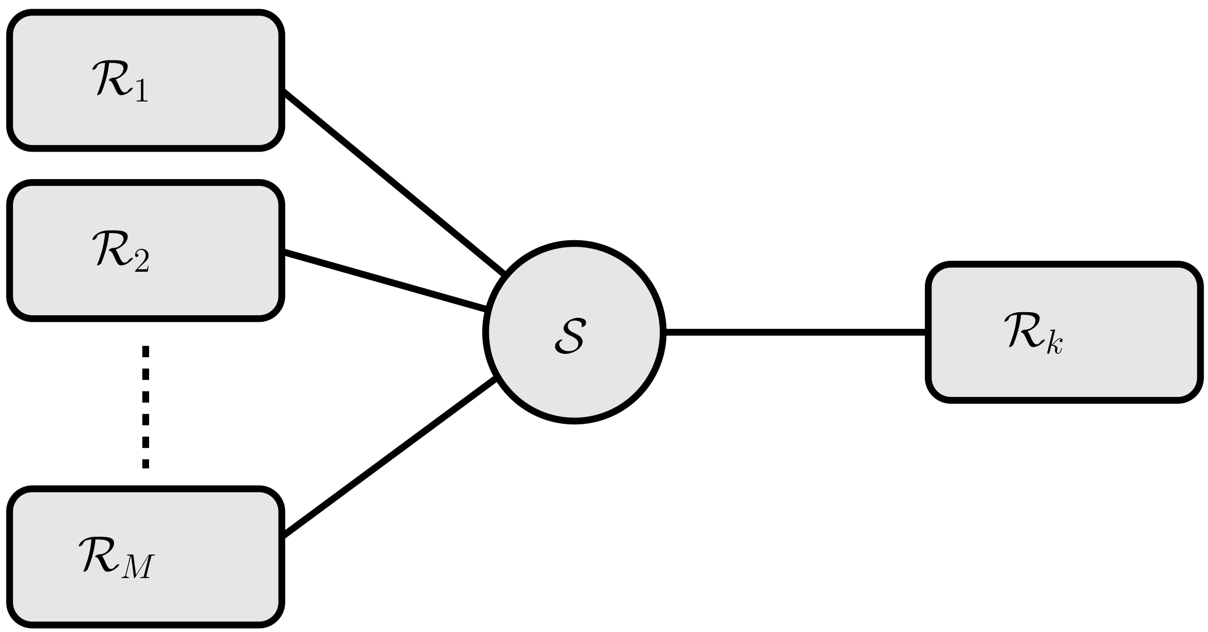
Relative entropy

$$S(\rho_t|\rho) = \mathrm{tr}(\rho_t(\log \rho_t - \log \rho))$$

$$= \langle \rho_t^{1/2}, \log \Delta_{\rho_t|\rho} \rho_t^{1/2} \rangle \geq 0.$$

$$\frac{1}{t} S(\rho_t|\rho) = \langle \Delta\sigma(t) \rangle = \frac{1}{t} \int_0^t \langle \sigma_s \rangle \mathrm{d}s.$$

OPEN QUANTUM SYSTEMS



$\mathcal{S} = \mathcal{R}_0$. Hilbert spaces $\mathcal{H}_k$, $k = 0, \cdots, M$. Hamiltonians H_k.

Initial states

$$\rho_k = \mathrm{e}^{-\beta_k H_k}/Z_k.$$

Composite system:

$$\mathcal{H} = \mathcal{H}_0 \otimes \cdots \otimes \mathcal{H}_M$$

$$\rho = \rho_0 \otimes \cdots \otimes \rho_M$$

$$H_{\mathrm{fr}} = \sum H_k,$$

$$H = H_{\mathrm{fr}} + V.$$

Energy change of $\mathcal{R}_k$ over the time interval $[0, t]$:

$$\Delta Q_k(t) = \frac{1}{t}(\mathrm{e}^{\mathrm{i}tH} H_k \mathrm{e}^{-\mathrm{i}tH} - H_k).$$

The energy flux observable

$$\Phi_k = \lim_{t \to 0} \Delta Q_k(t) = \mathrm{i}[H, H_k] = \mathrm{i}[V, H_k].$$

$$\Delta Q_k(t) = \frac{1}{t} \int_0^t \Phi_{ks} \mathrm{d}s.$$

The balance equation takes the familiar form:

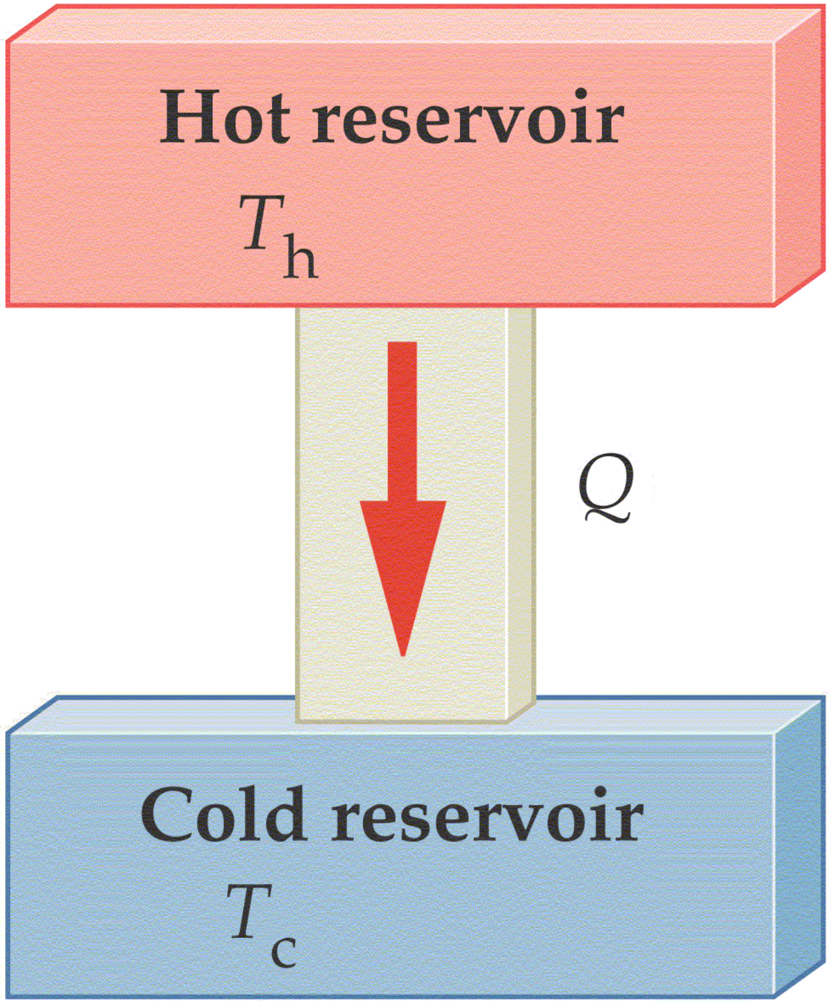
$$S = \sum \beta_k H_k + \text{const}$$

$$\Delta\sigma(t) = \sum \beta_k \Delta Q_k(t)$$

$$\sigma = \sum \beta_k \Phi_k$$

$$\langle \Delta\sigma(t) \rangle = \sum \beta_k \langle \Delta Q_k(t) \rangle \geq 0.$$

Heat flows from hot to cold.



Hot reservoir
T_h
Q
Cold reservoir
T_c

GOAL I

$$\langle \Delta\sigma(t)\rangle = \frac{1}{t}\int_0^t \langle \sigma_s\rangle \mathrm{d}s.$$

TD= Thermodynamic limit. Existence of the limit (steady state entropy production):

$$\langle \sigma\rangle_+ = \lim_{t\to\infty}\lim_{TD}\langle \Delta\sigma(t)\rangle$$

$\langle \sigma\rangle_+ \geq 0$. Strict positivity:

$$\langle \sigma\rangle_+ > 0.$$

GOAL II

More ambitious: non-equilibriium steady state (NESS). TD leads to C^* quantum dynamical system $(\mathcal{O}, \tau^t, \rho)$.

$$\rho_+(A) = \lim_{t\to\infty} \frac{1}{t}\int_0^t \rho(\tau^s(A))\mathrm{d}s.$$

$$\langle\sigma\rangle_+ = \rho_+(\sigma).$$

Structural theory:

$$\sigma_+ > 0 \quad \Leftrightarrow \quad \rho_+ \perp \rho.$$

THE REMARK OF RUELLE

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

The balance equation

$$\langle \Delta\sigma(t)\rangle = \sum \beta_k \langle \Delta Q_k(t)\rangle.$$

can (should?) be written differently.

$\mathcal{H}_{\setminus k} = \bigotimes_{j \neq k} \mathcal{H}_j$. State of the k-th subsystem at time t:

$$\rho_{kt} = \mathrm{tr}_{\mathcal{H}_{\setminus k}} \rho_t.$$

$$\Delta S_k(t) = \frac{1}{t}(S(\rho_{kt}) - S(\rho_k)).$$

$$\Delta \sigma_k(t)\rangle = \frac{1}{t} S(\rho_{kt} | \rho_k)$$

$$\Delta \widehat{S}(t) = \sum \Delta S_k(t)$$

$$\Delta \widehat{\sigma}(t) = \sum \Delta \sigma_k(t).$$

Obviously,

$$\Delta \widehat{\sigma}(t) \geq 0.$$

$\sum S(\rho_k) = S(\rho) = S(\rho_t)$ and by the sub-additivity:

$$\Delta \widehat{S}(t) \geq 0.$$

One easily verifies

$$\langle \Delta\sigma(t) \rangle = \Delta \widehat{S}(t) + \Delta\widehat{\sigma}(t).$$

Set

$$\mathrm{Ep}_+ = \lim_{t\to\infty} \lim_{TD} \Delta \widehat{S}(t)$$

$$\Delta\widehat{\sigma}_+ = \lim_{t\to\infty} \lim_{TD} \Delta\widehat{\sigma}(t).$$

OPEN PROBLEMS

Mathematical structure of the decomposition

$$\langle \sigma \rangle_+ = \mathrm{Ep}_+ + \Delta\widehat{\sigma}_+.$$

The existence of Ep_+ and $\Delta\widehat{\sigma}_+$ in concrete models (to be discussed latter).

When is $\Delta\widehat{\sigma}_+ = 0$? Ruelle: *Perhaps when the boundaries between the small system and the reservoirs are allowed to move to infinity. This limit is more of less imposed by physics, but seems hard to analyze mathematically.*
Another possibility: adiabatically switched interaction (quasi-static process)?

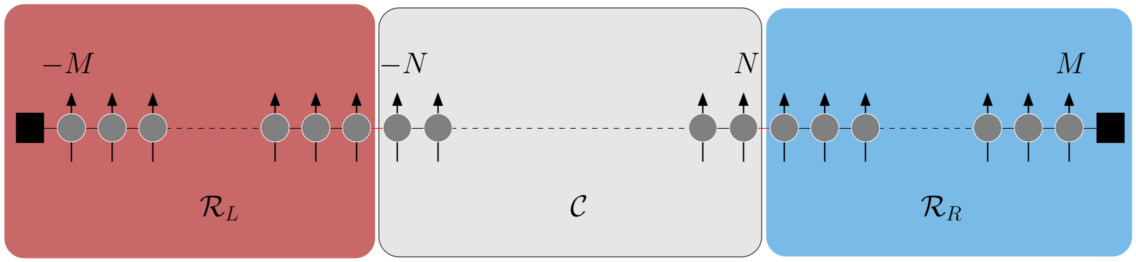
XY SPIN CHAIN

$\Lambda = [A, B] \subset \mathbb{Z}$, 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 $\mathcal{R}_{L/R}$: XY-chains on $\Lambda_L = [-M, -N-1]$ and $\Lambda_R = [N+1, M]$.

N fixed, thermodynamic limit $M \to \infty$.

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

The full Hamiltonian is

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

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

Initial state:

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

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

Fluxes and entropy production:

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

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

Araki-Ho, Ashbacher-Pillet $\sim$ 2000-2003

J-Landon-Pillet 2013: NESS exists and

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

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

Steady state heat fluxes:

$$\langle \Phi_L \rangle_+ + \langle \Phi_R \rangle_+ = 0$$

$$\langle \sigma \rangle_+ = \beta_L \langle \Phi_L \rangle_+ + \beta_R \langle \Phi_R \rangle_+.$$

$$\langle \Phi_L \rangle_+ = \frac{1}{4\pi} \int_{\mathbb{R}} |T(E)|^2 \frac{E \sinh(\Delta\beta E)}{\cosh \frac{\beta_L E}{2} \cosh \frac{\beta_R E}{2}} \mathrm{d}E.$$

Idea of the proof–Jordan-Wigner transformation.

$\mathcal{O}$ is transformed to the even part of $\mathrm{CAR}(\ell^2(\mathbb{Z}))$ generated by $\{a_x, a_x^* \,|\, x \in \mathbb{Z}\}$ acting on the fermionic Fock space $\mathcal{F}$ over $\ell^2(\mathbb{Z})$.

Transformed dynamics: generated by $\mathrm{d}\Gamma(h)$, where h is the Jacobi matrix

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

Φ_R (and similarly Φ_L, σ) is transformed to

$$\mathrm{i} J_N J_{N+1} (a_N^* a_{N+2} - a_{N+2}^* a_N)$$

$$\mathrm{i} J_N \lambda_{N+1} (a_N^* a_{N+1} - a_{N+1}^* a_N).$$

Decomposition

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

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

$$h = h_{\mathrm{fr}} + v_L + v_R,$$

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

The initial state ρ is transformed to the quasi-free state generated by

$$\frac{\mathbf{1}}{1+\mathrm{e}^{\beta_L h_L}} \oplus \frac{\mathbf{1}}{2N+1} \oplus \frac{\mathbf{1}}{1+\mathrm{e}^{\beta_R h_R}}.$$

The wave operators

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

exist and are complete.

The scattering matrix:

$$s = w_+^* w_- : \mathcal{H}_{\mathsf{ac}}(h_{\mathsf{fr}}) \to \mathcal{H}_{\mathsf{ac}}(h_{\mathsf{fr}})$$

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

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

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

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

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

$J_x = const$, $\lambda_x = const$ (or periodic)

$$|T| = \chi_{\sigma(h)}$$

Assumption:

h has no singular continuous spectrum

Open question: The existence and formulas for Ep_+ and $\Delta\widehat{\sigma}_+$.

Open question: NESS and entropy production if h has some singular continuous spectra. Transport in quasi-periodic structures.

HEISENBERG SPIN CHAIN

The Hamiltonian H of XY spin chain is changed to

$$H_P = H + P$$

where

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

The central part is now Heisenberg spin chain

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

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

Initial state remains the same. h is the old Jacobi matrix.

Fluxes and entropy production:

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

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

TD limit obvious. τ_P denotes the perturbed C^*-dynamics.

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

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

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

Theorem. Suppose that

$$\sup_{x\in[-N,N[} |K_x| < \bar{K}.$$

Then for all $A \in \mathcal{O}$,

$$\rho_+(A) = \lim_{t\to\infty} \rho(\tau_P^t(A))$$

exists.

Comments:

No time averaging. The constant $\bar{K}$ is essentially optimal. With change of the constant $\bar{K}$ the result holds for any P depending on finitely many $\sigma_x^{(3)}$:

$$P = \sum \prod K_{x_{i_1} \cdots x_{i_k}} \sigma_{x_{i_1}}^{(3)} \cdots \sigma_{x_{i_k}}^{(3)}.$$

The NESS ρ_+ is attractor in the sense that for any ρ-normal initial state ω,

$$\lim_{t \to \infty} \omega \circ \tau_P^t = \rho_+.$$

The map

$$(\{K_x\}, \beta_L, \beta_R) \mapsto \langle \sigma \rangle_+ = \rho_+(\sigma)$$

is real analytic. This leads to the strict positivity of entropy production.

Green-Kubo linear response formula holds for thermodynamical force $X = \beta_L - \beta_R$.

The above results are established in J-Pillet-Ogata (2007).

Bosonization Central Limit Theorem holds, J-Pautrat-Pillet (2009).

See also
Fröhlich-Merkli-Ueltschi: Dissipative transport: thermal contacts and tunnelling junctions (2003)

OPEN PROBLEM

The existence (and properties) of NESS

$$\rho_+(A) = \lim_{t\to\infty} \frac{1}{t}\int_0^t \rho(\tau_P^s(A))\mathrm{d}s$$

for all $\{K_x\} \in \mathbb{R}^{2N}$.

This is an open problem even if

$$P = K_0 a_0^* a_0 a_1^* a_1.$$

Dependence of $\langle\sigma\rangle_+$ on N?

Idea of the proof: Jordan-Wigner transformation: τ_P^t is generated by

$$\mathrm{d}\Gamma(h) + \frac{1}{2} \sum_{x \in [-N,N[} K_x (2a_x^* a_x - \mathbf{1})(2a_{x+1}^* a_{x+1} - \mathbf{1}).$$

One proves that

$$\gamma^+(A) = \lim_{t \to \infty} \tau^{-t} \circ \tau_P^t(A)$$

exists and is an $*$-automorphism of $\mathcal{O}$. The starting point is the Dyson expansion of $\tau^{-t} \circ \tau_P^t$. One then proceeds with careful combinatorial estimates of each term in the expansion (Botvich-Massen).

FINE FORM OF THE SECOND LAW

Finite dimensional setup. Time-reversal invariance.

Spectral resolution

$$\Delta\sigma(t) = \frac{1}{t}\int_0^t \sigma_s \mathrm{d}s = \sum \lambda P_\lambda.$$

Time-reversal implies

$$\dim P_\lambda = \dim P_{-\lambda}.$$

Entropy balance equation (the germ of the second law)

$$\frac{1}{t} S(\rho_t|\rho) = \langle \Delta\sigma(t) \rangle = \sum \lambda \mathrm{tr}(\rho P_\lambda) \geq 0.$$

Positive λ's are favoured. Heat flows from hot to cold.

BAD NEWS: Unlike in the classical case, the relation (fine form of the germ)

$$\frac{\mathrm{tr}(\rho P_{-\lambda})}{\mathrm{tr}(\rho P_{\lambda})} = \mathrm{e}^{-t\lambda}$$

FAILS.

Cummulant generating function:

$$\begin{aligned} e_{\mathrm{naive}}(\alpha) &= \log \mathrm{tr}(\rho \mathrm{e}^{-\alpha t \Delta\sigma(t)}) \\ &= \log \mathrm{tr}(\mathrm{e}^{-S} \mathrm{e}^{-\alpha(S_t - S)}). \end{aligned}$$

Equivalent form of bad news:

$$e_{\mathrm{naive}}(\alpha) = e_{\mathrm{naive}}(1-\alpha)$$

FAILS.

QUANTUM ENTROPIC FUNCTIONAL I

Kurchan, (Hal) Tasaki (2000), (Shuichi)Tasaki-Matsui (2003)

$$e_{\mathsf{fcs}}(\alpha) = \log \mathrm{tr}(\mathrm{e}^{-(1-\alpha)S} e^{-\alpha S_t}).$$

Renyi relative entropy:

$$e_{\mathsf{fcs}}(\alpha) = \log \mathrm{tr}(\rho_t^{1-\alpha} \rho^{\alpha}).$$

Time reversal invariance implies that the symmetry

$$e_{\mathsf{fcs}}(\alpha) = e_{\mathsf{fcs}}(1-\alpha)$$

HOLDS.

Tasaki-Matsui relative modular operator interpretation.

$\mathcal{O} = \mathcal{B}(\mathcal{H})$, $\langle A, B\rangle = \mathrm{tr}(A^*B)$. $\Omega_\rho = \rho^{1/2}$.

$$\Delta_{\rho_t|\rho}(A) = \rho_t A \rho^{-1}.$$

$$\begin{aligned} e_{\mathrm{fcs}}(\alpha) &= \log\langle \Omega_\rho, \Delta_{\rho_t|\rho}^{-\alpha}\Omega_\rho\rangle \\ &= \log \int_{\mathbb{R}} \mathrm{e}^{-\alpha t\varsigma}\mathrm{d}\mathbb{P}_t(\varsigma). \end{aligned}$$

Atomic probability measure $\mathbb{P}_t$ is the spectral measure for the operator

$$-\frac{1}{t}\log\Delta_{\rho_t|\rho}(A) = -\frac{1}{t}\log\Delta_{\rho|\rho}(A) - \Delta\sigma(t)A$$

and Ω_ρ.

$e_{\mathsf{fcs}}(\alpha) = e_{\mathsf{fcs}}(1-\alpha)$ is equivalent to

$$\frac{\mathbb{P}_t(-\varsigma)}{\mathbb{P}_t(\varsigma)} = \mathrm{e}^{-t\varsigma}.$$

Kurchan-Tasaki interpretation gives the physical meaning:

$e_{\mathrm{fcs}}(\alpha)$ is the cummulant generating function for the full counting statistics of the repeated quantum measurement of

$$S = -\log \rho = \sum sP_s$$

Measurement at $t = 0$ yields s with probability $\mathrm{tr}(\rho P_s)$.
State after the measurement:

$$\rho P_s / \mathrm{tr}(\rho P_s).$$

State at later time t:

$$\mathsf{e}^{-\mathsf{i}tH}\rho P_s \mathsf{e}^{\mathsf{i}tH}/\mathsf{tr}(\rho P_s).$$

Another measurement of S yields value s' with probability

$$\mathsf{tr}(P_{s'}\mathsf{e}^{-\mathsf{i}tH}\rho P_s \mathsf{e}^{\mathsf{i}tH})/\mathsf{tr}(\rho P_s).$$

The probability of measuring the pair (s, s') is

$$\mathsf{tr}(P_{s'}\mathsf{e}^{-\mathsf{i}tH}\rho P_s \mathsf{e}^{\mathsf{i}tH})$$

Probability distribution of the mean change of entropy

$$\varsigma = (s' - s)/t$$

is the spectral measure of Tasaki-Matsui:

$$\mathbb{P}_t(\varsigma) = \sum_{s'-s=t\varsigma} \mathrm{tr}(P_{s'} \mathrm{e}^{-\mathrm{i}tH} P_s \mathrm{e}^{\mathrm{i}tH}).$$

$e_{\mathrm{fcs}}(\alpha)$ is the cummulant generating function for $\mathbb{P}_t$. Note that

$$-\frac{1}{t} e'_{\mathrm{fcs}}(0) = \sum_{\varsigma} \varsigma \mathbb{P}_t(\varsigma) = \langle \Delta\sigma(t) \rangle.$$

QUANTUM ENTROPIC FUNCTIONAL II

J-Ogata-Pautrat-Pillet (2011).

$$\mathsf{e}_{\mathsf{var}}(\alpha) = \log \mathsf{tr}(\mathsf{e}^{-(1-\alpha)S-\alpha S_t}).$$

Time reversal implies

$$e_{\mathsf{var}}(\alpha) = e_{\mathsf{var}}(1-\alpha)$$

Variational characterization:

$$e_{\mathsf{var}}(\alpha) = -\inf_{\omega} \left(\alpha \mathsf{tr}(\omega(S_t - S)) + S(\rho|\omega)\right).$$

Golden-Thompson:

$$e_{\mathsf{var}}(\alpha) \leq e_{\mathsf{fcs}}(\alpha).$$

Herbert Stahl (2011): Bessis-Moussa-Villani conjecture.

There exist probability measure Q_t such that

$$e_{\mathsf{var}}(\alpha) = \log \int_{\mathbf{R}} \mathrm{e}^{-\alpha t \varsigma} \mathrm{d}Q_t(\varsigma).$$

$e_{\mathsf{var}}(\alpha) = e_{\mathsf{var}}(1-\alpha)$ implies

$$\frac{\mathrm{d}Q_t(-\varsigma)}{\mathrm{d}Q_t(\varsigma)} = \mathrm{e}^{-t\varsigma}.$$

Q_t is **not** an atomic measure.

Is this measure experimentally accessible (even in principle)?

Note that

$$-\frac{1}{t} e'_{\mathsf{var}}(0) = \sum_{\varsigma} \varsigma \mathbb{Q}_t(\varsigma) = \langle \Delta\sigma(t) \rangle.$$

ALGEBRAIC BMV CONJECTURE

$(\mathfrak{M}, \tau^t, \Omega)$ W^*-dynamical system on a Hilbert space $\mathcal{H}$. Ω is (τ, β)-KMS vector.

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

$V \in \mathfrak{M}$ selfadjoint, Ω_V the β- KMS vector for perturbed dynamics

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

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

The Pierls-Bogoluibov and Golden-Thompson inequality hold:

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

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

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

Finite systems:

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

REMARKS

- Mathematical structure of finite time theory deals directly with infinitely extended system within the framework of algebraic quantum statistical mechanics.

  Critical role: Modular theory of W^*-dynamical systems (Araki, Connes, Haagerup) and Araki-Masuda theory of non-commutative L^p-spaces (1982).

  Araki, H., Masuda, T. (1982). Positive cones and L^p-spaces for von Neumann algebras. Publ. RIMS, Kyoto Univ. **18**, 339–411.

- Benefit of unraveling the algebraic structure of entropic functionals: Quantum Ruelle transfer operators (J-Pillet (2011))

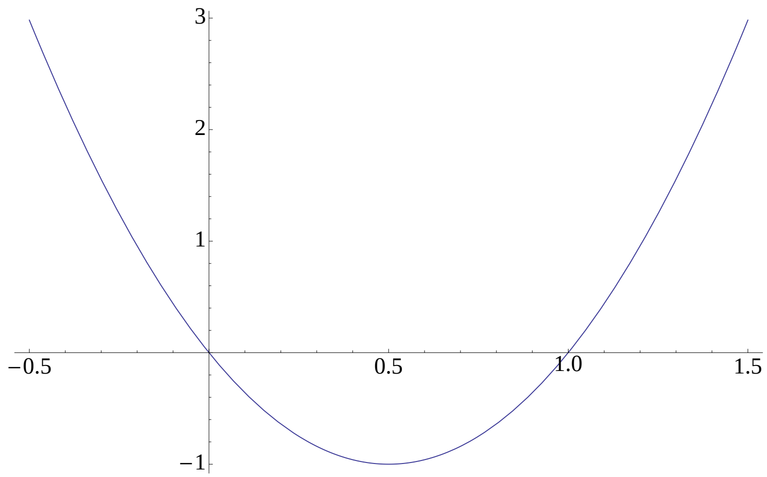
- Concrete models: Thermodynamic limit of the finite time finite volume structures.

- The existence and regularity of ($p =$ fcs, var)

$$e_{p+}(\alpha) = \lim_{t\to\infty} \frac{1}{t} e_{pt}(\alpha)$$

  is a difficult problem in physically interesting models.
  Link with quantum Ruelle resonances.

- Closed formulas in the XY-chain case (J-Landon-Pillet (2013))



$$e'_{p+}(0) = -\langle\sigma\rangle_+, \qquad e'_{p+}(1) = \langle\sigma\rangle_+$$

IMPLICATIONS

- $p =$ fcs, the large deviation principle and central limit theorem for the full counting statistics of entropy/energy/charge transport.
  Pioneering work: W. De Roeck (2009).

- $p =$ var. The large deviation principle and central limit theorem for the BMV Q_t. Quantum version of Gallavotti's linear response theory (generalized symmetries). The Green-Kubo formulas, Onsager reciprocity relations and the Fluctuation-Dissipation Theorem follow from those symmetries (alternative derivation: J-Ogata-Pillet (2006)).

- Many topics have not been discussed!

RECENT DEVELOPMENTS (ONE LOOSE END CLOSED)

- 2022 paper Benoist, Bruenau, J, Panati, Pillet.

- FCS $\Leftrightarrow$ ancilla quantum state trajectory tomography

- Novel observational status of FCS + novel class of quantum transfer operators.

- entropic quantum trajectory stability and Quantum Gallavotti-Cohen theory (entropic fluctuations wrt NESS)

- next week talk of Annalisa Panati!