Mathematical Theory of Non Equilibrium Quantum Statistical Mechanics

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Slides of the lectures and several review papers related to the lectures are posted at

http://www.math.mcgill.ca/jaksic/GOETTINGEN.html

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

David Ruelle (2008)

ENTROPY PRODUCTION OBSERVABLE

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

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

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

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

BALANCE EQUATION

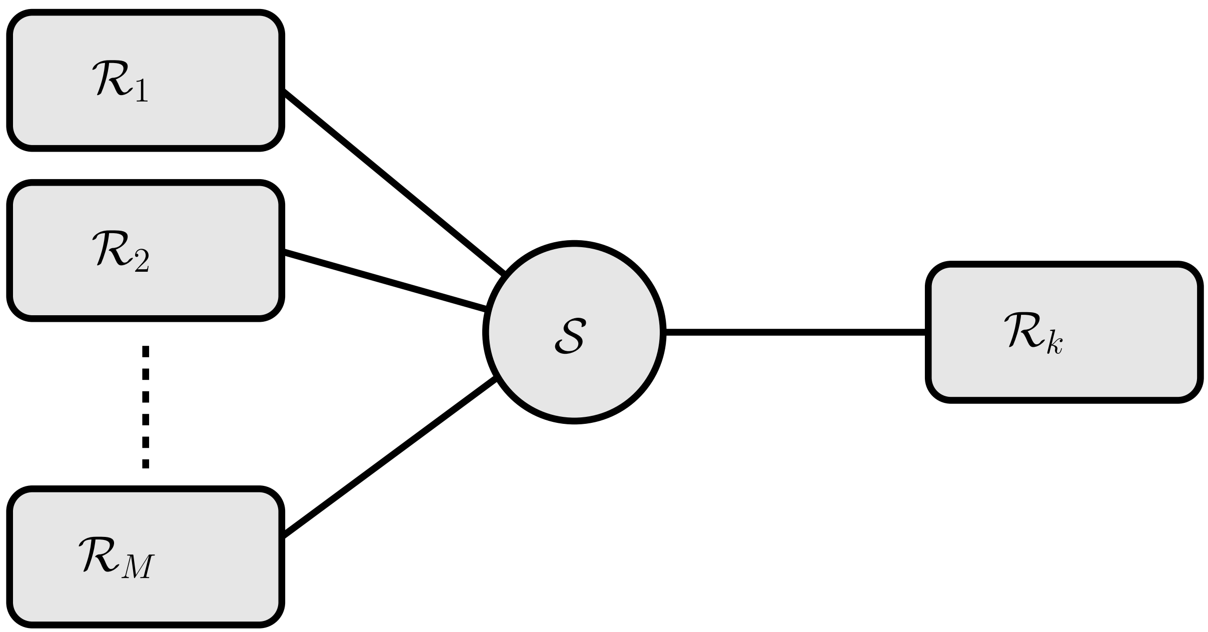
Relative entropy

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

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

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

OPEN QUANTUM SYSTEMS



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.

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

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

Clausius type decomposition.

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

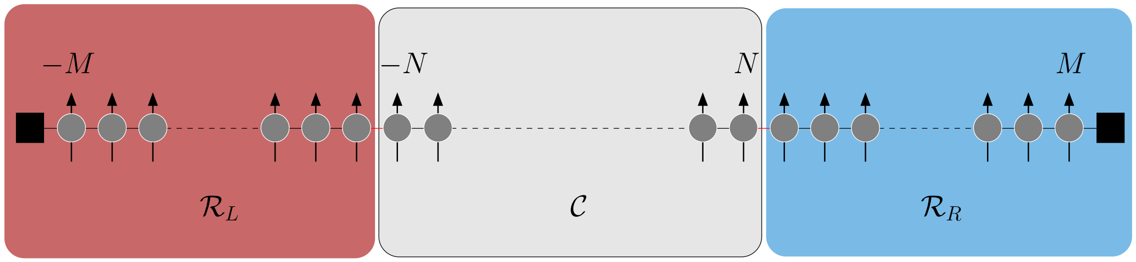
$\Lambda = [A, B] \subset \mathbb{Z}$, Hilbert space $\mathcal{H}_\Lambda = \bigotimes_{x\in\Lambda} \mathbb{C}^2$.

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 $H_{\text{fr}} = H_{\Lambda_L} + H_{\Lambda_\mathcal{C}} + H_{\Lambda_R}$.

The full Hamiltonian is

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

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

Initial state:

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

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

Fluxes and entropy production:

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

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

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

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

$\Delta\beta = \beta_L - \beta_R$. 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

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

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 $X = \beta_L - \beta_R$ (J-Pillet-Ogata)

Bosonization Central Limit Theorem holds (J-Pautrat-Pillet)

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).

The transport theory of non-equilibrium quantum statistical mechanics leads to an insight regarding two basic questions of spectral theory:

What is absolutely continuous spectrum?

What is localization?

WHAT IS AC SPECTRUM?

(1) Bruneau L., Jaksic V., Pillet C.-A.: Landauer-Bütttiker formula and Schrödinger conjecture, CMP 2013

(2) Jaksic V., Landon B., Panati A.: A note on reflectionless Jacobi matrices, CMP 2014

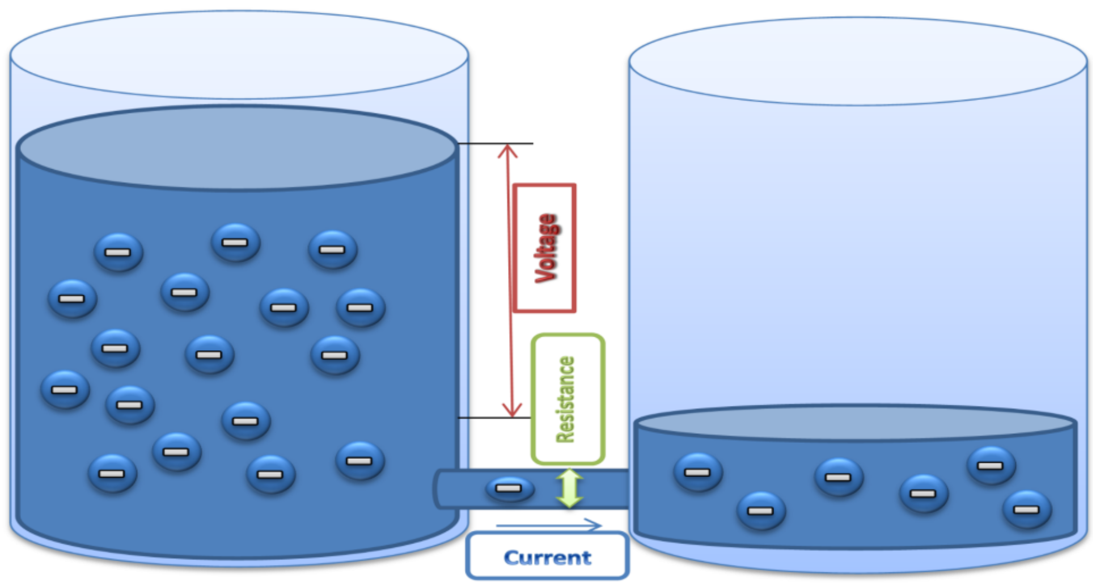
(3) Bruneau L., Jaksic V., Last Y., Pillet C.-A.: Landauer-Bütttiker and Thouless conductance, CMP 2015

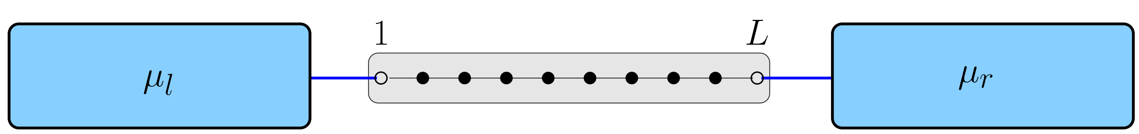
(4) Bruneau L., Jaksic V., Last Y., Pillet C-A.: Conductance and absolutely continuous spectrum of 1D samples, CMP 2016

(5) Bruneau L., Jaksic V., Last Y., Pillet C-A.: Crystaline conductance and absolutely continuous spectrum of 1D samples, LMP 2016

(6) Bruneau L., Jaksic V., Last Y., Pillet C-A.: What is AC spectrum? ICMP 2015.

PHYSICAL PICTURE





MATHEMATICAL MODEL

- Sample: $\mathcal{H}_L = \ell^2([1, L])$, $h_L = -\Delta + v$.

- Reservoirs: One electron data: $(\mathcal{H}_{l/r}, h_{l/r}, \psi_{l/r})$.
  $\mathcal{H}_{l/r} = L^2(\mathbb{R}, \mathrm{d}\nu_{l/r})$, $h_{l/r} = E$, $\psi_{l/r} = 1$.

- One electron reservoirs + sample system:

$$\mathcal{H} = \mathcal{H}_l \oplus \mathcal{H}_L \oplus \mathcal{H}_r, \qquad h_0 = h_l \oplus h_L \oplus h_r,$$

$$h = h_0 + v_T,$$

$$v_T = \lambda\Big(|\psi_l\rangle\langle\delta_1| + |\delta_1\rangle\langle\psi_l| + |\psi_r\rangle\langle\delta_L| + |\delta_L\rangle\langle\psi_r|\Big)$$

- Electron gas:
  Fock space $\Gamma_-(\mathcal{H})$, Hamiltonian $H = \mathrm{d}\Gamma(h)$,
  Algebra of observables $CAR(\mathcal{H})$, state ω_{μ_r,μ_l}.

- Charge current observable:

$$J = -\mathrm{i}[H, N_l], \qquad J_t = \mathrm{e}^{\mathrm{i}tH} J \mathrm{e}^{-\mathrm{i}tH}$$

- Steady state current:

$$\langle J \rangle = \lim_{T\to\infty} \frac{1}{T} \int_0^T \omega_{\mu_r,\mu_l}(J_t)\mathrm{d}t.$$

$$\langle J \rangle = \lim_{T\to\infty} \frac{1}{T} \left[\omega_{\mu_r,\mu_l}(N_l) - \omega_{\mu_r,\mu_l}(\mathrm{e}^{\mathrm{i}TH} N_l \mathrm{e}^{-\mathrm{i}TH}) \right].$$

LANDAUER-BÜTTIKER FORMULA

- $$\langle J \rangle = \int_{\mu_r}^{\mu_l} \mathcal{D}(L,E)\mathrm{d}E$$

- $$\mathcal{D}(L,E) = 2\pi\lambda^4 |\langle \delta_1, (h-E-\mathrm{i}0)^{-1}\delta_L\rangle|^2 \frac{\mathrm{d}\nu_{l,\mathrm{ac}}}{\mathrm{d}E}(E)\frac{\mathrm{d}\nu_{r,\mathrm{ac}}}{\mathrm{d}E}(E)$$

- Origin: Scattering theory of the one-particle pair (h, h_0).

  Aschbacher W., Jaksic V., Pautrat Y., Pillet C.-A.: J. Math. Phys., 48 (2007), 032101.
  Nenciu, G.: J. Math. Phys. 48, 033302 (2007).

THOULESS FORMULA

- Special case of the LB-formula. Crystaline reservoirs.
  $h = h_{L,\text{per}}$ on $\ell^2(\mathbb{Z})$.

- Reflectionless transport. $\mathcal{D}(L,E) = (2\pi)^{-1}$ for $E \in \text{sp}(h_{L,\text{per}})$, 0 otherwise.

- Thouless formula:
$$\langle \mathcal{T} \rangle = \frac{1}{2\pi} |\text{sp}(h_{L,\text{per}}) \cap (\mu_r, \mu_l)|.$$

-
$$\langle J \rangle \lesssim \langle \mathcal{T} \rangle$$

GOAL

- Extended sample: $h_S = -\Delta + v$ on $\ell^2(\mathbb{Z}_+)$.
  $\mathrm{sp}_{\mathrm{ac}}(h_S)$.
  $\Sigma_{\mathrm{ac}}(h_S)$: the essential support of the ac spectrum of h_S.

- Mathematical characterization of the conducting regime $\Leftrightarrow$ Physical characterization of the conducting regime.

- The energies in $\mathrm{sp}_{\mathrm{ac}}(h_S)$ and $\Sigma_{\mathrm{ac}}(h_S)$ should be precisely the energies at which the charge transport of the finite samples is non-vanishing in the limit $L \to \infty$.

LINEAR RESPONSE

- $\mu_r = E$, $\mu_l = E + \varepsilon$. Ohm's law

$$\langle J \rangle = \varepsilon \mathcal{D}(L, E) + o(1).$$

-

$$\mathfrak{T} = \{E \mid \liminf_{L \to \infty} \mathcal{D}(L, E) > 0\}.$$

- Bruneau, J., Pillet (2013): Conjecture

$$\Sigma_{\mathrm{ac}} = \mathfrak{T}$$

- $T(L,E)$–transfer matrix of $h_{\mathcal{S}}$,

$$T(L,E) = \begin{bmatrix} v(L) - E & -1 \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} v(1) - E & -1 \\ 1 & 0 \end{bmatrix}$$

- Bruneau, J., Pillet (2013): Result

$$\mathfrak{T} = \{E \mid \sup_L \|T(L,E)\| < \infty\}.$$

$\mathfrak{T} \subset \Sigma_{\mathrm{ac}}$.

- $\Sigma_{\mathrm{ac}} = \mathfrak{T}$ turns to the Schrödinger Conjecture.

COUNTEREXAMPLE

- A. Avila.: On the Kotani-Last and Schrödinger Conjectures, J. Amer. Math. Soc. 28 (2015), 579-616.

- The counterexample is in the ergodic setting: $|\Sigma_{\mathrm{ac}} \setminus \mathfrak{T}| > 0$ with probability one.

- In the ergodic setting, the Kotani theory gives (Bruneau, J.)

$$\Sigma_{\mathrm{ac}} = \{E \,|\, \limsup_{L\to\infty} \mathcal{D}(L,E) > 0\}$$

and (Deift-Simon)

$$\Sigma_{\mathrm{ac}} = \left\{E \,|\, \limsup_{L\to\infty} \frac{1}{L} \sum_{\ell=1}^{L} \|T(\ell,E)\|^2 < \infty \right\}.$$

THEOREM

$\langle J \rangle = \langle J \rangle_{L,\mu_r,\mu_l}$, $\langle \mathfrak{T} \rangle = \langle \mathfrak{T} \rangle_{L,\mu_r,\mu_l}$.

The following statements are equivalent.

(A) $\mathrm{sp}_{\mathrm{ac}}(h_S) \cap (\mu_r, \mu_l) = \emptyset$.

(B) $\lim_{L\to\infty} \langle J \rangle_{L,\mu_r,\mu_l} = 0$.

(C) $\lim_{L\to\infty} \langle \mathfrak{T} \rangle_{L,\mu_r,\mu_l} = 0$.

Moreover, if $\mathrm{sp}_{\mathrm{ac}}(h_S) \cap (\mu_r, \mu_l) \neq \emptyset$, then

$$\liminf_{L\to\infty} \langle J \rangle_{L,\mu_r,\mu_l} > 0, \qquad \liminf_{L\to\infty} \langle \mathfrak{T} \rangle_{L,\mu_r,\mu_l} > 0.$$

PERSPECTIVES

- The role of reflectionless

- Kotani and Remling theory

- Many body theory

IDEAS OF THE PROOF

- Key Lemma: $\mathrm{sp}_{\mathrm{ac}}(h_{\mathcal{S}}) \cap (\mu_r, \mu_l) = \emptyset$ iff

$$\lim_{L\to\infty} \int_{\mu_r}^{\mu_l} \|T(L,E)\|^{-2} \mathrm{d}E = 0. \tag{1}$$

- The proof proceeds by showing that the statements (B) and (C) are equivalent to (1).

- Proof of the Lemma: The key ingredient is the result of Carmona, Krutikov-Remling, Simon: If ν_D is the spectral measure for h_S and δ_1 with D. b.c. and $u = (1,0)^T$, then

$$\frac{1}{\pi}\|T(L,E)u\|^{-2}\mathrm{d}E \to \mathrm{d}\nu_D(E).$$

- Given the Lemma, the proof of $(A) \Leftrightarrow (B)$ follows from the Last-Simon result: given a sequence $L_k \to \infty$,

$$\Sigma_{\text{ac}} \subset \{E \mid \liminf_{k\to\infty} \|T(L_k, E)\| < \infty\},$$

and Bruneau-J-Pillet result:

$$\{E \mid \lim_{k\to\infty} \mathcal{D}(L_k, E) = 0\} = \{E \mid \lim_{k\to\infty} \|T(L_k, E)\| = \infty\}.$$

- In the ergodic setting the equivalence $(A) \Leftrightarrow (C)$ was proven in Yoram Last 1994 PhD thesis.

- One of the key ingredients of Last's proof was the estimate:

$$\limsup_{L\to\infty} |\mathrm{sp}_{\mathrm{ac}}(h_{L,\mathrm{per}}) \cap (\mu_r, \mu_l)| \leq |\mathrm{sp}_{\mathrm{ac}}(h_S) \cap (\mu_r, \mu_l)|$$

that holds with probability one. Proof: the Kotani theory.

- Although motivated by the implication $(C) \Rightarrow (A)$ and the study of the Thouless conductance, (2) is stronger than one needs for this purpose.

- Independent of its motivation, the above relation was shown to have important consequences for the spectral theory of quasi-periodic operators:
Last, Y.: A relation between a.c. spectrum of ergodic Jacobi matrices and the spectra of periodic approximants. Commun. Math. Phys. **151**, 183–192 (1993).

- Gestezsy-Simon extended Last's result to deterministic full line operators. Their argument does not work for the half line operators.

- For the half-line case we prove

$$\limsup_{L\to\infty} |\mathrm{sp}_{\mathrm{ac}}(h_{\mathrm{per},L})\cap(\mu_r,\mu_l)| \leq C|\mathrm{sp}_{\mathrm{ac}}(h_S)\cap(\mu_r,\mu_l)|^{\frac{1}{5}},$$

where $C = 5\left(\frac{\pi^2(1+\pi)^4}{4}\right)^{1/5} \simeq 18.7$; That suffices for $(C) \Rightarrow (A)$.

- Back to the electron gas picture:
  Fock space $\Gamma_-(\mathcal{H})$
  Algebra of observables $CAR(\mathcal{H})$
  State ω_{μ_r,μ_l}.
  Interaction

$$V = \sum_{x,y\in[1,L],|x-y|=1} a_x^* a_y^* a_y a_x$$

  Hamiltonian: $H = \mathrm{d}\Gamma(h) + V$.
  Current observable:

$$J = -\mathrm{i}[H, N_l], \qquad J_t = \mathrm{e}^{\mathrm{i}tH} J \mathrm{e}^{-\mathrm{i}tH}.$$

- Def: Localization regime on (μ_r, μ_l):

$$\langle J \rangle_+ = \limsup_{L\to\infty} \limsup_{T\to\infty} \frac{1}{T} \int_0^T \omega_{\mu_r,\mu_l}(J_t) \mathrm{d}t = 0.$$

- Def: Conducting regime on (μ_r, μ_l):

$$\langle J \rangle_- = \liminf_{L\to\infty} \liminf_{t\to\infty} \frac{1}{T} \int_0^T \omega_{\mu_r,\mu_l}(J_t) \mathrm{d}t > 0.$$

- $V = 0$: equivalent to absence/presence of ac spectrum on (μ_r, μ_l).

PROBLEM: 1D MANY BODY LOCALIZATION

Suppose that $\{v(x)\}_{x \in \mathbb{Z}_+}$ are i.i.d. random variables (with density). Is it true for all μ_r and μ_l,

$$\langle J \rangle_+ = 0.$$

One can go further (with definitions and conjectures): Linear response theory, many body Lyapunov exponent, many body Kotani theory, any D, ...

But no results (proofs) worth mentioning...

STEP 0

Replace the interaction V with

$$\widehat{V} = a_1^* a_2^* a_2 a_1.$$

Prove that in this ”trivial” case

$$\langle J \rangle_+ = 0.$$

Completely open.

ENTROPIC FLUCTUATIONS

- J., Ogata, Pautrat, Pillet:
  ”Entropic fluctuations in non-equlibrium quantum statistical mechanics. An Introduction.”
  In Quantum Theory from Small to Large Scales, Les Houches Proceeding (2012)

- J., Pillet, Rey-Bellet:
  ”Entropic Fluctuations in Statistical Mechanics I. Classical Dynamical Systems.” Nonlinearity (2011)

NAIVE FLUCTUATION RELATION FAILS

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

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

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

BAD NEWS: The fluctuation relation

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

FAILS.

Cummulant generating function:

$$e_{\text{naive}}(\alpha) = \log \mathrm{tr}(\rho \mathrm{e}^{-\alpha t \Delta\sigma(t)})$$

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

Equivalent form of bad news:

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

FAILS.

QUANTUM ENTROPIC FUNCTIONAL I

Kurchan (2000), 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.

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

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

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

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.

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

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

Kurchan interpretation gives the physical meaning:

$e_{\text{fcs}}(\alpha)$ is the cummulant generating function for the full counting statistics (Levitov-Lesovik) of the repeated quantum measurement of $S = -\log \rho$.

$$S = \sum sP_s$$

Measurement at $t = 0$ yields s with probability $\mathtt{tr}(\rho P_s)$.

State after the measurement:

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

State at later time t:

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

Another measurement of S yields value s' with probability

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

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

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

Probability distribution of the mean change of entropy

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

is the spectral measure of Tasaki-Matsui:

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

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

QUANTUM ENTROPIC FUNCTIONAL II

J-Ogata-Pautrat-Pillet.

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

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

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

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:

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

INTERPOLATING FUNCTIONALS

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

$$e_p(\alpha) = \log \operatorname{tr} \left(\mathrm{e}^{-\frac{1-\alpha}{p} S} \mathrm{e}^{-\frac{2\alpha}{p} S_t} \mathrm{e}^{-\frac{1-\alpha}{p} S} \right)^{p/2}$$

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

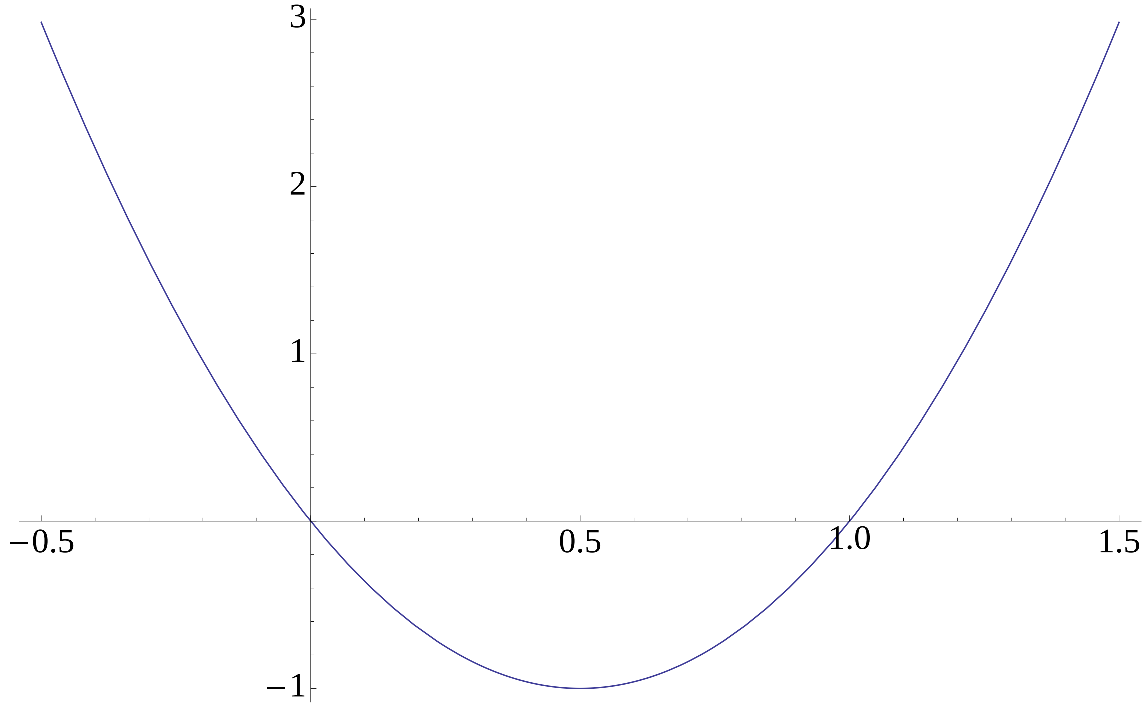
- $e_2(\alpha) = e_{\mathrm{fcs}}(\alpha)$.
- $e_\infty(\alpha) = \lim_{p\to\infty} e_p(\alpha) = e_{\mathrm{var}}(\alpha)$.
- $e_p(\alpha) = e_p(1-\alpha)$

- $e_p(0) = e_p(1) = 0$.

- $\alpha \mapsto e_p(\alpha)$ is convex.

- $e_p'(0) = -S(\rho_t|\rho)$, $e_p'(1) = S(\rho_t|\rho)$.

- $[1, \infty] \ni p \mapsto e_p(\alpha)$ is decreasing (strictly): (Araki)-Lieb-Thirring.


3
2
1
−1
−0.5
0.5
1.0
1.5

- Interpolating functionals motivated recent works in quantum information: M.R. Audenaert, N. Datta: α-z-relative Renyi entropies.
  For $\nu, \zeta > 0$, set

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

  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.

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

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

$$U_p(t)A = A_{-t}\mathrm{e}^{\frac{1}{p}S_{-t}}\mathrm{e}^{-\frac{1}{p}S}.$$

Properties:

$$U_p(t_1 + t_2) = U_p(t_1)U_p(t_2)$$

$$U_p(-t)AU_p(t) = A_t$$

$$\|U_p(t)A\|_p = \|A\|_p.$$

Crucial property:

$$e_p(\alpha) = \log \|U_{p/\alpha}(t)\mathbf{1}\|_p^p.$$

GOALS

- Mathematical structure of finite time theory that deals directly with infinitely extended system within the framework of algebraic quantum statistical mechanics. Modular theory of W^*-dynamical systems (Araki, Connes, Haagerup).

  Critical role: Araki-Masuda theory of non-commutative L^p-spaces.

  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.

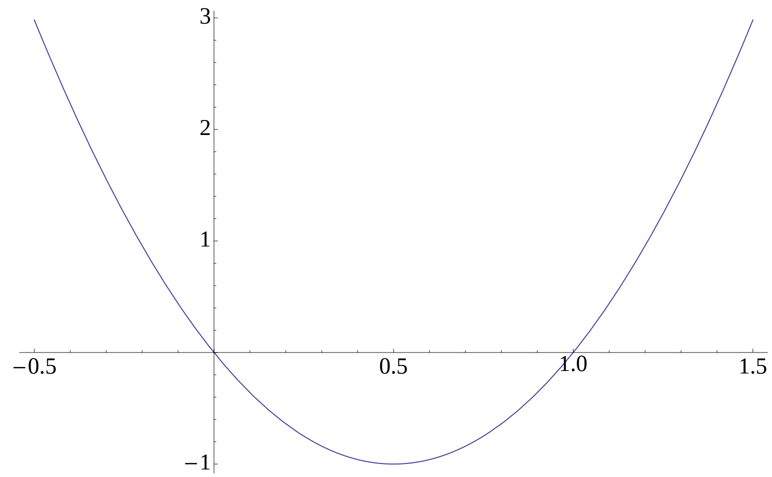
- Concrete models: Thermodynamic limit of the finite time finite volume structures.

- The existence and regularity of

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

  Difficult problem in physically interesting models. Link with quantum Ruelle resonances.

$e_{p+}(\alpha)$ inherits all the listed properties of $e_{pt}(\alpha)$.



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

- Implications. $p = 2$, the large deviation principle and central limit theorem for the full counting statistics of entropy/energy/charge transport. The symmetry $\alpha \to 1 - \alpha$ in the linear regime (small α, linear response) yields the Green-Kubo formulas and Onsager reciprocity relations energy and charge fluxes. The Fluctuation-Dissipation Theorem follows.

- $p = \infty$. The large deviation principle and central limit theorem for the BMV Q_t. Quantum version of Gallavotti's linear response theory.

BACK TO XY CHAIN

Two additional functionals:

(I) (Evans-Searles) Fluctuations with respect to the initial state:

$$C_t(\alpha) = \lim_{M\to\infty} \log \mathrm{tr}\left(\rho \mathrm{e}^{-\alpha \int_0^t \sigma_s \mathrm{d}s}\right).$$

(II) (Gallavotti-Cohen) Steady state fluctuations: $\rho_t = \mathrm{e}^{-\mathrm{i}tH}\rho\mathrm{e}^{\mathrm{i}tH}$.

$$C_{t+}(\alpha) = \lim_{T\to\infty} \lim_{M\to\infty} \log \mathrm{tr}\left(\rho_T \mathrm{e}^{-\alpha \int_0^t \sigma_s \mathrm{d}s}\right).$$

Naive quantizations of the classical entropic functionals.

After the TD limit

$$\begin{aligned} C_t(\alpha) &= \log \rho\left(\mathrm{e}^{-\alpha \int_0^t \sigma_s \mathrm{d}s}\right) \\ &= \log \int_{\mathbb{R}} \mathrm{e}^{-\alpha t \varsigma} \mathrm{d}P_t(\varsigma), \end{aligned}$$

$$\begin{aligned} C_{t+}(\alpha) &= \log \rho_+\left(\mathrm{e}^{-\alpha \int_0^t \sigma_s \mathrm{d}s}\right) \\ &= \log \int_{\mathbb{R}} \mathrm{e}^{-\alpha t \varsigma} \mathrm{d}P_{t+}(\varsigma). \end{aligned}$$

$P_{t/t+}$ is the spectral measure for ρ/ρ_+ and $\frac{1}{t}\int_0^t \sigma_s \mathrm{d}s$.

THEOREM

Assumption: Jacobi matrix h has purely ac spectrum.

(1)

$$C(\alpha) = \lim_{t\to\infty} \frac{1}{t} C_t(\alpha) = \lim_{t\to\infty} \frac{1}{t} C_{t+}(\alpha)$$

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

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

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

(2)

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

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

(3) The functionals $C(\alpha), e_{p+}(\alpha)$ are real-analytic and strictly convex.
$C(0) = e_{p+}(0) = 0$ and

$$C'(0) = e'_{p+}(0) = -\langle\sigma\rangle_+.$$

(4)

$$C''(0) = e''_2(0) = \frac{1}{2}\int_{-\infty}^{\infty} \Big\langle (\sigma_t - \langle\sigma\rangle_+)(\sigma - \langle\sigma\rangle_+)\Big\rangle_+ \mathrm{d}t.$$

(5) The function

$$[1,\infty] \ni p \mapsto e_{p+}(\alpha)$$

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 $e_{p+}(\alpha)$ does not depend on p and

$$e_{p+}(\alpha) = C(\alpha) =$$

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

Phenomenon: ”Entropic triviality.”

(6) If h is not reflectionless, $C(1) > 0$.

(7) The Central Limit Theorem and Large Deviation Principle hold for measures P_t, P_{t+}, $\mathbb{P}_t$, Q_t.

$P_{t/t_+} \to \delta_{\langle\sigma\rangle_+}, \mathbb{P}_t, Q_t \to \delta_{\langle\sigma\rangle_+}$. Gärtner-Ellis theorem.

$$P_t(B) \simeq P_{t+}(B) \simeq \mathrm{e}^{-t \inf_{\varsigma\in B} I(\varsigma)},$$
$$\mathbb{P}_t(B) \simeq \mathrm{e}^{-t \inf_{\varsigma\in B} \mathbb{I}(\varsigma)},$$
$$Q_t(B) \simeq \mathrm{e}^{-t \inf_{\varsigma\in B} \mathcal{J}(\varsigma)}$$

$$I(\varsigma) = -\inf_{\alpha\in\mathbb{R}} \left(\alpha\varsigma + C(\alpha)\right),$$

$$\mathbb{I}(\varsigma) = -\inf_{\alpha\in\mathbb{R}} \Big(\alpha\varsigma + e_{2+}(\alpha)\Big),$$

$$\mathcal{J}(\varsigma) = -\inf_{\alpha\in\mathbb{R}} \Big(\alpha\varsigma + e_{\infty+}(\alpha)\Big)$$

Fluctuation Relation implies

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

etc.

OPEN PROBLEM

Suppose that $J_x = J > 0$ for all x.

$$hu_x = J(u_{x+1} + u_{x-1}) + \lambda_x u_x$$

discrete Schrödinger operator.

Davies-Simon (1978): h is called homogenuous if it is reflectionless and has purely a.c. spectrum.

> *We feel that the theory of homogeneous Hamiltonians is worthy of further study.*

Does there exist h with purely a.c. spectrum which is not reflectionless?

HEISENBERG CHAIN

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

Given $\delta > 0$ there exists $\epsilon > 0$ such that if $|\bar{K}| < \epsilon$,

$$e_{p+}(\alpha)$$

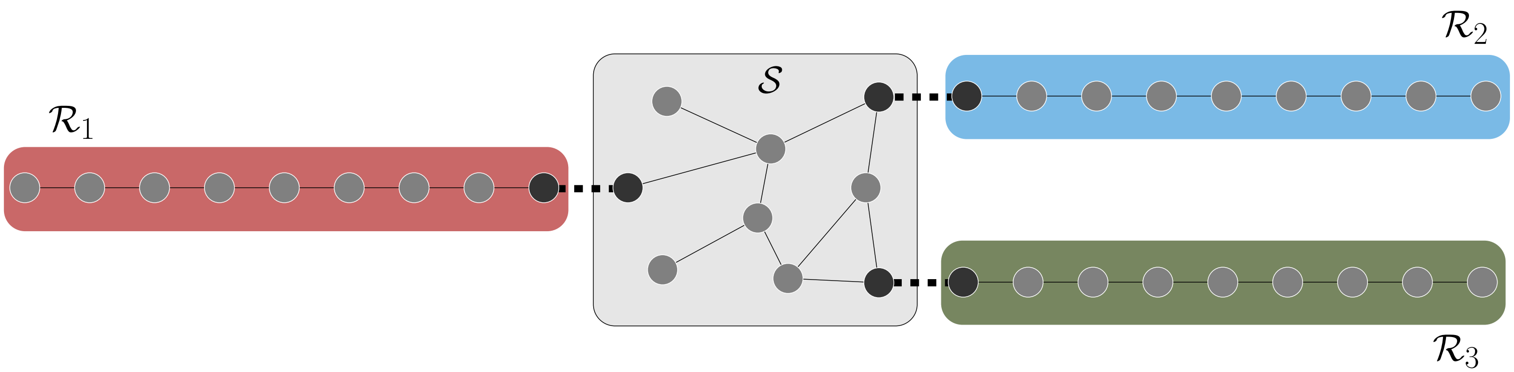
exists for $p = 2, \infty$ and $\alpha \in]-\delta, 1+\delta[$.

$(\{K_x\}, \alpha) \mapsto e_{p+}(\alpha)$ is real analytic.

CLT and local LDP for $\mathbb{P}_t$ and Q_t.

Proof: Combination of De Roeck-Kupianien dynamical polymer expansion and combinatorial estimates of J-Pautrat-Pillet.

ELECTRONIC BLACK BOX MODEL



MCLENNAN-ZUBAREV DYNAMICAL ENSEMBLES

Open systems:

$$\rho_t = \mathrm{e}^{-S_{-t}} = \mathrm{e}^{-\sum \beta_k (H_k + \int_0^t \Phi_{k(-s)} \mathrm{d}s)}$$

ρ_t– Gibbs state at inverse temperature 1 for

$$\sum \beta_k (H_k + \int_0^t \Phi_{k(-s)}) \mathrm{d}s.$$

TD limit: ρ_t is KMS-state for the dynamics generated by

$$\delta_t(\cdot) = \sum \beta_k \delta_k(\cdot) + \int_0^t [\Phi_{k(-s)}, \cdot] \mathrm{d}s$$

NESS ρ_+ is the KMS state for the dynamics generated by

$$\delta_+(\cdot) = \sum \beta_k \left(\delta_k(\cdot) + \int_0^\infty [\Phi_{k(-s)}, \cdot] \mathrm{d}s \right)$$

Aschbacher-Pillet, Ogata-Matsui, Tasaki-Matsui.

XY-chain, $J_x = const$, $\lambda_x = 0$,

$$\beta = (\beta_L + \beta_R)/2, \qquad \gamma = (\beta_R - \beta_L)/2.$$

ρ_+ is β-KMS state for Hamiltonian

$$H + \frac{\delta}{\beta} K$$

$$K = j(x-y) \frac{1}{2\mathrm{i}} \sum_{x<y} \left(\sigma_x^{(1)} \sigma_{x+1}^{(3)} \cdots \sigma_{y-1}^{(3)} \sigma_y^{(2)} - \text{h.c.} \right)$$

where j is the Fourier transform of $|\cos\theta|$.

$$e_{2t}(\alpha) = \log \mathrm{tr}(\mathrm{e}^{-(1-\alpha)S}\mathrm{e}^{-\alpha S_t}).$$

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

In open systems:

$$e_{2t}(\alpha) = \log \mathrm{tr}\left(\mathrm{e}^{-(1-\alpha)\sum \beta_k H_k}\mathrm{e}^{-\alpha \sum \beta_k (H_k + \int_0^t \Phi_{ks}\mathrm{d}s)}\right).$$

$$e_{\infty t}(\alpha) = \log \mathrm{tr}\left(\mathrm{e}^{-\sum \beta_k (H_k + \alpha \int_0^t \Phi_{ks}\mathrm{d}s.}\right).$$

Similarly for other $e_{pt}(\alpha)$. The entropic functionals can be viewed as deformations McLennan-Zubarev dynamical ensembles.

ENTROPIC GEOMETRY (UNDER CONTRUCTION)

David Ruelle: Extending the definition of entropy to nonequilibrium steady states. Proc. Nat. Acad. Sci. 100 (2003).

Outside of equilibrium entropy has curvature.

An old idea. Ruppeiner geometry (1979).

G. Ruppeiner (1995): Riemannian geometry in thermodynamic fluctuation theory. Reviews of Modern Physics 67 (3): 605659

Older:

B. Effron: Defining the curvature of the statistical problem. The Annals of Statistics (1975), 1189-1242.

Even older:

Rao, C.R: (1945) Information and accuracy attainable in the estimation of statistical parameter. Bull. Calcutta Math. Soc. 37.

Information geometry. Monograph:

Amari-Nagaoka: Methods of information geometry (2000)

For our purposes:

G. Crooks (2007): Measuring thermodynamic length. PRL **99**.

Parameter manifold: $(\beta_1, \cdots, \beta_M)$.

$$e''_{p+}(0) = \sum_{j,k} \beta_j \beta_k L_{pjk}.$$

This introduces a (possibly degenerate) metric on the tangent space at $(\beta_1, \cdots, \beta_M)$.

$p = 2$. metric is induced by the CLT variance of CLT for the full counting statistics.

$$L_{2jk} = \frac{1}{2} \int_{-\infty}^{\infty} \rho_+ \Big((\Phi_{js} - \rho_+(\Phi_j))(\Phi_{ks} - \rho_+(\Phi_k)) \Big) \, \mathrm{d}s.$$

In equilibrium $\beta_1 = \cdots = \beta_M$, L_{2jk} are Onsager transport coefficents.

At $p = \infty$, twist to Bogoluibov-Kubo-Mari inner product.

The induced norms $\| \cdot \|_p$ are monotone in p.

Crooks thermodynamical path out of equilibrium.

RELATIONS WITH QUANTUM INFORMATION THEORY

Landauer principle: the energy cost of erasing quantum bit of information by action of a thermal reservoir at inverse temperature T is $\geq kT \log 2$ with the equality for quasi-static processes.

Full counting statistics, $e_{2,+}(\alpha) =$ the Chernoff error exponent in the quantum hypothesis testing of the arrow of time, i.e., of the family of states $\{\rho_t, \rho_{-t}\}_{t>0}$.

J., Ogata-Pillet-Seiringer.: Quantum hypothesis testing and non-equilibrium statistical mechanics, Rev. Math. Phys, 24 (6) (2012), 1-67

Parameter estimation, Fisher entropies, entropic/information geometry?

STEADY STATE FLUCTUATION RELATIONS

Classical statistical mechanics: Dynamical system (M, ϕ_t, ρ).

Observable: $f : M \to \mathbb{R}$. $\rho(f) = \int_M f \mathrm{d}\rho$. Time evolution

$$f_t = f \circ \phi_t$$

$$\rho_t = \rho \circ \phi_{-t}.$$

Phase space contraction:

$$\Delta_{\rho_t|\rho} = \frac{\mathrm{d}\rho_t}{\mathrm{d}\rho}.$$

Entropy production observable

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

$$\log \Delta_{\rho_t|\rho} = \int_0^t \sigma_{-s} \mathrm{d}s.$$

$$S(\rho_t|\rho) = \int_M \log \Delta_{\rho_t|\rho} \mathrm{d}\rho_t = \int_0^t \rho(\sigma_s) \mathrm{d}s.$$

Classical open systems:

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

$$\Phi_k = \{V, H_k\}.$$

Evans-Searles entropic functional:

$$e_t(\alpha) = \log \int_M \mathrm{e}^{-\alpha \int_0^t \sigma_s \mathrm{d}s} \mathrm{d}\rho.$$

Time-reversal invariance.

Evans-Searles fluctuation relation:

$$e_t(\alpha) = e_t(1 - \alpha).$$

Let P_t be the probability distribution of

$$\frac{1}{t} \int_0^t \sigma_s$$

with respect to ρ.

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

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

CLT and LDP are with respect to ρ.

Important: The classical counterpart of the theory of quantum entropic fluctuations described so far is the Evans-Searles fluctuation relation.

Gallavotti-Cohen fluctuation relation: Related but also very different.

NESS: weak limit

$$\rho_+(f) = \lim_{t\to\infty} \rho_t(f).$$

$\rho_+(\sigma) > 0 \Leftrightarrow \rho_+ \perp \rho$.

Gallavotti-Cohen entropic functional:

$$\hat{e}_t(\alpha) = \log \int_M \mathrm{e}^{-\alpha \int_0^t \sigma_s \mathrm{d}s} \mathrm{d}\rho_+.$$

Finite time fluctuation relation

$$\hat{e}_t(\alpha) = \hat{e}_t(1-\alpha)$$

does not hold.
It is even possible that $\hat{e}_t(1) = \infty$ for $t > 0$ (chain of harmonic oscillators).

$$\widehat{e}_+(\alpha) = \lim_{t\to\infty} \frac{1}{t}\widehat{e}_t(\alpha).$$

Gallavotti-Cohen fluctuation relation: for Anosov diffeomprhisms of compact manifolds the symmetry

$$\widehat{e}_+(\alpha) = \widehat{e}_+(1-\alpha)$$

is restored. In this case

$$\widehat{e}_+(\alpha) = e_+(\alpha).$$

General Gallavotti-Cohen fluctuation relation.

Principle of regular entropic fluctuations.Exchange of limits:

$$\begin{aligned}
e_+(\alpha) &= \lim_{t\to\infty} \frac{1}{t} \log \int_M \mathrm{e}^{-\alpha \int_0^t \sigma_s \mathrm{d}s} \mathrm{d}\rho \\
&= \lim_{t\to\infty} \frac{1}{t} \log \int_M \mathrm{e}^{-\alpha \int_u^{u+t} \sigma_s \mathrm{d}s} \mathrm{d}\rho \\
&= \lim_{t\to\infty} \frac{1}{t} \log \int_M \mathrm{e}^{-\alpha \int_0^t \sigma_s \mathrm{d}s} \mathrm{d}\rho_u \\
&= \lim_{t\to\infty} \lim_{u\to\infty} \frac{1}{t} \log \int_M \mathrm{e}^{-\alpha \int_0^t \sigma_s \mathrm{d}s} \mathrm{d}\rho_u \\
&= \lim_{t\to\infty} \frac{1}{t} \log \int_M \mathrm{e}^{-\alpha \int_0^t \sigma_s \mathrm{d}s} \mathrm{d}\rho_+ \\
&= \widehat{e}_+(\alpha).
\end{aligned}$$

OPEN PROBLEM

Gallavotti-Cohen fluctuation relation in quantum statistical mechancs.

Two obvious routes:

Tasaki-Matsui: $(\mathcal{H}, \pi, \Omega_\rho)$ GNS-representation induced ρ,

$$\log \Delta_{\rho_t|\rho} = \log \Delta_{\rho|\rho} + \int_0^t \sigma_{-s} \mathrm{d}s.$$

$$\begin{aligned} e_{2t}(\alpha) &= \log \int_{\mathbb{R}} \mathrm{e}^{-\alpha t \varsigma} \mathbb{P}_t(\varsigma) \\ &= \log \langle \Omega_\rho, \Delta^{\alpha}_{\rho_t|\rho} \Omega_\rho \rangle \\ &= \log \langle \Omega_\rho, \mathrm{e}^{\alpha\left(\log \Delta_{\rho|\rho} - \int_0^t \sigma_s \mathrm{d}s\right)} \Omega_\rho \rangle \end{aligned}$$

$(\mathcal{H}_+, \pi_+, \Omega_{\rho_+}),$

$$\widehat{e}_{2t}(\alpha) = \log\langle \Omega_{\rho_+}, \mathrm{e}^{\alpha\left(\log \Delta_{\rho_+|\rho_+} - \int_0^t \sigma_s \mathrm{d}s\right)} \Omega_{\rho_+}\rangle$$
$$= \log \int_{\mathbb{R}} \mathrm{e}^{-\alpha t \varsigma} \mathrm{d}\widehat{\mathbb{P}}_t(\varsigma).$$

$$\widehat{e}_{2+}(\alpha) = \lim_{t\to\infty} \frac{1}{t} \widehat{e}_{2t}(\alpha).$$

XY chain:

$$\widehat{e}_{2+}(\alpha) = e_{2+}(\alpha).$$

Same for locally interacting case.

Missing: Physical interpretation. Repeated quantum measurement procedure incompatible with NESS structure.

One possibility: Indirect measurements. Work in preparation Bruneau, J., Pillet

Bauer M., Bernard D., Phys. Rev. A84, (2011) Convergence of repeated quantum non-demolition measurements and wave function collapse.

M. Bauer, T. Benoist, D. Bernard, Repeated Quantum Non-Demolition Measurements: Convergence and Continuous Time Limit, Ann. Henri Poincar 14 (2013) 639 67

One difficulty in quantum optic experiments is to measure a system without destroying it. For example to count a number of photons usually one would need to convert each photon into an electric signal. To avoid such destruction one can use non demolition measurements. Instead of measuring directly the system, quantum probes interact with it and are then measured. The interaction is tuned such that a set of system states are stable under the measurement process.

This situation is typically the one of Serge Haroche's (2012 Nobel prize in physics) group experiment inspired the work I will present. In their experiment they used atoms as probes to measure the number of photons inside a cavity without destroying them.

Abstract of T. Benoist talk at McGill (2014)

$p = \infty$. Slightly more satisfactory.

$$e_{\infty t} = -\inf_{\omega \ll \rho} \left(S(\omega|\rho) + \alpha \int_0^t \omega(\sigma_s) \mathrm{d}s \right).$$

$$\widehat{e}_{\infty t} = -\inf_{\omega \ll \rho_+} \left(S(\omega|\rho_+) + \alpha \int_0^t \omega(\sigma_s) \mathrm{d}s \right).$$

Again, in the cases where one can compute (XY, etc):

$$\widehat{e}_{\infty +}(\alpha) = e_{\infty +}(\alpha).$$

TOPICS NOT DICSUSSED

Weak coupling limit (Davies 1974, Lebowitz-Spohn 1978, J-Pillet-Westrich 2014)

Repeated interactions systems

Pauli-Fierz systems (finite level atom coupled to bosonic reservoirs).

Classical statistical mechanics.

Landauer Erasing Principle

Refinements of the 1st law of thermodynamics

CONCLUSIONS