Rigorous scattering approach to quasifree fermionic systems out of equilibrium

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1. Motivation

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?
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 $\tau^t \in \text{Aut}(\mathfrak{A})$
- Normalized positive $\omega \in \mathfrak{A}^*$

Math E.g. $\mathfrak{A} = \mathcal{L}(\mathfrak{H})$ with $\tau^t(A) = e^{itH} A e^{-itH}$ and mixed state $\omega(A) = \text{tr}(\varrho A)$
3. Quasifree fermionic systems

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]:
\[(1 + \gamma)\sigma^x_i \sigma^x_{i+1} + (1 - \gamma)\sigma^y_i \sigma^y_{i+1} \text{ vs. } a_i^* a_{i+1} + a_{i+1}^* a_i + \gamma(a_i^* a_{i+1} + a_{i+1} a_i)\]

**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:

<table>
<thead>
<tr>
<th>Def: Selfdual CAR [Araki 1971]</th>
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<td>The generators ( B(F') ) with ( F \in \mathcal{F} ) of a selfdual CAR algebra ( \mathfrak{A} ) over a complex 1-particle Hilbert space ( \mathcal{F} ) endowed with an antiunitary involution ( J ) satisfy:</td>
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<tr>
<td>- ( \mathcal{F} \ni F \mapsto B(F') \in \mathfrak{A} ) is complex linear</td>
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<td>- ( B^*(F) = B(JF) )</td>
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<td>- ( {B^*(F), B(G)} = (F, G)_1 )</td>
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</table>

**MATH** Natural framework (\(*\)-isomorphic with CAR algebra over the range of any basis projection):
\[\mathcal{F} = \mathfrak{h} \oplus \bar{\mathfrak{h}} \text{ with } Jf_1 \oplus f_2 = \bar{f}_2 \oplus \bar{f}_1 \text{ and } B(f_1 \oplus f_2) = a^*(f_1) + a(\bar{f}_2)\]

**PHYS** Broken gauge invariance (e.g. XY)
3. Quasifree fermionic systems

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:

\[
\tau^t(B(F)) = B(e^{itH}F)
\]

**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:

\[
\omega(B(F_1)B(F_2)\ldots B(F_{2n})) = \text{pf}\left(\left[(JF_i, RF_j)\right]_{i,j\in\{1,\ldots,2n\}}\right)
\]

**PHYS** Gauge invariance: \( R \) is diagonal w.r.t. \( \mathfrak{H} = \mathfrak{h} \oplus \mathfrak{h} \)
4. Scattering approach to NESS

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

The NESS associated with $\omega_0$ and $\tau^t$ are the limits for $T \to \infty$ of

$$\frac{1}{T} \int_0^T dt \, \omega_0 \circ \tau^t$$

**MATH** Weak-$\ast$ topology: $B_{A_1,\ldots,A_n} \varepsilon(\omega) = \{ \omega' \in \mathcal{A}^* \mid |\omega'(A_i) - \omega(A_i)| < \varepsilon \text{ for all } i \}$

**PHYS** Inherent imprecision of measurements

We specialize to the fundamental paradigm for quasifree fermionic systems:

**Def: Nonequilibrium setting**

- The 1-particle Hilbert space reads $\mathcal{H} = \mathcal{H}_L \oplus \mathcal{H}_S \oplus \mathcal{H}_R$
- The dynamics $\tau_0^t$, generated by $H_0$, propagates the decoupled system
- The quasifree state $\omega_0$, induced by $R_0$, describes the decoupled system with reservoirs in thermal equilibrium at temperatures $T_L \neq T_R$
- The dynamics $\tau^t$, generated by $H$, couples the reservoirs to the sample

**PHYS** Configuration space $\mathcal{Z} = \mathcal{Z}_L \cup \mathcal{Z}_S \cup \mathcal{Z}_R$ (e.g. XY)

**MATH** KMS state: $\omega(A \tau^{i\beta}(B)) = \omega(BA)$ (on entire analytic subalgebra)
4. Scattering approach to NESS

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

If the coupling satisfies $H - H_0 \in L^1(\mathfrak{H})$, there exists a unique NESS $\omega_+$ associated with $\omega_0$ and $\tau^t$ whose 2-point operator has the form

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

**MATH: The wave operator from scattering theory is defined by:**

$$W_+ = s - \lim_{t \to +\infty} e^{-itH_0} e^{itH} 1_{ac}(H)$$

**Ingredients of the Proof:**

- Since $\omega_0$ is quasifree, we analyze the 2-point function
- The spectral decomposition (with $1_{sc}(H) = 0$) and Kato-Rosenblum theory yields the scattering contribution since, as $[H_0, R_0] = 0$, we can write:

$$\omega_0(\tau^t [B(F)B(G)]) = (e^{-itH_0} e^{itH} JF, R_0 e^{-itH_0} e^{itH} G)$$

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

**MATH** Well-developed techniques from scattering theory (in particular, the stationary approach)
The next 3 examples succinctly illustrate rigorous scattering theory in action:

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

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

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

\[
\frac{1}{2\delta} \, \text{Ep}(\omega_+) = \int_T \text{dk} \, |V_+ H| \left[ \rho_L(|H|) - \rho_R(|H|) \right]
\]

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

**PHYS** Strict positivity of the entropy production

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**Thm 2: Weak coupling** [A 2013]

The entropy production \( \sigma_\delta \) in the van Hove weak coupling regime \( \lambda \to 0 \) is related to the microscopic entropy production as

\[
\text{Ep}(\omega_+) = \sigma_\delta \lambda^2 + \mathcal{O}(\lambda^4)
\]

**MATH** Regularity through the stationary approach

**PHYS** Triviality of commutants implies strict positivity of the van Hove entropy production
5. Transport properties

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

$$\partial_\mu E_p(\omega_+) = C_\delta \mu \log(\mu) + O(\mu)$$

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]


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!