# Entropy Production in the Two-Sided XYh Chain

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# 1. Introduction

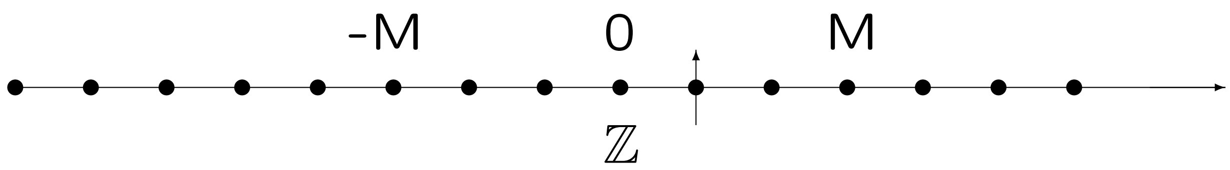
## 1.1 Content

Properties of steady states for finite systems coupled to thermal reservoirs in non-equilibrium quantum statistical mechanics, in particular:

The one-dimensional, two-sided, and anisotropic XYh model:

$$H = -\frac{1}{4}\sum_{x\in\mathbb{Z}}\Big((1+\gamma)\sigma_1^{(x)}\sigma_1^{(x+1)} + (1-\gamma)\sigma_2^{(x)}\sigma_2^{(x+1)} + 2\lambda\sigma_3^{(x)}\Big)$$

• Inifinite chain of spins interacting anisotropically with two nearest neighbors and with external magnetic field: $\gamma$ and $\lambda$



## Results

- Construction of the unique non-equilibrium steady state (NESS) for the XYh chain perturbed by compact decoupling using *scattering theory*
- Independence of the NESS of the size of the finite system
- Structural properties of the NESS: primary, modular, non-KMS, quasi-free, singular,...
- Long range decay of correlation functions

- Strictly positive entropy production !

$\Rightarrow$ NESS thermodynamically non-trivial !

## 1.2 Physics of the XYh Chain

Non-equilibrium thermodynamics as phenomenological macroscopic field theory has its roots in phenomenological laws as, e.g.:

- Viscous flow (Newton, 1687)
- Heat conduction (Fourier, 1822)
- Electrical conduction (Ohm, 1826)
- Diffusion (Fick, 1855)

Low dimensional spin systems:

- Anomalous thermal transport coefficients in Green-Kubo theory and experiments on $SrCuO_2$, $Sr_2CuO_3$,...(XYZ):

Quantum integrability of the system !

- $PrCl_3$ (XY)

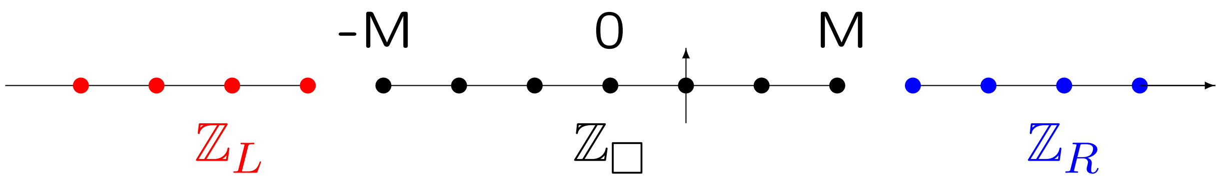
## 1.3 Non-equilibrium Setting

Remove spin-spin coupling across the two bounds $(-M-1,-M)$ and $(M,M+1)$

$\Rightarrow$ New dynamics w.r.t. $H_0$: Free

$\Rightarrow$ Three noninteraction subsystems with respective $(\tau_L,\beta_L)$, $(\tau_\Box,0)$, and $(\tau_R,\beta_R)$-KMS states:

$$\omega_0^{M,\beta_L,\beta_R} := \omega_L^{\beta_L} \otimes \omega_\Box \otimes \omega_R^{\beta_R}$$




$\Rightarrow$ Infinite half-chains $\mathbb{Z}_L$, $\mathbb{Z}_R$ play role of thermal reservoirs to which finite subsystem $\mathbb{Z}_\Box$ is attached via coupling $V := H - H_0$

• NESS [R 2000]

Quantum dynamical systems:

(1) Free $(\mathfrak{S}, \tau_0)$ with $\tau_0$-invariant state $\omega_0$

(2) Perturbed $(\mathfrak{S}, \tau)$

$$\Sigma_+(\omega_0) := \text{weak}^*\text{lim-pt} \left\{ \frac{1}{T} \int_0^T dt\, \omega_0 \circ \tau^t,\ T > 0 \right\}$$

Non-empty, weak*-compact subset of the weak*-compact set of states $\mathcal{E}(\mathfrak{S})$ on $\mathfrak{S}$ ($\mathfrak{S}$ contains $\mathbf{1}$) of $\tau$-invariant Non-Equilibrium Steady States (NESS)

## 2. The Model

### 2.1 Kinematics

- Observables $\mathfrak{S}$

Uniformly hyperfinite quasi-local $C^*$ algebra $\mathfrak{S}$ over $\mathbb{Z}$, i.e.:
Associate Hilbert space $\mathcal{H}_x := \mathbb{C}^2$ for $x$ in index set $\mathbb{Z}$, and

$$\mathcal{H}_\Lambda := \bigotimes_{x \in \Lambda} \mathcal{H}_{\{x\}},$$

for $\Lambda$ in directed set of finite subsets of $\mathbb{Z}$ (direction by inclusion; orthogonality relation by disjointness)
Corresponding full matrix algebra of observables:

$$\mathfrak{S}_\Lambda := \mathcal{B}(\mathcal{H}_\Lambda)$$

$*$-algebra with $C^*$ norm for arbitrary $\mathcal{L} \subset \mathbb{Z}$:

$$\mathfrak{S}^0_{\mathcal{L}} := \bigcup_{\Lambda \subset \mathcal{L}} \mathfrak{S}_\Lambda$$

$C^*$ completion $\Rightarrow$ Infinite tensor product of $\mathcal{B}(\mathcal{H}_{\{x\}})$, $x \in \mathcal{L}$:

$$\mathfrak{S}_{\mathcal{L}} := \overline{\mathfrak{S}^0_{\mathcal{L}}}$$

Pauli matrices $\sigma_1, \sigma_2, \sigma_3$ generate $\mathcal{B}(\mathcal{H}_{\{x\}}) \Rightarrow \mathfrak{S}_\Lambda$: Algebra of polynomials in

$$\sigma^{(x)}_\alpha := \cdots \otimes \mathbf{1} \otimes \mathbf{1} \otimes \sigma_\alpha \otimes \mathbf{1} \otimes \mathbf{1} \otimes \cdots , \; x \in \Lambda$$

$\Rightarrow \mathfrak{S}_{\mathcal{L}}$: Uniform limit of polynomials in $\sigma^{(x)}_\alpha$, $x \in \mathcal{L}$; $\mathfrak{S} := \mathfrak{S}_{\mathbb{Z}}$

Fix $M \geq 0$:

$$\mathfrak{S}_L := \mathfrak{S}_{\{x < -M\}}, \; \mathfrak{S}_\Box := \mathfrak{S}_{\{-M \leq x \leq M\}}, \; \mathfrak{S}_R := \mathfrak{S}_{\{x > M\}}$$

## 2.2 Dynamics

- Local XY Hamiltonian

$$H_\Lambda := \sum_{X \subset \Lambda} \phi(X)$$

- Interaction

$$\phi(X) := \begin{cases} -\frac{1}{2}\lambda\sigma_3^{(x)}, & X = \{x\}, \\ -\frac{1}{4}\{(1+\gamma)\sigma_1^{(x)}\sigma_1^{(x+1)} + (1-\gamma)\sigma_2^{(x)}\sigma_2^{(x+1)}\}, & X = \{x, x+1\}, \\ 0, & \text{otherwise} \end{cases}$$

Short range, two-body

- Magnetic field strength, anisotropy:

$$\lambda \in \mathbb{R}, \qquad \gamma \in ]-1, 1[$$

$\Rightarrow$ Genuinely quantum mechanical !

• Perturbed time evolution

$$\tau_\Lambda^t(A) := \mathrm{e}^{itH_\Lambda} A\, \mathrm{e}^{-itH_\Lambda},\ A \in \mathfrak{S}$$

$\Rightarrow$ Norm continuous group of local $*$-automorphisms of $\mathfrak{S}$

$\phi$ short range, two-body $\Rightarrow$ TD limit exists:

$$\tau^t(A) := \lim_{\Lambda \uparrow \mathbb{Z}} \tau_\Lambda^t(A),\ A \in \mathfrak{S}$$

$\Rightarrow$ Perturbed $C^*$-dynamical $XY$ system $(\mathfrak{S}, \tau)$

• Free time evolution

Perturbation: $V := \phi(\{-M-1, -M\}) + \phi(\{M, M+1\})$

$\Rightarrow$ Free $C^*$-dynamical $XY$ system $(\mathfrak{S} = \mathfrak{S}_L \otimes \mathfrak{S}_\square \otimes \mathfrak{S}_R, \tau_0)$:

$$\tau_0^t = \tau_L^t \otimes \tau_\square^t \otimes \tau_R^t$$

## 2.3 Araki-Jordan-Wigner

- $\theta_-$ $\in \mathrm{Aut}(\mathfrak{S})$: $\theta_-(\sigma_\alpha^{(x)}) := \begin{cases} -\sigma_\alpha^{(x)}, & \alpha = 1,2, \quad x \leq 0 \\ \sigma_\alpha^{(x)}, & \alpha = 1,2, \quad x > 0 \\ \sigma_\alpha^{(x)}, & \alpha = 3, \quad\;\; x \in \mathbb{Z} \end{cases}$

- Two-sided $C^*$ algebra $\mathfrak{A} := \langle \mathfrak{S}, T \rangle$ for $T \notin \mathfrak{S}$:

$$T = T^* \qquad T^2 = \mathbf{1} \qquad TA = \theta_-(A)T$$

$\Rightarrow \mathfrak{A} = \mathfrak{S} + T\mathfrak{S}$

- CAR algebra $\mathfrak{F} := \langle a_x, a_x^* \,|\, x \in \mathbb{Z} \rangle$

$$a_x := TS^{(x)}(\sigma_1^{(x)} - i\sigma_2^{(x)})/2 \qquad a_x^* = TS^{(x)}(\sigma_1^{(x)} + i\sigma_2^{(x)})/2$$

$$S^{(x)} := \begin{cases} \sigma_3^{(1)} \cdots \sigma_3^{(x-1)}, & x > 1 \\ \mathbf{1}, & x = 1 \\ \sigma_3^{(x)} \cdots \sigma_3^{(0)}, & x < 1 \end{cases}$$

- $\theta \in$ Aut$(\mathfrak{A})$: $\theta(\sigma_\alpha^{(x)}) := \begin{cases} -\sigma_\alpha^{(x)}, & \alpha = 1,2 \\ \sigma_\alpha^{(x)}, & \alpha = 3 \end{cases}$ , $\theta(T) := T$

$\Rightarrow \mathfrak{S}_\pm := \{A \in \mathfrak{S} \,|\, \theta(A) = \pm A\}$ and $\mathfrak{F}_\pm := \{A \in \mathfrak{F} \,|\, \theta(A) = \pm A\}$
Note: $\mathfrak{S}_+$ is $C^*$ subalgebra, and $\tau_0^t \mathfrak{S}_+ \subset \mathfrak{S}_+$, $\tau^t \mathfrak{S}_+ \subset \mathfrak{S}_+$
Furthermore:

$$\mathfrak{S}_+ = \mathfrak{F}_+, \qquad \mathfrak{S}_- = T\mathfrak{F}_-$$

- The interaction is even, $\phi(X) \in \mathfrak{F}_+$:

$$\phi(X) = \begin{cases} -\frac{1}{2}\lambda(2a_x^* a_x - 1), & X = \{x\} \\ \frac{1}{2}\{a_x^* a_{x+1} + a_{x+1}^* a_x + \gamma(a_x^* a_{x+1}^* + a_{x+1} a_x)\}, & X = \{x, x+1\} \\ 0, & \text{otherwise} \end{cases}$$

## 2.4 Bogoliubov Automorphisms

• Self-dual CAR algebra $\mathfrak{F}_{sd}(\mathfrak{h}, J)$ [A 71]

$\mathfrak{h}$: Complex Hilbert space, $J$: Antiunitary involution on $\mathfrak{h}$

$\mathfrak{F}^0_{sd}(\mathfrak{h}, J) := \langle B(f), B^*(f), \mathbf{1} \,|\, f \in \mathfrak{h} \rangle$:

$$\begin{array}{ll} (1) & B(f) \text{ is complex linear in } f \\ (2) & \{B^*(f), B(g)\} = (f, g)\,\mathbf{1} \\ (3) & B^*(f) = B(Jf) \end{array}$$

$\Rightarrow \mathfrak{F}_{sd}(\mathfrak{h}, J) := \overline{\mathfrak{F}}^0_{sd}(\mathfrak{h}, J)$ $C^*$ completion w.r.t. unique $C^*$ norm

Here:

$\mathfrak{h} = \ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z})$, $\mathfrak{h} \ni f =: (f_+, f_-)$

$J: (f_+, f_-) \mapsto (\bar{f}_-, \bar{f}_+)$

$B(f) := \sum_{x \in \mathbb{Z}} \Big( f_+(x)\, a^*_x + f_-(x)\, a_x \Big)$

$\Rightarrow \mathfrak{F} = \mathfrak{F}_{sd}(\mathfrak{h}, J)$: Self-dual algebra generated by polynomials in $B(f)$

• Implementing the dynamics

Finite rank operator $k := \sum_{j=1}^{n} f_j\,(g_j,\,\cdot\,) \mapsto \mathbf{B}(k) := \sum_{j=1}^{n} B(f_j)\,B^*(g_j)$

If $k + Jk^*J = 0$:

$$\mathrm{e}^{t\mathbf{B}(k)/2}\,B(f)\,\mathrm{e}^{-t\mathbf{B}(k)/2} = B(\mathrm{e}^{tk}f)$$

Here:

$H_\Lambda = \mathbf{B}(h_\Lambda)/2$ and $h_\Lambda = \sum_{X\subset\Lambda}\varphi(X)$ with $\varphi(\{x\}) = -\lambda\,|x\rangle\langle x| \otimes \sigma_3$, $\varphi(\{x,x+1\}) = c_x \otimes \sigma_3 - \gamma s_x \otimes \sigma_2$

$\Rightarrow$ TD limit:

$$\tau^t(B(f)) = B(\mathrm{e}^{ith}f),\ h = (\cos\xi - \lambda)\otimes\sigma_3 - \gamma\sin\xi\otimes\sigma_2$$

Analogously for decoupled dynamics $\tau_0^t$:

$h_0 = h - v = h_L \oplus h_\Box \oplus h_R$ on $\mathfrak{h} = \ell^2(\mathbb{Z}_L)\otimes\mathbb{C}^2 \oplus \ell^2(\mathbb{Z}_\Box)\otimes\mathbb{C}^2 \oplus \ell^2(\mathbb{Z}_R)\otimes\mathbb{C}^2$

for $v := \varphi(\{-M-1,-M\}) + \varphi(\{M,M+1\})$

## 2.5 Quasi-free States

- State $\omega$ on $\mathfrak{F}_{sd}(\mathfrak{h}, J)$ quasi-free:

$$\omega(B(f_1)\cdots B(f_{2n})) = \sum_{\pi\in S_{2n}} \mathrm{sign}(\pi) \prod_{j=1}^{n} \omega(B(f_{\pi(2k-1)})B(f_{\pi(2k)}))$$

for $\pi(2k), \pi(2k+1) > \pi(2k-1)$, and $\omega(B(f_1)\cdots B(f_{2n+1})) = 0$

[A 71]: $\omega_T$ quasi-free $\Leftrightarrow$
(1) $0 \le T = T^* \le \mathbf{1}$ (2) $T + JTJ = \mathbf{1}$: $\omega_T(B^*(f)B(g)) = (f, Tg)$

- Example:

$k = k^*$ on $\mathfrak{h}$, $k + JkJ = 0$ and $\tau_k^t(B(f)) := B(e^{itk}f) \Rightarrow T := (1 + e^{\beta k})^{-1}$
satisfies (1), (2) and $\omega_T$ is $(\tau_k, \beta)$-KMS

- Here:

$\omega_0^{M,\beta_L,\beta_R} = \omega_{T_0}$ for $T_0 = (1 + e^{k_0})^{-1}$, and $k_0 := \beta_L h_L \oplus 0 \oplus \beta_R h_R$

## 3. Results

### 3.1 Existence and Uniqueness of NESS

**Theorem 1**

Let $\beta_L, \beta_R \in \mathbb{R}$, $M \in \mathbb{N}$. Then:

$$\Sigma_+(\omega_0^{M,\beta_L,\beta_R}) \;=\; \{\omega_+^{\beta_L,\beta_R}\}$$

**Proof Theorem 1**

- $\beta_L = \beta_R =: \beta$ [A 84] $\Rightarrow \omega_+^{\beta_L,\beta_R}$ unique $(\tau,\beta)$-KMS, and RTE
- $\beta_L \neq \beta_R$ Scattering theory $\Rightarrow$ Møller $\gamma_+(A) := \lim_{t\to\infty} \tau_0^{-t}\tau^t(A)$ exists in norm, and, for $\Omega_- := \mathrm{s}-\lim_{t\to\infty} \mathrm{e}^{-ith_0}\,\mathrm{e}^{ith}$:

$$\gamma_+(B(f)) = B(\Omega_- f)$$

$\Rightarrow \omega_+^{\beta_L,\beta_R} := \omega_0^{M,\beta_L,\beta_R} \circ \gamma_+$ $\square$

## 3.2 Further Properties of $\omega_+^{\beta_L,\beta_R}$

Main Theorem 2

$\omega_+^{\beta_L,\beta_R} \in \mathcal{E}(\mathfrak{F})$ has 2-point function $\omega_+^{\beta_L,\beta_R}(B^*(f)B(g)) = (f, T_+ g)$ with

$$T_+ = (1 + e^{k_+})^{-1}, \quad k_+ := (\beta + \delta\, \mathrm{sign} v_-)h$$

where

$$\beta := (\beta_R + \beta_L)/2, \quad \delta := (\beta_R - \beta_L)/2;$$

i.e.:

$\beta_\alpha$-Gibbs distribution if particle stems from $\alpha$-reservoir in the past, $\alpha = L, R$.

## Proof of Theorem 2

Structure of $\omega_+^{\beta_L,\beta_R} \Rightarrow T_+ = \Omega_+^* T_0 \Omega_+$

- Partial wave operators $\Omega_\alpha$, asymptotic projections $P_\alpha$

Natural injection: $i_\alpha \colon \ell^2(\mathbb{Z}_\alpha) \otimes \mathbb{C}^2 \to \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$, $\alpha = L, R$:

$$\Omega_\alpha := \mathrm{s} - \lim_{t\to\infty} \mathrm{e}^{-ith_\alpha}\, i_\alpha^*\, \mathrm{e}^{ith} \qquad P_\alpha := \mathrm{s} - \lim_{t\to\infty} \mathrm{e}^{-ith}\, i_\alpha i_\alpha^*\, \mathrm{e}^{ith}$$

(1) [Kato-Birman] $\Rightarrow$ Existence

(2) $\Omega_- = \sum_{\alpha\in\{L,R\}} i_\alpha\, \Omega_\alpha$

(3) $h_\alpha\, \Omega_\alpha = \Omega_\alpha\, h$

(4) $P_\alpha = \Omega_\alpha^* \Omega_\alpha$

(5) $P_L + P_R = I$

(6) $[P_\alpha, h] = 0$

From $T_0 = (1 + e^{k_0})^{-1}$ with $k_0 := \beta_L\, h_L \oplus 0 \oplus \beta_R\, h_R$, and (1)-(6):

$$T_+ = (1 + e^{k_+})^{-1} \qquad k_+ = \beta\, h + \delta\, (P_R - P_L)\, h$$

• Asymptotic velocity $v_-$

Set $x := -i\partial_\xi \otimes \mathbf{1}$, $x_t := \mathrm{e}^{-ith} x\, \mathrm{e}^{ith}$, $p := -i[h, x]$, and $p_t := \mathrm{e}^{-ith} p\, \mathrm{e}^{ith}$

First: $\sigma(h) = \sigma_{ac}(h) \Rightarrow P_R - P_L = \mathrm{s} - \lim_{t\to\infty} \operatorname{sign} \frac{x_t}{t}$

Second: Compute $x_t$ via $\dot{x}_t = p_t$ by $p = \mathbf{p} \cdot \sigma, h = \mathbf{h} \cdot \sigma$, and SU(2)-SO(3) homomorphism

$(\mu := \mathbf{p}{\cdot}\mathbf{h}/\mathbf{h}{\cdot}\mathbf{h}$, $\mathbf{h}(\xi) := (0, -\gamma \sin \xi, \cos \xi - \lambda)$, $\mathbf{p}(\xi) := (0, -\gamma \cos \xi, -\sin \xi))$

$\Rightarrow \mathrm{s} - \lim_{t\to\infty} \frac{x_t}{t} = \mu h$ on common core

$\Rightarrow$ s-res-$\lim_{t\to\infty} \frac{x_t}{t} = \mu h =: v_-$ asymptotic velocity

Third: $\sigma(\mu h) = \sigma_{ac}(\mu h) \Rightarrow$ Main Theorem 2:

$$P_R - P_L = \operatorname{sign} v_-$$

$\square$

Theorem 3

The unique NESS $\omega_+^{\beta_L,\beta_R}$ is:

(1) attractive

(2) independent of $M$

(3) translation invariant

(4) primary

(5) modular

(6) quasi-free

(7) KMS for $\tau$, iff $\beta_L = \beta_R$

(8) singular w.r.t. $\omega_0^{M,\beta_L,\beta_R}$, if $\beta_L \neq \beta_R$

## Proof Theorem 3

(1) attractive: $\lim_{t\to\infty}\omega_0^{M,\beta_L,\beta_R}(\tau^t(A)) = \omega_+^{\beta_L,\beta_R}(A)$, $A \in \mathfrak{S}$

(2),(3) $T_+$ independent of $M$, commutes with translations

(4),(5) $\sigma(T_+) = \sigma_{ac}(T_+)$, textcolormagenta[A 71]

(6) $\omega_+^{\beta_L,\beta_R} = \omega_0^{M,\beta_L,\beta_R} \circ \gamma_+$

(7) [A 84]

(8) (4), [J,P 2002], Theorem 4

$\square$

## 3.3 Entropy production

Entropy production in NESS $\omega_+^{\beta_L,\beta_R} \in \Sigma_+(\omega_0^{M,\beta_L,\beta_R})$ [J,P 2001]:

$$\mathrm{Ep}(\omega_+^{\beta_L,\beta_R}) := \beta_L\,\omega_+^{\beta_L,\beta_R}(\Phi_L) + \beta_R\,\omega_+^{\beta_L,\beta_R}(\Phi_R)$$

$\Phi_L = -i[H, H_L]$, $\Phi_R = -i[H, H_R]$: Heat fluxes $\mathbb{Z}_L$, $\mathbb{Z}_R \to \mathbb{Z}_\square$

Theorem 4

$$\begin{aligned}
\mathrm{Ep}(\omega_+^{\beta_L,\beta_R}) &= \frac{\delta}{4}\int_0^{2\pi}\frac{d\xi}{2\pi}\,|\mathbf{p}\cdot\mathbf{h}|\,\frac{\mathrm{sh}\,\delta|h|}{\mathrm{ch}^2(\beta|h|/2)+\mathrm{sh}^2(\delta|h|/2)} \\
\mathrm{Ep}(\omega_+^{\beta_L,\beta_R}) &> 0 \qquad \text{if } \beta_L \neq \beta_R
\end{aligned}$$

Proof Theorem 4

Explicit computations ! $\square$

## 3.4 Correlation functions

Longitudinal correlations:

$$C_3^T(x) := \omega_+^{\beta_L,\beta_R}(\sigma_3^{(0)}\sigma_3^{(x)}) - \omega_+^{\beta_L,\beta_R}(\sigma_3^{(0)})^2$$

Theorem 5

$$0 < \limsup_{x\to\infty} |x^2\, C_3^T(x)| < \infty$$

Proof Theorem 5

Araki-Jordan-Wigner $\Rightarrow$ Fermionic 4-point function

Wick expansion $\Rightarrow C_3^T(x) = 4\,\det \check{T}_+(x)$

Analysis of singularities in $\check{T}_+(x)$ ! $\square$

## 4. Outlook

• Correlation functions long range out of equilibrium ?!
For Longitudinal correlations:

$$0 < \limsup_{x \to \infty} |x^2 C_3^T(x)| < \infty$$

• Long range effective Hamiltonian through conserved charges !
• Integrability of the system, selection of NESS, and Fourier Law ?
• Central limit theorems
• Gallavotti-Cohen fluctuation of the entropy production
• Onsager on graph systems
• Functional analysis and modular theory: Ergodic properties
• ...

We are at the beginning only of a rigorous treatment of quantum statistical systems out of thermal equilibrium...