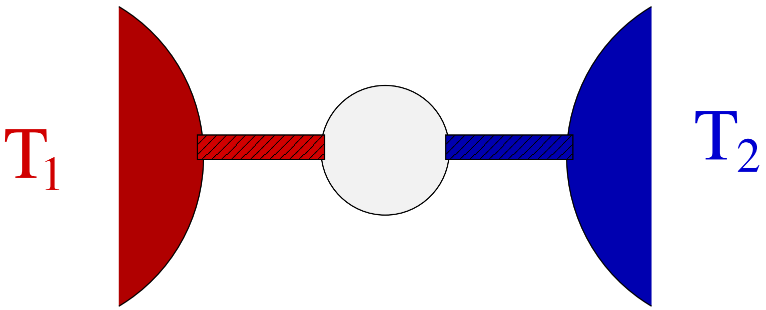
A Short Introduction to the Mathematical Theory of Nonequilibrium Quantum Statistical Mechanics



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Part 1: General Theory

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1. Basic concepts of C^*-algebraic quantum statistical mechanics
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1. C^*-algebraic quantum statistical mechanics

[Bratteli-Robinson], [Jakšić-Pillet 02], [A-Jakšić-Pautrat-Pillet 06],...

1.1 C^*-dynamical systems $(\mathcal{O}, \tau)$

• observables

(unital) C^*-algebra $\mathcal{O}$

Banach $*$-algebra (complete w.r.t. submultiplicative norm $\|\cdot\|$, involution $*$) with $\|A^*A\| = \|A\|^2$

• dynamics

strongly continuous group τ^t of $*$-automorphisms of $\mathcal{O}$

$\mathbb{R} \ni t \mapsto \tau^t(A) \in \mathcal{O}$ continuous w.r.t $\|\cdot\|$ for all $A \in \mathcal{O}$

Example $\mathcal{L}(\mathcal{H})$ with $\|A\| = \sup_{\|\psi\|=1} \|A\psi\|$ and $\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}$ and $H^* = H \in \mathcal{L}(\mathcal{H})$

1.2 States ω

- $\omega \in \mathcal{O}^*$

continuous linear functional on $\mathcal{O}$ with $\omega(\mathbf{1}) = 1$ (normalized) and $\omega(A^*A) \geq 0$ (positive)

- $\mathcal{E}(\mathcal{O})$

set of states

convex weak*-compact subset of $\mathcal{O}^*$ with neighborhood base $U_{A_j,\epsilon}(\omega) = \{\omega' \colon |\omega'(A_j) - \omega(A_j)| < \epsilon\}$

- (τ, β)-KMS state

$(\mathcal{O}, \tau)$ C^*-dynamical system, $\beta > 0$.

$$\omega(A\tau^{\mathrm{i}\beta}(B)) = \omega(BA)$$

$A, B \in \mathcal{D}$ norm dense, τ-invariant $*$-subalgebra of $\mathcal{O}_\tau$ "entire analytic elements for τ":
$A \in \mathcal{O}_\tau :\Leftrightarrow \mathbb{R} \ni t \mapsto \tau^t(A)$ extends to an entire analytic function

interpretation: systems in thermal equilibrium at temperature $1/\beta$

Example (i.g. formal) Gibbs state $\omega(A) = \mathrm{tr}(\mathrm{e}^{-\beta H} A)/Z$ (e.g. finite system, Fermi: unique)

1.3 GNS representation [Gelfand-Naimark-Segal]

- $\omega \in \mathcal{E}(\mathcal{O})$. exists unique cyclic representation $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ of $\mathcal{O}$ s.t.

$$\omega(A) = (\Omega_\omega, \pi_\omega(A)\Omega_\omega)$$

$\pi_\omega : \mathcal{O} \to \mathcal{L}(\mathcal{H}_\omega)$ $*$-morphism:
$\pi_\omega(\alpha A + \beta B) = \alpha\pi_\omega(A) + \beta\pi_\omega(B)$, $\pi_\omega(AB) = \pi_\omega(A)\pi_\omega(B)$, $\pi_\omega(A^*) = \pi_\omega(A)^*$

Ω_ω cyclic: $\{\pi_\omega(A)\Omega_\omega \,|\, A \in \mathcal{O}\}$ dense in $\mathcal{H}_\omega$

uniqueness up to unitary equivalence: $U\pi_\omega(A)\Omega_\omega := \pi'_\omega(A)\Omega'_\omega$

$\mathcal{H}_\omega$: positive semidefinite $\langle A, B\rangle := \omega(A^*B)$, left ideal $\mathcal{I}_\omega := \{A \in \mathcal{O} \,|\, \omega(A^*A) = 0\}$, equivalence classes $[A] := \{A + I \,|\, I \in \mathcal{I}_\omega\}$, scalar product $([A], [B]) := \langle A, B\rangle$
$\pi_\omega(a)[B] := [AB]$
$\Omega_\omega := [1]$

- $\eta \in \mathcal{E}(\mathcal{O})$ ω-normal $:\Leftrightarrow$ exists density matrix $\rho \in \mathcal{L}(\Omega_\omega)$:

$$\eta(A) = \mathrm{tr}(\rho\, \pi_\omega(A))$$

$\mathcal{N}_\omega$ set of all ω-normal states

1.4 (Concrete) von Neumann algebra

- commutant

$\mathcal{H}$ Hilbert space, $\mathcal{M} \subset \mathcal{L}(\mathcal{H})$.

$$\mathcal{M}' := \{A \in \mathcal{L}(\mathcal{H}) \mid [A, M] = 0,\ M \in \mathcal{M}\}$$

$\mathcal{M} \subset \mathcal{M}'' = \mathcal{M}^{(iv)} = \mathcal{M}^{(vi)} = \ldots$ and $\mathcal{M}' = \mathcal{M}''' = \mathcal{M}^{(v)} = \mathcal{M}^{(vii)} = \ldots$

- von Neumann algebra over $\mathcal{H}$

$$\mathcal{M}'' = \mathcal{M}$$

Examples $\mathcal{L}(\mathcal{H})$; not $\mathcal{L}^\infty(\mathcal{H})$ since $\mathcal{L}^\infty(\mathcal{H})' = \mathbb{C}\mathbf{1}$

$\mathcal{M}$ von Neumann algebra over $\mathcal{H}$, $\Omega \in \mathcal{H}$, $\mathcal{M}\Omega := \{A\Omega \mid A \in \mathcal{M}\}$

- $\Omega \in \mathcal{H}$ cyclic $:\Leftrightarrow \overline{\mathcal{M}\Omega} = \mathcal{H}$
- $\Omega \in \mathcal{H}$ separating $:\Leftrightarrow \Omega \in \ker A \Rightarrow A = 0$

1.5 Tomita-Takesaki theory

- $\mathcal{M}$ von Neumann algebra over $\mathcal{H}$, $\Omega \in \mathcal{H}$ cyclic and separating
- transfer $*$-involution on $\mathcal{M}$ to dense subspace $\mathcal{M}\Omega$ of $\mathcal{H}$:

$\theta : \mathcal{M} \to \mathcal{M}\Omega$, $A \mapsto A\Omega$ $\quad$ θ injective (Ω separating), $\mathcal{M}\Omega$ dense (Ω cyclic)

$$S_0 : \mathcal{M}\Omega \to \mathcal{M}\Omega, \qquad S_0 A\Omega = A^*\Omega \qquad \begin{array}{ccc} \mathcal{M} & \overset{\theta^{-1}}{\longleftarrow} & \mathcal{M}\Omega \\ * \downarrow & & \downarrow S_0 \\ \mathcal{M} & \overset{\theta}{\longrightarrow} & \mathcal{M}\Omega \end{array}$$

- modular conjugation J, modular operator Δ associated with $(\mathcal{M}, \Omega)$

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

polar decomposition of closure $S := \overline{S}_0$, J unique antiunitary, Δ unique positive selfadjoint

- [Tomita-Takesaki] $J\mathcal{M}J = \mathcal{M}'$ and $\Delta^{\mathrm{i}t}\mathcal{M}\Delta^{-\mathrm{i}t} = \mathcal{M}$
- here: $\mathcal{M} \equiv \mathcal{M}_\omega := \pi_\omega(\mathcal{O})'' \subseteq \mathcal{L}(\mathcal{H}_\omega)$.
- $\omega \in \mathcal{E}(\mathcal{O})$ modular $:\Leftrightarrow$ Ω_ω is separating for $\mathcal{M}_\omega$

Example (τ, β)-KMS state (Schwarz reflection principle, reformulation of KMS conditions)

1.6 Standard Liouvillean

$(\mathcal{O}, \tau)$ C^*-dynamical system, $\omega \in \mathcal{E}(\mathcal{O})$ modular.
$\Rightarrow$ exists unique self-adjoint standard Liouvillean L on $\mathcal{H}_\omega$ s.t.

$$\pi_\omega(\tau^t(A)) = \mathrm{e}^{\mathrm{i}tL}\pi_\omega(A)\mathrm{e}^{-\mathrm{i}tL}, \quad \mathrm{e}^{-\mathrm{i}tL}\mathcal{P} \subset \mathcal{P}$$

natural cone $\mathcal{P} = \overline{\{AJA\Omega_\omega \,|\, A \in \mathcal{M}_\omega\}}$

$\eta \in \mathcal{N}_\omega$ and τ-invariant $\Rightarrow$ exists unique $\Omega_\eta \in \ker L \cap \mathcal{P}$ s.t. $\eta(A) = (\Omega_\eta, \pi_\omega(A)\Omega_\eta)$

1.7 Quantum statistical mechanics and modular theory

- $\ker L = \{0\} \Rightarrow$ no ω-normal τ-invariant states
- Quantum Koopmanism: spec L encodes some ergodic properties

Example $\lim_{|t|\to\infty} \eta(\tau^t(A)) = \omega(A)$ for all $\eta \in \mathcal{N}_\omega$ and all $A \in \mathcal{O}$ "returns to equilibrium (RTE)"

$\Leftrightarrow$ spec L is absolutely continuous up to simple eigenvalue 0

- $\Delta_\omega = \mathrm{e}^{\mathcal{L}_\omega}$. [Takesaki] ω is (τ, β)-KMS $\Leftrightarrow \mathcal{L}_\omega = -\beta L$

1.8 Local perturbations

$(\mathcal{O},\tau)$ C^*-dynamical system.

- local perturbation $V = V^* \in \mathcal{O}$
- generator δ_V of perturbed dynamics $\tau^t := \mathrm{e}^{t\delta}$ from $\tau_0^t = \mathrm{e}^{t\delta_0}$

$$\delta(A) := \delta_0(A) + \mathrm{i}[V, A]$$

generators δ_0, δ: $*$-derivation of $\mathcal{O}$: $\delta(A^*) = \delta(A)^*,\ \delta(AB) = \delta(A)B + A\delta(B),\ A, B \in \mathcal{D}(\delta)$

- Dyson series

$$\tau^t(A) = \tau_0^t(A) + \sum_{n\geq 1} \mathrm{i}^n \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \ldots \int_0^{t_{n-1}} \mathrm{d}t_n\, [\tau_0^{t_n}(V), [\ldots[\tau_0^{t_1}(V), \tau_0^t(A)]\ldots]]$$

- $(\mathcal{O},\tau)$ is C^*-dynamical system

- ω modular. standard Liouvillean for perturbed dynamics

$$L_V = L + V - JVJ$$

$\mathrm{dom}(L_V) = \mathrm{dom}(L)$ and L standard Liouvillean for τ

1.9 Examples

Finite quantum systems

- C^*-dynamical systems $(\mathcal{O}, \tau)$, $(\mathcal{O}, \tau_V)$ $\mathcal{H} = \mathbb{C}^N$, $\mathcal{O} = \mathcal{L}(\mathcal{H})$, $H = H^*$

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

- State ρ density matrix on $\mathcal{H}$, any $\omega \in \mathcal{E}(\mathcal{O})$ of the form

$$\omega(A) = \mathrm{tr}(\rho A)$$

Example unique (τ, β)-KMS state, $\beta > 0$: $\rho = \mathrm{e}^{-\beta H}/\mathrm{tr}(\mathrm{e}^{-\beta H})$

- GNS representation $\lambda_j \geq 0$ eigenvalues and ψ_j eigenvectors of ρ

$$\mathcal{H}_\omega = \mathcal{H} \otimes \mathcal{H}, \quad \pi_\omega(A) = A \otimes \mathbf{1}, \quad \Omega_\omega = \sum_j \sqrt{\lambda_j}\, \psi_j \otimes \psi_j$$

- Modular structure

$$J(\psi \otimes \phi) = \bar{\phi} \otimes \bar{\psi}, \quad \mathcal{L}_\omega = \log \Delta_\omega = \log \rho \otimes \mathbf{1} - \mathbf{1} \otimes \log \rho$$

- Standard Liouvillean

$$L = H \otimes \mathbf{1} - \mathbf{1} \otimes H$$

Free Fermi gas

- C^*-dynamical system$(\mathcal{O},\tau)$ 1-Fermion: Hilbert space $\mathfrak{h}$, Hamiltonian h

Examples free non-relativistic spinless electron of mass m: $\mathfrak{h} = L^2(\mathbb{R}^3), l^2(\mathbb{Z}^3)$, $h = -\frac{\hbar^2}{2m}\Delta$

Fock space $\mathfrak{F}(\mathfrak{h})$, bounded annihilation, creation operators $a(f), a^*(f)$
$\mathcal{O} = \mathrm{CAR}(\mathfrak{h})$ generated by $a^\sharp(f), f \in \mathfrak{h}$

$$\tau^t(A) = \mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma(h)} A \mathrm{e}^{-\mathrm{i}t\mathrm{d}\Gamma(h)}$$

$\mathrm{d}\Gamma$ second quantization of h, and $\tau^t(a^\sharp(f)) = a^\sharp(\mathrm{e}^{\mathrm{i}th} f)$

- Quasifree, gauge-invariant state $T^* = T \in \mathcal{L}(\mathfrak{h})$, $0 \leq T \leq \mathbf{1}$

$$\omega(a^*(f_1)...a^*(f_n)a(g_1)...a(g_m)) = \delta_{mn} \det \left[(g_i, T f_j)\right]$$

completely determined by 2-point function

$$\omega(a^*(f)a(g)) = (g, Tf)$$

Examples $T = F(h)$: Fermi gas with energy density $F(E)$, e.g., $T = (1 + \mathrm{e}^{\beta h})^{-1}$: unique (τ, β)-KMS state, cf. XY (Pfaffian for *self-dual* CAR, cf. XY)

- GNS representation [Araki-Wyss 63] N number operator, Ω Fock vacuum

$$\begin{aligned} \mathcal{H}_\omega &= \mathfrak{F}(\mathfrak{h}) \otimes \mathfrak{F}(\mathfrak{h}), \qquad \Omega_\omega = \Omega \otimes \Omega, \\ \pi_\omega(a(f)) &= a((\mathbf{1} - T)^{1/2} f) \otimes \mathbf{1} + (-1)^N \otimes a^*(\bar{T}^{1/2} \bar{f}) \end{aligned}$$

- Modular structure

$$\begin{aligned} J(\psi \otimes \phi) &= U\bar{\phi} \otimes U\bar{\psi}, \qquad U = (-1)^{N(N-1)/2} \\ \mathcal{L}_\omega &= \log \Delta_\omega = \mathrm{d}\Gamma(S) \otimes \mathbf{1} - \mathbf{1} \otimes \mathrm{d}\Gamma(S), \qquad S = \log T(1 - T)^{-1} \end{aligned}$$

- Standard Liouvillean

$$L = \mathrm{d}\Gamma(h) \otimes \mathbf{1} - \mathbf{1} \otimes \mathrm{d}\Gamma(h)$$

Lattice spin systems

cf. 6.

2. Nonequilibrium steady states (NESS) [Ruelle 00]

$(\mathcal{O}, \tau_0)$ C^*-dynamical system, $\omega_0 \in \mathcal{E}(\mathcal{O})$, V local perturbation.

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

• non-empty, weak*-compact subset of the weak*-compact set of states $\mathcal{E}(\mathcal{O})$ ($\mathcal{O}$ unital) containing τ-invariant NESS

• Abelian averaging: $\lim_{\epsilon \to 0+} \epsilon \int_0^\infty \mathrm{d}t \, \mathrm{e}^{-\epsilon t} \omega_0 \circ \tau^t$

useful for spectral deformation

• [A-Jakšić-Pautrat-Pillet 06] ω_0 factor, weak asymptotic abelianness in mean. $\eta \in \mathcal{N}_{\omega_0} \Rightarrow \Sigma_+(\eta) = \Sigma_+(\omega_0)$

$\mathcal{M}_{\omega_0} \cap \mathcal{M}'_{\omega_0} = \mathbb{C}1$, and $\lim_{T \to \infty} \frac{1}{T} \int_0^T \mathrm{d}t \, \eta([\tau^t(A), B]) = 0$ for all $A, B \in \mathcal{O}$ and all $\eta \in \mathcal{N}_{\omega_0}$

• structural properties of NESS, spectral characterization...

Example ω_0 modular, ker L_V contains separating vector for $\mathcal{M}_{\omega_0} \Rightarrow \Sigma_+(\omega_0) \subset \mathcal{N}_{\omega_0}$

The response of the system to a local perturbation depends strongly on the nature of the initial state ω_0.

System near equilibrium:

ω_0 is (τ, β)-KMS, $\eta \in \mathcal{N}_{\omega_0}$. expect

$$\lim_{t\to\infty} \eta(\tau^t(A)) = \omega(A) \quad \text{where } \omega \text{ is } (\tau, \beta) - \text{KMS}$$

- ergodic problem reduces to spectral analysis of Liouvillean L_V
- conceptually clear, spectral analysis done for few systems only

System far from equilibrium:

ω_0 is *not* normal w.r.t. some KMS state

- conceptual framework not well understood, the following two approaches to the construction of NESS are used (rigorous literature):

the scattering approach, and the spectral approach

3. The scattering approach to NESS [Ruelle 00]

- Møller morphism $(\mathcal{O}, \tau_0)$ C^*-dynamical system, V local perturbation.

$$\gamma_+ = \lim_{t\to\infty} \tau_0^{-t} \circ \tau^t$$

algebraic analog of Hilbert space wave operator $\Omega_+ = \mathrm{s} - \lim_{t\to\infty} \mathrm{e}^{\mathrm{i}tH} \mathrm{e}^{-\mathrm{i}tH_0} 1_{\mathrm{ac}}(H_0)$

NESS ω_0 τ_0-invariant. $\Rightarrow$ $\omega_+ = \omega_0 \circ \gamma_+ \in \Sigma_+(\omega_0)$

Example ω_0 is (τ_0, β)-KMS $\Rightarrow$ ω_+ is (τ, β)-KMS

- algebraic Cook criterion for the existence of γ_+

$$\int_0^\infty \mathrm{d}t \, \|[V, \tau^t(A)]\| < \infty$$

A in dense subset of $\mathcal{O}$, and $|f(x) - f(y)| = |\int_x^y \mathrm{d}t \, f'(t)| \le \int_x^y \mathrm{d}t \, |f'(t)| \to 0$ for $f' \in L^1(\mathbb{R})$

difficult to verify in physically interesting models

Examples [A-Pillet 03], [A-Jakšić-Pautrat-Pillet 07] reduction to 1-particle Hilbert space scattering problem for quasifree systems; [Botvich-Malyshev 83] locally perturbed Fermi gas

4. The spectral approach to NESS [Jakšić-Pillet 02]

$\ker L_V$ provides information about ω_0-normal, τ-invariant states; but thermodynamically interesting NESS *not* in $\mathcal{N}_{\omega_0}$!

usual approach: scattering theory

C-Liouvillean L^*

$(\mathcal{O}, \tau_0)$ C^*-dynamical system, ω_0 modular, τ_0-invariant,
V local perturbation. assumptions about analytic continuation of $\Delta_{\omega_0}^{\mathrm{i}t} V \Delta_{\omega_0}^{-\mathrm{i}t}$, etc.

$$\mathsf{L}^* = L + V - J\Delta^{-1/2} V \Delta^{1/2} J$$

implements perturbed time evolution $\tau^t(A) = \mathrm{e}^{\mathrm{i}t\mathsf{L}^*} A \mathrm{e}^{-\mathrm{i}t\mathsf{L}^*}$, and $\Omega_{\omega_0} \in \ker \mathsf{L}$

(Abelian) NESS are weak* limit points of $\epsilon\,\omega_{\mathrm{i}\epsilon}$ for $\epsilon \to 0^+$, where

$$\omega_z(A) = \mathrm{i} \int_0^\infty \mathrm{d}t\ \mathrm{e}^{\mathrm{i}zt}\, \omega_0(\tau^t(A)) = (\Omega_{\omega_0}, A(\mathsf{L}^* - z)^{-1} \Omega_{\omega_0})$$

$\Rightarrow$ NESS described by resonance of L^* !

5. Entropy production [Jakšić-Pillet 02]

$(\mathcal{O}, \tau_0)$ C^*-dynamical system, ω_0 τ_0-invariant, V local perturbation, C^*-dynamics σ_0 with generator δ_0 s.t. ω_0 is $(\sigma_0, -1)$-KMS.

mean entropy production rate in NESS $\omega_+ \in \Sigma_+(\omega)$

$$\text{Ep}\,(\omega_+) := \omega_+(\delta_0(V))$$

Example [Open system] small system $\mathcal{S}$ coupled to extended thermal reservoirs $\mathcal{R}_k$:

$\omega_0 = \otimes_k \omega_k$, ω_k is (τ_k, β_k)-KMS, $\sigma_0^t = \otimes_k \tau_k^{-\beta_k t}$, $\delta_0 = -\sum_k \beta_k \delta_k$

$\Rightarrow$ $\text{Ep}(\omega_+) = -\sum_k \beta_k \phi_k$ with $\phi_k := \omega_+(\delta_k(V))$ heat flux leaving $\mathcal{S}$

- entropy production as asymptotic rate of decrease of relative entropy

$\int_0^T \mathrm{d}t\ \omega_0 \circ \tau^t(\delta_0(V)) = \text{Ent}(\omega_0|\omega_0) - \text{Ent}(\omega_0 \circ \tau^T|\omega_0)$

- $\text{Ep}(\omega_+) \geq 0$
- ω_+ ω_0-normal $\Rightarrow$ $\text{Ep}(\omega_+) = 0$

equivalence under weak ergodicity condition

Part 2: Some Applications

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6. Application of the scattering approach: XY model
7. Further applications

6. Application of the scattering approach: XY model

• “integrable” models as essential tools in development of equilibrium statistical mechanics - *out* of equilibrium: dynamics crucial

• XY model one of few systems for which explicit knowledge of dynamics available: ”integrable”

due to Jordan-Wigner transformation ⇒ free fermions

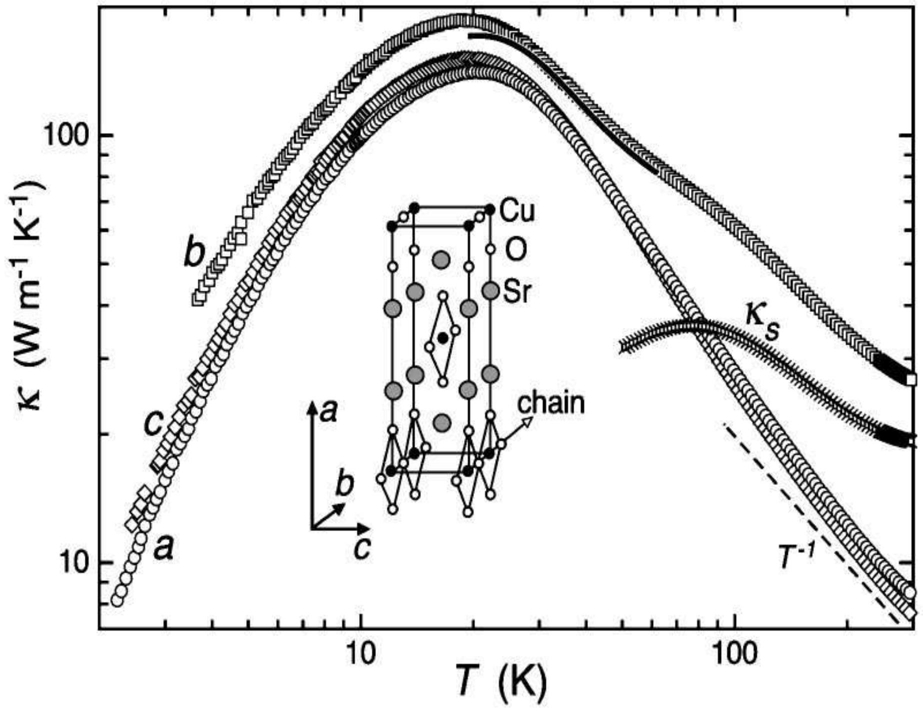
• integrability may be traced back to infinite family of charges

master symmetries [Barouch-Fuchssteiner 85], [Araki 90]

• integrability relates to anomalous transport:

theory: overlap of current with charges prevents current-current correlation to decay to zero ⇒ ”ideal thermal conductivity”
numerics: Fourier law violated for “integrable” systems
experiment: anomalous transport properties in low-dimensional magnetic systems, e.g. Heisenberg spin models

• Sr_2CuO_3



• one of the best physical realizations of $1d, S = 1/2$ XYZ Heisenberg model: interchain/intrachain interaction: $\sim 10^{-5}$ ($PrCl_3$: XY)

• [Sologubenko et al. 00] anomalously enhanced conductivity along chain

electric insulator; T high: spinons $\gg$ phonons, limited by defects & phonons

XY chain

infinite chain of spins interacting anisotropically with two nearest neighbors and with external magnetic field: $\gamma \in (-1,1)$, $\lambda \in \mathbb{R}$

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

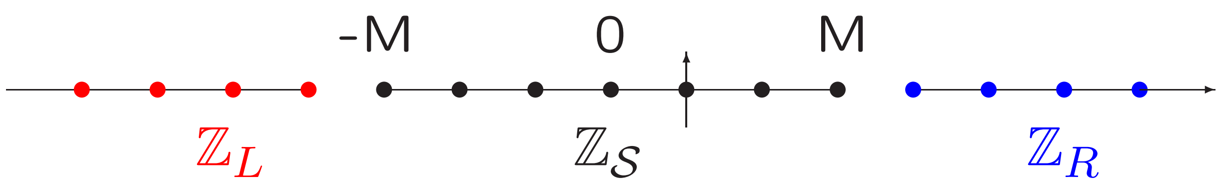
6.1 Nonequilibrium setting [A-Pillet 03]

remove bonds at the two sites $\pm M$

$\Rightarrow$ 3 decoupled subsystems with (τ_L, β_L), $(\tau_{\mathcal{S}}, 0)$, (τ_R, β_R)-KMS states

$$\omega_0 = \omega_L^{\beta_L} \otimes \omega_{\mathcal{S}} \otimes \omega_R^{\beta_R}$$

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



6.2 Observables

quasi-local C^*-algebra $\mathfrak{S}$ over $\mathbb{Z}$

$$\mathcal{H}_\Lambda = \bigotimes_{x\in\Lambda} \mathcal{H}_{\{x\}}, \quad \mathfrak{S}_\Lambda = \mathcal{L}(\mathcal{H}_\Lambda)$$

associate Hilbert space $\mathcal{H}_{\{x\}} = \mathbb{C}^2$ to $x \in \mathbb{Z}$, finite subset Λ of $\mathbb{Z}$

infinite tensor product of $\mathcal{L}(\mathcal{H}_{\{x\}})$ for x in arbitrary subset $\mathcal{Z}$ of $\mathbb{Z}$:

$$\mathfrak{S}_\mathcal{Z} = \overline{\bigcup_{\Lambda\subset\mathcal{Z}} \mathfrak{S}_\Lambda}$$

observables as limits of polynomials in Pauli matrices $\sigma_\alpha^{(x)}$, $\alpha = 0, 1, 2, 3$

Pauli matrices $\sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, $\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $\sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$, $\sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ generate $\mathcal{L}(\mathcal{H}_{\{x\}})$

and $\sigma_\alpha^{(x)} = \cdots \otimes \mathbf{1} \otimes \mathbf{1} \otimes \sigma_\alpha \otimes \mathbf{1} \otimes \mathbf{1} \otimes \cdots$

$$\mathfrak{S} = \mathfrak{S}_\mathbb{Z}, \quad \mathfrak{S}_L = \mathfrak{S}_{\{x<-M\}}, \quad \mathfrak{S}_\mathcal{S} = \mathfrak{S}_{\{-M\leq x\leq M\}}, \quad \mathfrak{S}_R = \mathfrak{S}_{\{x>M\}}$$

6.3 Dynamics

- local XY Hamiltonian $H_\Lambda = \sum_{X\subset\Lambda} \Phi(X)$, interaction $\Phi : X \to \mathfrak{S}_X$:

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

- thermodynamic limit of local perturbed dynamics:

$$\tau_\Lambda^t(A) = \mathrm{e}^{\mathrm{i}tH_\Lambda} A \mathrm{e}^{-\mathrm{i}tH_\Lambda}, \qquad \tau^t = \lim_{\Lambda\to\mathbb{Z}} \tau_\Lambda^t$$

exists since interaction short range, two-body $\Rightarrow$ defines perturbed C^*-dynamical system $(\mathfrak{S}, \tau)$

- free dynamics from local perturbation

$V = \Phi(\{-M-1, -M\}) + \Phi(\{M, M+1\})$ $\Rightarrow$ defines free C^*-dynamical system $(\mathfrak{S}, \tau_0)$

$$\mathfrak{S} = \mathfrak{S}_L \otimes \mathfrak{S}_{\mathcal{S}} \otimes \mathfrak{S}_R, \qquad \tau_0^t = \tau_L^t \otimes \tau_{\mathcal{S}}^t \otimes \tau_R^t$$

6.4 Jordan-Wigner transformation [Jordan-Wigner 28], [Araki 84]

$$a_x := TS^{(x)}(\sigma_1^{(x)} - \mathrm{i}\sigma_2^{(x)})/2, \quad S^{(x)} = \begin{cases} \sigma_3^{(1)} \cdots \sigma_3^{(x-1)}, & x > 1 \\ \mathbf{1}, & x = 1 \\ \sigma_3^{(x)} \cdots \sigma_3^{(0)}, & x < 1 \end{cases}$$

CAR $\mathfrak{A}(\mathfrak{h})$ with $\mathfrak{h} = \ell^2(\mathbb{Z})$: $\{a_x, a_y\} = 0$ and $\{a_x, a_y^*\} = \delta_{xy}$ (T for *two*-sided chain)

- interaction becomes quadratic

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

- dynamics become Bogoliubov automorphisms

$$\tau^t(B(f)) = B(\mathrm{e}^{ith} f), \quad \tau_0^t(B(f)) = B(\mathrm{e}^{ith_0} f)$$

[Araki 71] self-dual CAR: $B(f) = a^*(f_1) + a(\bar{f}_2)$ for $f = (f_1, f_2) \in \mathfrak{h}^{\oplus 2}$

- 1-particle Hamiltonians Fourier variable ξ , V (self-dual) 2nd quantization of v

$$h = (\cos\xi - \lambda) \otimes \sigma_3 + \gamma \sin\xi \otimes \sigma_2, \quad h_0 = h - v = h_L \oplus h_{\mathcal{S}} \oplus h_R$$

6.5 Existence and uniqueness of NESS

Theorem

Let $\beta_L, \beta_R > 0$, $M \in \mathbb{N}$. Then:

$$\Sigma_+(\omega_0) \;=\; \{\omega_+\}$$

Proof

- [Araki 84] $\beta_L = \beta_R \equiv \beta$: ω_+ unique (τ, β)-KMS (RTE)
- [Kato-Birman] time dependent scattering theory for trace class type perturbations: $1_{\mathrm{ac}}(h) = 1$, $v \in \mathcal{L}^0$

$\Rightarrow W_\pm(h, h_0) = \text{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}th}\,\mathrm{e}^{-\mathrm{i}th_0} 1_{\mathrm{ac}}(h_0)$ exist and are complete

completeness: $\mathrm{ran}\, W_\pm(h, h_0) = \mathfrak{h}^{(\mathrm{ac})}$ (isometricity and intertwining)

$$\gamma_+(B(f)) = \lim_{t\to\infty} \tau_0^{-t}(\tau^t(B(f))) = \lim_{t\to\infty} B(\mathrm{e}^{-\mathrm{i}th_0}\mathrm{e}^{\mathrm{i}th} f) = B(W_-^* f)$$

$\Rightarrow$ $\omega_+ = \omega_0 \circ \gamma_+$ quasifree NESS $\square$

6.6 NESS density

Theorem

ω_+ has 2-point function $\omega_+(B^*(f)B(g)) = (f, T_+ g)$ with density

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

v_- asymptotic velocity, $\beta = (\beta_R + \beta_L)/2$ and $\delta = (\beta_R - \beta_L)/2$

Proof

- $\omega_+ = \omega_0 \circ \gamma_+ \Rightarrow T_+ = W_- T_0 W_-^*$
- partial wave operators w_α, asymptotic projections P_α

$j_\alpha \colon \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2 \to \ell^2(\mathbb{Z}_\alpha) \otimes \mathbb{C}^2$, $\alpha = L, R$: canonical projections

$$w_\alpha^* = \underset{t\to-\infty}{\mathrm{s-lim}}\ \mathrm{e}^{ith_\alpha} j_\alpha \mathrm{e}^{-ith}, \qquad P_\alpha = \underset{t\to-\infty}{\mathrm{s-lim}}\ \mathrm{e}^{ith} j_\alpha^* j_\alpha \mathrm{e}^{-ith}$$

[Kato-Birman], [Davies-Simon] $\Rightarrow$ existence and completeness of P_α, and

$W_-^* = \sum_{\alpha\in\{L,R\}} j_\alpha^* W_\alpha^*$, $h_\alpha W_\alpha^* = W_\alpha^* h$, $P_\alpha = W_\alpha W_\alpha^*$, $P_L + P_R = I$, $[P_\alpha, h] = 0$

• ω_0 quasifree with density $T_0 = (1+e^{-k_0})^{-1}$, $k_0 = \beta_L h_L \oplus 0 \oplus \beta_R h_R$

$$T_+ = (1+e^{k_+})^{-1}, \quad k_+ = \beta h + \delta \underbrace{(P_R - P_L)}_{= \text{sign}\, v_-} h$$

$v_- = \text{s-res-lim}_{t\to\infty} x_t/t$ strong resolvent sense, $x = -\mathrm{i}\partial_\xi \otimes \mathbf{1}$, $x_t = \mathrm{e}^{-\mathrm{i}th} x \mathrm{e}^{\mathrm{i}th}$

• explicitely computable:

$$\text{sign}\, v_- = \text{sign}(2\lambda \sin\xi - (1-\gamma^2)\sin 2\xi)\sqrt{(\cos\xi - \lambda)^2 + \gamma^2 \sin^2\xi} \otimes \sigma_0$$

Fourier variable ξ

□

Remarks

• since $k_+ = \beta_L h P_L \oplus \beta_R h P_R$, NESS ω_+ describes mixture of two independent species: "left-movers" from ran P_R carry β_R, "right-movers" from ran P_L carry β_L

• further properties: ω_+ is attractive, independent of M, translation invariant, factor, modular, quasifree, KMS iff $\beta_L = \beta_R$, singular w.r.t. ω_0

Does ω_+ have nontrivial thermodynamics in the sense that its entropy production is strictly positive?

6.7 Entropy production

entropy production in the open system:

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

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

Theorem

$$\mathrm{Ep}(\omega_+) = \frac{\delta}{4} \int_0^{2\pi} \frac{\mathrm{d}\xi}{2\pi} |\kappa| \frac{\mathrm{sh}\,\delta\mu}{\mathrm{ch}^2(\beta\mu/2) + \mathrm{sh}^2(\delta\mu/2)} > 0 \text{ iff } \beta_L \neq \beta_R$$

$\kappa(\xi) = 2\mathbf{p} \cdot \mathbf{h} = 2\lambda \sin\xi - (1-\gamma^2)\sin 2\xi$ and $\mu(\xi) = \sqrt{(\cos\xi - \lambda)^2 + \gamma^2 \sin^2\xi}$

Proof explicit computation! □

Remark

• first rigorous application of Ruelle's scattering approach to a thermodynamically nontrivial system

7. Further applications

7.1 Quasifree fermionic systems [A-Jakšić-Pautrat-Pillet 07]

NESS interaction of trace class type, no singular continuous spectrum

initial state τ_0^t-invariant and quasifree with density ϱ_0:

$$\omega_+(\mathrm{d}\Gamma(c)) = \mathrm{tr}(\varrho_+ c) \text{ with } \varrho_+ = W_- \varrho_0 W_-^* + \sum_{\varepsilon \in \sigma_{\mathrm{pp}}(h)} 1_\varepsilon(h) \varrho_0 1_\varepsilon(h)$$

Landauer-Büttiker formalism derives from Ruelle's approach:

$$\omega_+(\Phi_q) = \int_{\sigma_{\mathrm{ac}}(h_0)} \frac{\mathrm{d}\varepsilon}{2\pi}\, \mathrm{tr}(\varrho_0(\varepsilon)[q(\varepsilon) - S^*(\varepsilon) q(\varepsilon) S(\varepsilon)])$$

$\Rightarrow$ Landauer Büttiker formula
$\Rightarrow$ entropy production
$\Rightarrow$ kinetic transport koefficients, Onsager relations

7.2 Weak coupling theory [A-Spohn 06]

Entropy production   algebraic criterion which ensures strict positivity in the weak coupling limit:

$$\{H_{\mathcal{S}}, Q_j\}' = \mathbb{C}1 \quad \Rightarrow \quad \mathrm{Ep}(\omega_+^\lambda) = \lambda^2 \sigma(\rho_0) + \mathcal{O}(\lambda^3) > 0$$

7.3 Correlations [A-Barbaroux 06], [A 07]

Spatial spin-spin correlations   decay rate out of equilibrium: spectral condition on quasifree density implies exponential decay

break translation invariance [A in progress]

von Neumann entropy density   asymptotic behavior: "left-movers" and "right-movers"

7.4 More...

intermediate times, interacting systems, phase transitions, symmetries, fluctuations,...