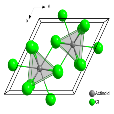
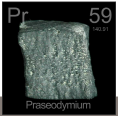
Rigorous scattering approach to quasifree fermionic systems out of equilibrium





Walter H. Aschbacher

Université de Toulon, Aix Marseille Univ, CNRS, CPT, Toulon, France

IWNET 2018 Sint-Michielsgestel – July 6, 2018

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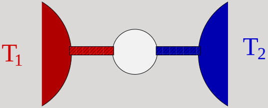
Open systems: Fundamental paradigm

A confined sample is suitably coupled to two thermal reservoirs at different temperatures:



We want to study the following natural questions:

PHYS

- Is the coupled system approaching a unique state for large times?
- If so, how does this asymptotic state relate to the underlying scattering process?
- Does it carry a nonvanishing heat flux?

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How to describe our paradigm from first principles?

- An extended thermal reservoir has a large number N of degrees of freedom
- Idealization: $N \notin \mathbb{N}$

  MATH 2 approaches: TD limit of finite systems, directly infinite systems
- If $N \notin \mathbb{N}$, no universal Hilbert space description available due to the existence of inequivalent representations (unlike $N \in \mathbb{N}$)

  MATH E.g. Araki-Wyss GNS representation of quasifree fermionic systems

Our algebraic formulation has the following 3 ingredients:

[1930s: von Neumann, Murray, Gelfand, Segal, etc.]

Def: Observables, dynamics, and states

- Unital C^*-algebra $\mathfrak{A}$
- Strongly continuous group $\tau^t \in \mathrm{Aut}(\mathfrak{A})$
- Normalized positive $\omega \in \mathfrak{A}^*$

MATH E.g. $\mathfrak{A} = \mathcal{L}(\mathfrak{H})$ with $\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}$ and mixed state $\omega(A) = \mathrm{tr}(\varrho A)$

Quasifree fermions play an important role (in and) out of equilibrium:

- They allow for a powerful description by means of scattering theory on the one-particle Hilbert space which underlies the observable algebra
- They are realized in nature
  PHYS E.g. Metallic solids in the independent electron approximation
  E.g. XY spin chain (also XX if $\gamma = 0$) [Lieb *et al.* 1961, Araki 1984]:
  $(1+\gamma)\sigma_i^x\sigma_{i+1}^x + (1-\gamma)\sigma_i^y\sigma_{i+1}^y$ vs. $a_i^* a_{i+1} + a_{i+1}^* a_i + \gamma(a_i^* a_{i+1}^* + a_{i+1} a_i)$
  $PrCl_3$: Cover page! [e.g. Culvahouse *et al.* 1969, D'Iorio *et al.* 1983]

We next specify the 3 ingredients for quasifree fermionic systems:

Def: Selfdual CAR [Araki 1971]

The generators $B(F)$ with $F \in \mathfrak{H}$ of a selfdual CAR algebra $\mathfrak{A}$ over a complex 1-particle Hilbert space $\mathfrak{H}$ endowed with an antiunitary involution J satisfy:

- $\mathfrak{H} \ni F \mapsto B(F) \in \mathfrak{A}$ is complex linear
- $B^*(F) = B(JF)$
- $\{B^*(F), B(G)\} = (F, G)1$

MATH Natural framework ($*$-isomorphic with CAR algebra over the range of any basis projection):

$$\mathfrak{H} = \mathfrak{h} \oplus \mathfrak{h} \quad \text{with} \quad J f_1 \oplus f_2 = \bar{f}_2 \oplus \bar{f}_1 \quad \text{and} \quad B(f_1 \oplus f_2) = a^*(f_1) + a(\bar{f}_2)$$

PHYS Broken gauge invariance (e.g. XY)

The other 2 ingredients are as follows:

Def: Bogoliubov dynamics

The quasifree dynamics on the selfdual CAR algebra $\mathfrak{A}$ generated by the Hamiltonian $H \in \mathcal{L}(\mathfrak{H})$ with $H^* = H$ and $JHJ = -H$ is given by:

$$\tau^t(B(F)) = B(\mathrm{e}^{\mathrm{i}tH}F)$$

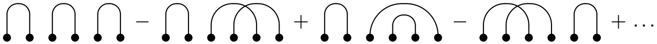
MATH C^*-dynamical system: $(\mathfrak{A}, \tau^t)$
Strong continuity: $2\|B(F)\|^2 = \|F\|^2 + [\|F\|^4 - |(F, JF)|^2]^{\frac{1}{2}} \leq 2\|F\|^2$

Def: Quasifree state

The quasifree state induced by the 2-point operator $R \in \mathcal{L}(\mathfrak{H})$ with $R^* = R$, $0 \leq R \leq 1$, and $JRJ = 1 - R$, is an even state given by:

$$\omega(B(F_1)B(F_2)\dots B(F_{2n})) = \mathrm{pf}\big([(JF_i, RF_j)]_{i,j\in\{1,\dots,2n\}}\big)$$

MATH Pfaffian: $\mathrm{pf}(A) = \sum_\pi \mathrm{sign}(\pi) \prod_{i=1}^n A_{\pi(2i-1),\pi(2i)}$, summing over pairings:



$\pi = (123456)$ $\pi = (123546)$ $\pi = (123645)$ $\pi = (132456)$

PHYS Gauge invariance: R is diagonal w.r.t. $\mathfrak{H} = \mathfrak{h} \oplus \mathfrak{h}$

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Def: Nonequilibrium steady state (NESS) [Ruelle 2001]

The NESS associated with ω_0 and τ^t are the limits for $T \to \infty$ of

$$\frac{1}{T}\int_0^T \mathrm{d}t \ \omega_0 \circ \tau^t$$

MATH Weak-$*$ topology: $\mathcal{B}_{A_1,\dots,A_n;\varepsilon}(\omega) = \{\omega' \in \mathfrak{A}^* \mid |\omega'(A_i) - \omega(A_i)| < \varepsilon \text{ for all } i\}$

PHYS Inherent imprecision of measurements

We specialize to the fundamental paradigm for quasifree fermionic systems:

Def: Nonequilibrium setting

- The 1-particle Hilbert space reads $\mathfrak{H} = \mathfrak{H}_L \oplus \mathfrak{H}_\mathcal{S} \oplus \mathfrak{H}_R$
- The dynamics τ_0^t, generated by H_0, propagates the decoupled system
- The quasifree state ω_0, induced by R_0, describes the decoupled system with reservoirs in thermal equilibrium at temperatures $T_L \neq T_R$
- The dynamics τ^t, generated by H, couples the reservoirs to the sample

PHYS Configuration space $\mathbb{Z} = \mathbb{Z}_L \cup \mathbb{Z}_\mathcal{S} \cup \mathbb{Z}_R$ (e.g. XY)

MATH KMS state: $\omega(A\tau^{\mathrm{i}\beta}(B)) = \omega(BA)$ (on entire analytic subalgebra)

Thm: NESS [A-Pillet 2003, A 2018 ip]

If the coupling satisfies $H - H_0 \in \mathcal{L}^1(\mathfrak{H})$, there exists a unique NESS ω_+ associated with ω_0 and τ^t whose 2-point operator has the form

$$R_+ = W_+^* R_0 W_+ + \sum_{\lambda \in \sigma_{\mathrm{pp}}(H)} 1_\lambda(H) R_0 1_\lambda(H)$$

MATH/PHYS The wave operator from scattering theory is defined by:

$$W_+ = \mathrm{s} - \lim_{t \to +\infty} \mathrm{e}^{-\mathrm{i}tH_0} \mathrm{e}^{\mathrm{i}tH} 1_{\mathrm{ac}}(H)$$

Ingredients of the *Proof*:

- Since ω_0 is quasifree, we analyze the 2-point function
- The spectral decomposition (with $1_{\mathrm{sc}}(H) = 0$) and Kato-Rosenblum theory yields the scattering contribution since, as $[H_0, R_0] = 0$, we can write:

$$\omega_0(\tau^t[B(F)B(G)]) = (\mathrm{e}^{-\mathrm{i}tH_0} \mathrm{e}^{\mathrm{i}tH} JF, R_0 \mathrm{e}^{-\mathrm{i}tH_0} \mathrm{e}^{\mathrm{i}tH} G)$$

- Averaging yields the $1_{\mathrm{pp}}(H)$-contribution and, generally, a non-quasifree NESS

MATH Well-developed techniques from scattering theory (in particular, the stationary approach)

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The next 3 examples succinctly illustrate rigorous scattering theory in action:

PHYS E.g. the translation invariant XY/XX chains

Thm 1: Entropy production [A-Pillet 2003, A *et al.* 2007, A 2018 ip]

The heat flux, i.e., the NESS expecation value of the extensive energy current observable describing the energy flow from one reservoir into the sample, is

$$\frac{1}{2\delta}\,\mathrm{Ep}(\omega_+) = \int_{\mathbb{T}} \mathrm{d}k\ |V_+ H|\ [\rho_L(|H|) - \rho_R(|H|)]$$

MATH L/R movers: Fermi exponent $\beta H + \delta \mathrm{sign}(V_+) H$ with asymptotic velocity V_+

PHYS Strict positivity of the entropy production

Thm 2: Weak coupling [A 2013]

The entropy production σ_δ in the van Hove weak coupling regime $\lambda \to 0$ is related to the microscopic entropy production as

$$\mathrm{Ep}(\omega_+) = \sigma_\delta \lambda^2 + \mathcal{O}(\lambda^4)$$

MATH Regularity through the stationary approach

PHYS Triviality of commutants implies strict positivity of the van Hove entropy production

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Thm 3: Nonequilibrium phase transitions [A 2016, 2018 ip]

If the sample is exposed to a local external magnetic field $\mu \to 0$, the entropy production exhibits a second order quantum phase transition

$$\partial_\mu \mathrm{Ep}(\omega_+) = C_\delta \, \mu \log(\mu) + \mathcal{O}(\mu)$$

PHYS Ehrenfest type classification

The following properties have also been rigorously derived:

- Landauer-Büttiker: Heat flux through the 1-particle S-matrix (entropy production, linear response,...) [A *et al.* 2007]
- Correlations: Asymptotic regimes or upper bounds (spin-spin, efp, von Neumann entropy), broken translation invariance [A 2010, 2011]

  MATH Subtle problems from Toeplitz theory due to nonequilibrium symbol singularities

Quasifree fermionic systems are rich:

A lot more to come!

- Nonequilibrium phase transitions: Universality classes
- Entropy production: Symmetries and C^* structural properties
- Correlations: Perturbation theory

Thank you!