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ZENTRUM MATHEMATIK

Algebraic Approach to Open Quantum Systems

Habilitation thesis written by

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Contents

Organization of the thesis

The present habilitation thesis deals with the rigorous algebraic approach to non-equilibrium quantum statistical mechanics I've been involved in recently. The main body of the thesis consists of original research articles (Chapters 2 to 9) to which I prepend an overview (Chapter 1) whose goal is twofold. It is supposed to serve, first, as a general introduction to non-equilibrium quantum statistical mechanics and, second, as a condensed presentation of our work on the specific models of Chapters 2 to 9 within the framework of the foregoing general theory.

More precisely, in Section 2 of Chapter 1, I explain the C^*-algebraic approach to non-equilibrium quantum statistical mechanics. In Section 3, the general framework of Section 2 is specialized to the important case of open systems, a setting which serves as paradigm for the study of systems out of equilibrium. In Sections 4 to 8, these general concepts are applied to the class of quasi-free models (besides Section 7 which is of greater generality). In order to keep the overview sufficiently short, we omit most of the details in the main text. If, however, it is felt that more details have to be given, they are put into footnotes. Moreover, the proofs, if displayed at all, are sketched only. Detailed proofs can be found in the Chapters 2 to 9.

Acknowledgments

It is a great pleasure to warmly thank all of my collaborators for the enriching cooperation.

Chapter 1

Overview

1 Introduction

Since a few years, there is a renewed interest in the field of rigorous non-equilibrium quantum statistical mechanics (cf. [7, 27] for example for a brief introduction). At the heart of this activity is the construction of the so-called *non-equilibrium steady state* (NESS) and the corresponding mean *entropy production rate* (EPR). Although a time independent approach to the construction of NESS has become available recently (cf. [27, 28]), most of the work described in this overview uses the more traditional approach making use of time dependent scattering theory on the algebra of observables (cf. [38, 39]).[1] Furthermore, the models we consider are so-called *open systems*. An open system configuration consists of a *sample* system being frequently finite dimensional or at least confined, and an extended *reservoir* (also called *environment*) which, in turn, may consist of several subreservoirs, cf. Figure 1.

For the sake of concreteness, we start off, wherever possible, with the discussion of a particular open system, the so-called *XY chain* (cf. [3, 4]) which is a special instance of the class of Heisenberg spin models in one dimension (cf. [33]). In due course, we will extend the exposition to the more general *electronic black box* (EBB) model which is a quasi-free fermionic system whose dynamics act by so-called *Bogoliubov* evolutions (cf. [7, 9]).[2] As a consequence, the problem of constructing a NESS boils down to a scattering problem in the one-particle Hilbert space

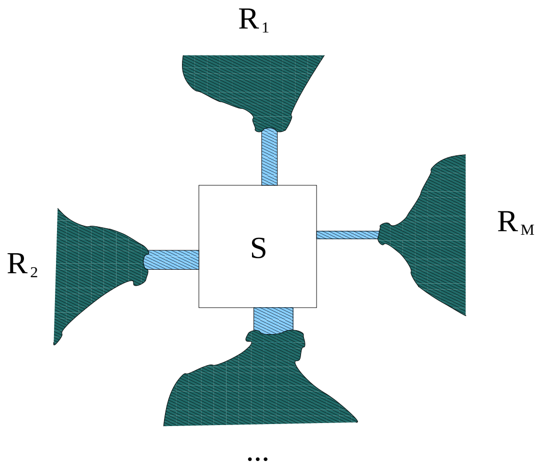

Figure 1: The sample $\mathcal{S}$ coupled to M reservoirs $\mathcal{R}_j$.

over which the observable algebra is built. For our choice of couplings between the sample and the reservoirs[3], we are left with a problem from time dependent scattering theory for perturbations of trace class type.

Then, having a (unique) NESS at our disposal, we can study the thermodynamics of an open system. First and foremost, we are interested in the existence of non-vanishing steady heat[4] fluxes across the sample. This is equivalent to show that the mean EPR in this NESS is strictly positive. Whereas, in certain cases, it is possible to do that in the full microscopic model (cf. [28, 4, 7]), we rely, in other cases, on the *weak coupling* (or *van Hove*) description which allows to extract the leading order contribution to the mean EPR for sufficiently small couplings (cf. [5, 7]). Of course, for this purpose, we have to make sure that the weak coupling regime can indeed be rigorously related to the microscopic description (cf. [28, 7]).
Moreover, we will see that the scattering approach naturally leads to the so-called *Landauer-Büttiker theory* which expresses such fluxes (and, hence, the mean EPR) by means of the scattering operator of the underlying scattering process. Using this theory, we derive the *Onsager reciprocity relations* (ORR) and the

[1] The algebraic framework allows for a “coordinate free” description of the thermodynamic limit of a local system.

[2] Occasionally, we will report on results in a particular EBB model, the so-called *simple* EBB (SEBB) model treated in [7].

[3] Symbolized by the shaded tube in Figure 1.

[4] or matter or charge etc.

Green-Kubo fluctuation-dissipation formula (GKF) of linear response theory (cf. [9]). Linear response theory provides an approximation of the physical situation where the non-equilibrium configuration is not too far from equilibrium.
Finally, we study *correlation functions* which describe the spatial interdependence of typical observables in systems out of equilibrium (and in more general quasi-free systems) using Toeplitz theory. Whereas, for some type of correlations (spin-spin, emptiness formation), we establish spectral criteria on the density of the quasi-free (non-equilibrium) state which guarantee exponential decay in the limit of large space separation (cf. [6, 10, 11, 12]), we directly determine the exact asymptotic behavior for others (von Neumann entropy, cf. [8]). Moreover, we recently started the investigation of a specific temporal correlation function in quasi-free systems, namely the generating function of the Gallavotti-Cohen symmetry (cf. [13]).

2 General framework

In this Section, we first explain the general set-up used in the algebraic description of a quantum mechanical system, namely the objects representing its algebra of observables, its physical states, and its dynamics. Afterwards, we introduce a particular state, the NESS, which has already been mentioned in the Introduction. Finally, the mean EPR in a NESS is defined as the rate of change of the so-called *relative entropy*.

Algebraic quantum statistical mechanics

The physical observables of a quantum mechanical system are elements of a C^*-algebra $\mathcal{O}$ with identity[5], whereas the time evolution is defined to be a strongly continuous group τ^t of $*$-automorphisms[6] of $\mathcal{O}$.[7] We denote the group of $*$-automorphism of $\mathcal{O}$ by $\mathrm{Aut}(\mathcal{O})$. Such a τ^t is called a *C^*-dynamics* and the pair $(\mathcal{O},\tau)$ a *C^*-dynamical system* (cf. [17, p.136]).

Remark 1 Note that it is not possible to assume the dynamics to be strongly continuous for all quantum mechanical systems, e.g. for free bosons, the dynamics is σ-weakly continuous only (cf. [18, p.57]).[8] But, since we are treating free fermionic systems in the following whose dynamics are strongly continuous, we restrict our discussion to C^*-dynamical systems.

A state ω is a normalized[9] positive[10] linear functional on $\mathcal{O}$. We denote by $\mathcal{E}(\mathcal{O})$ the set of all states on $\mathcal{O}$.[11] For most computational purposes, we have to choose some Hilbert space "coordinatization", i.e. we have to leave the representation independent formulation in terms of C^*-algebras. A useful coordinatization is established with the help of the so-called *GNS theorem*[12] which, for any state $\omega \in \mathcal{E}(\mathcal{O})$, asserts the existence (and uniqueness[13]) of a representation π_ω of the C^*-algebra $\mathcal{O}$ on some Hilbert space $\mathcal{H}_\omega$ s.t.

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

for some cyclic[14] vector $\Omega_\omega \in \mathcal{H}_\omega$. W.r.t. this representation, we can introduce the following two types of states. First, for a given $\omega \in \mathcal{E}(\mathcal{O})$, a linear functional

[5]A *C^*-algebra* $\mathcal{O}$ is an algebra (over $\mathbb{C}$ here) equipped with an involution $*$ and a submultiplicative norm $\|\cdot\|$ which is complete and has the property

$$\|A^*A\| = \|A\|^2.$$

An identity 1 is an element of $\mathcal{O}$ such that $1A = A1 = A$.

[6]A $*$-automorphism of $\mathcal{O}$ is a bijective $*$-morphism of $\mathcal{O}$ into itself.

[7] More precisely, τ is a strongly continuous representation of the additive group $\mathbb{R}$ in $\mathrm{Aut}(\mathcal{O})$, i.e. $\tau^t \in \mathrm{Aut}(\mathcal{O})$ with

$$\tau^0 = 1, \quad \tau^s\tau^t = \tau^{s+t},$$

and the map $\mathbb{R} \ni t \mapsto \tau^t(A) \in \mathcal{O}$ is continuous in norm.

[8]This is then called a *W^*-dynamical system*.

[9]I.e. $\omega(1) = 1$.

[10]I.e. $\omega(A^*A) \geq 0$. Note that ω is continuous if ω is positive (cf. [17, p.49]). Hence, $\omega \in \mathcal{O}^*$, where $\mathcal{O}^*$ is the Banach space dual of $\mathcal{O}$.

[11]$\mathcal{E}(\mathcal{O})$ is a convex subset of $\mathcal{O}^*$. Moreover, it is compact in the weak-$*$ topology (cf. [17, p.53]).

[12]The Gelfand-Naimark-Segal theorem (cf. [18, p.56]).

[13]Up to unitary equivalence.

[14]I.e. the set $\{\pi_\omega(A)\Omega_\omega : A \in \mathcal{O}\}$ is dense in $\mathcal{H}_\omega$.

$\omega' \in \mathcal{O}^*$ is called ω*-normal* iff there exists a trace class operator $\rho' \in \mathcal{L}^1(\mathcal{H}_\omega)$[15] s.t.

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

We denote by $\mathcal{N}_\omega$ the set of all ω-normal states. Second, a state $\omega \in \mathcal{E}(\mathcal{O})$ is called a *factor state* iff its enveloping von Neumann algebra[16] $\mathfrak{M}_\omega = \pi_\omega(\mathcal{O})''$ is a factor.[17] Moreover, again representation independent, we define the following states used later on. Let $(\mathcal{O}, \tau)$ be a C^*-dynamical system, $\omega \in \mathcal{E}(\mathcal{O})$, $\beta \in \mathbb{R}$, and $\mathfrak{D}_\beta = \{z \in \mathbb{C} : \min\{0, \beta\} < \mathrm{Im} z < \max\{0, \beta\}\}$. A state ω is a (τ, β)*-KMS state*[18] iff, for any $A, B \in \mathcal{O}$, there exists a holomorphic function $F_{A,B}$ on $\mathfrak{D}_\beta$ which is bounded and continuous on the closure $\overline{\mathfrak{D}}_\beta$ with boundary values[19]

$$\begin{aligned} F_{A,B}(t) &= \omega(A\tau_t(B)), \\ F_{A,B}(t+i\beta) &= \omega(\tau_t(B)A). \end{aligned}$$

Finally, a state $\omega \in \mathcal{E}(\mathcal{O})$ is called *modular* iff there exists a C^*-dynamics σ_ω^t on $\mathcal{O}$ s.t. ω is a $(\sigma_\omega, -1)$-KMS state.

Non-equilibrium steady states

We now address our main question of how to set up the frame for the description of systems which are out of equilibrium. First and foremost, we have to provide a definition of what could make up a sensible class of non-equilibrium states. Following [38, 39], we define the class of *non-equilibrium steady states* (NESS) as follows.

Definition 2 (cf. [38, 39]) *Let $(\mathcal{O}, \tau)$ be a C^*-dynamical system, and let $\omega_0 \in \mathcal{E}(\mathcal{O})$ be a given reference state. Then, the "NESS associated with ω_0 and τ" are defined to be the limit points in the weak-$*$ topology of the net*[20]

$$\frac{1}{T} \int_0^T \mathrm{d}t \; \omega_0 \circ \tau^t, \quad T > 0. \tag{1}$$

The set of NESS associated with ω_0 and τ is denoted by $\Sigma_+(\omega_0, \tau)$.[21]

One may wonder to what extent the set $\Sigma_+(\omega_0, \tau)$ depends on the reference state ω_0. On physical grounds, one expects that it remains unchanged if ω_0 is replaced by some ω_0' which is not too far from ω_0, and if we assume ω_0 to be sufficiently regular.

Theorem 3 (cf. [7]) *Let $(\mathcal{O}, \tau)$ be a C^*-dynamical system, and let $\omega_0 \in \mathcal{E}(\mathcal{O})$ be a factor state which is "weakly asymptotic abelian in mean".*[22] *Then,*

$$\Sigma_+(\omega_0', \tau) = \Sigma_+(\omega_0, \tau) \quad \text{if } \omega_0' \in \mathcal{N}_{\omega_0}.$$

Next, we turn our attention to the construction of NESS. As described in the Introduction, we will make use of the time dependent scattering method. The central object of this approach is the so-called *Møller morphism*, the analog in the C^*-algebraic setting of the wave operator in Hilbert space scattering theory. To do so, let $(\mathcal{O}, \tau_0)$ be a C^*-dynamical system and $V = V^* \in \mathcal{O}$ a so-called *local perturbation*. W.r.t. such a perturbation V, we define the perturbed C^*-

[15] We denote by $\mathcal{L}(\mathcal{H})$ and $\mathcal{L}^1(\mathcal{H})$ the bounded operators and the trace class operators on the Hilbert space $\mathcal{H}$, respectively.

[16] A *von Neumann algebra* $\mathfrak{M}$ on a Hilbert space $\mathcal{H}$ is a $*$-subalgebra of $\mathcal{L}(\mathcal{H})$ (with the adjoint operation as involution) such that $\mathfrak{M}'' = \mathfrak{M}$. Here,

$$\mathfrak{M}' = \{A \in \mathcal{L}(\mathcal{H}) : [A, B] = 0 \text{ for all } B \in \mathfrak{M}\}$$

is called the *commutant* of $\mathfrak{M}$, where $[A, B] = AB - BA$ denotes the commutator of A and B. Moreover, $\mathfrak{M}'' = (\mathfrak{M}')'$ is the so-called *bicommutant*.

[17] A von Neumann algebra $\mathfrak{M}$ on $\mathcal{H}$ is a *factor* iff its center $\mathfrak{Z}(\mathfrak{M}) = \mathfrak{M} \cap \mathfrak{M}'$ is trivial, i.e. if $\mathfrak{Z}(\mathfrak{M}) = \mathbb{C}1$.

[18] KMS stands for Kubo-Martin-Schwinger.

[19] Cf. [18, p.81]. If $\beta = 0$, we set $\overline{\mathfrak{D}}_\beta = \mathbb{R}$.

[20] For the directed system with T in the index set $(0, \infty)$ (and ordering "$\leq$").

[21] $\Sigma_+(\omega_0, \tau)$ is a non-empty, weak-$*$ compact subset of $\mathcal{E}(\mathcal{O})$ whose elements are τ*-invariant*, i.e.

$$\omega \circ \tau^t = \omega.$$

In general, for a C^*-dynamical system $(\mathcal{O}, \tau)$, we denote by $\mathcal{E}(\mathcal{O}, \tau)$ the τ-invariant states in $\mathcal{E}(\mathcal{O})$.

[22] I.e. $\lim_{T \to \infty} \int_0^T \mathrm{d}t \, \omega_0'([\tau^t(A), B])/T = 0$ for all $\omega_0' \in \mathcal{N}_{\omega_0}$.

dynamics $\tau^t \in \mathrm{Aut}(\mathcal{O})$ by Dyson's series,

$$\begin{aligned}\tau^t(A) &= \tau_0^t(A) \\ +\sum_{n\geq 1} i^n \left(\prod_{j=0}^{n-1}\int_0^{t_j}\mathrm{d}t_{j+1}\right) &\mathrm{ad}_n(t_n,...,t_1,t),\end{aligned} \qquad (2)$$

where we set $t_0 = t$ and make use of the definition

$$\begin{aligned}\mathrm{ad}_1(t_1,t) &= [\tau_0^{t_1}(V), \tau_0^t(A)], \\ \mathrm{ad}_n(t_n,...,t_1,t) &= [\tau_0^{t_n}(V), \mathrm{ad}_{n-1}(t_{n-1},...,t_1,t)].\end{aligned}$$

The following theorem formulates the algebraic analog of *Cook's criterion* in Hilbert space scattering theory (cf. [43, p.84]).

Theorem 4 (cf. [37, 7]) *Let the C^*-dynamical system $(\mathcal{O},\tau)$ be "asymptotically integrable w.r.t. the local perturbation V" generating the perturbed dynamics τ, i.e. assume that*

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

for all A in a dense subset of $\mathcal{O}$. Then,

$$\gamma_+ = \mathrm{s}-\lim_{t\to\infty} \tau_0^{-t}\circ\tau^t \qquad (3)$$

exists and defines a monomorphism[23] *which is called the "Møller morphism" on $\mathcal{O}$.*

As soon as we are assured, in one way or another, of the existence of the Møller morphism (as it will be the case in the models treated below), the following basic observation for a τ_0-invariant reference state ω_0 immediately leads to the construction of the unique NESS.

Theorem 5 (cf. [7]) *Let $(\mathcal{O},\tau_0)$ be a C^*-dynamical system, $\omega_0 \in \mathcal{E}(\mathcal{O},\tau_0)$ a reference state, and V a local perturbation. Then, if the Møller morphism γ_+ exists, there exists a unique NESS $\omega_+ \in \Sigma_+(\omega_0,\tau)$ of the form*

$$\omega_+ = \omega_0 \circ \gamma_+.$$

[23] I.e. an injective homomorphism. More precisely, γ_+ is an isometric $*$-endomorphism which is, in general, not surjective.

Proof We note that, due to the τ_0-invariance of ω_0,

$$\frac{1}{T}\int_0^T \mathrm{d}t \ \omega_0\circ\tau^t = \frac{1}{T}\int_0^T \mathrm{d}t \ \omega_0\circ(\tau_0^{-t}\circ\tau^t),$$

where on the left hand side we have the definition of a NESS from (1), and, on the right hand side, we use (3). □

Entropy production rate

The mean *entropy production rate* (EPR) is defined with the help of the concept of the so-called *relative entropy*. On the analogy of the relative entropy of two measures[24], the relative entropy of a density matrix[25] ρ' on a Hilbert space $\mathcal{H}$ w.r.t. the density matrix ρ is defined as

$$\mathrm{Ent}(\rho'|\rho) = \mathrm{tr}(\rho'(\log\rho - \log\rho')).$$

It has the two properties (cf. [18, p.268])

$$\mathrm{Ent}(\rho'|\rho) \leq 0, \quad \mathrm{Ent}(\rho'|\rho) = 0 \text{ iff } \rho' = \rho.$$

In order to define the relative entropy for two more general states in $\mathcal{E}(\mathcal{O})$, one makes use of the *relative modular operator* from Tomita-Takesaki's modular theory of von Neumann algebras.[26] It turns out that, in this generalization, the foregoing two properties still hold.

The following theorem serves as motivation for the subsequent definition of the mean EPR.

[24] For a probability measure μ' (on some convex compact subset of the Euclidean space) which is absolutely continuous w.r.t. the Lebesgue measure μ (or for more general Radon measures), the relative entropy of μ' w.r.t. μ is defined by (cf. [18, p.267])

$$\mathrm{Ent}(\mu'|\mu) = -\mu'\left(\log\frac{\mathrm{d}\mu'}{\mathrm{d}\mu}\right).$$

[25] A *density matrix* (or *statistical operator*) is an $A \in \mathcal{L}(\mathcal{H})$ s.t.

$$A \geq 0, \quad A \in \mathcal{L}^1(\mathcal{H}), \quad \mathrm{tr}\,A = 1.$$

[26] Cf. [18, p.276] for the case of so-called faithful normal states. A state $\omega \in \mathcal{E}(\mathcal{O})$ is called *faithful* iff $\omega(A^*A) > 0$ for all nonzero $A \in \mathcal{O}$.

Theorem 6 (cf. [26]) *Let* $(\mathcal{O}, \tau_0)$ *be a* C^**-dynamical system,* $\omega_0 \in \mathcal{E}(\mathcal{O}, \tau_0)$ *a modular state for a* C^**-dynamics* $\sigma^t_{\omega_0}$ *with generator* δ_{ω_0}[27]*, and* $V \in \mathrm{dom}\,(\delta_{\omega_0})$ *a local perturbation generating the perturbed* C^**-dynamics* τ*. Then, for any* $\omega_0' \in \mathcal{N}_{\omega_0}$*,*

$$\frac{1}{T}\int_0^T \mathrm{d}t\ \omega_0'(\tau^t(\delta_{\omega_0}(V))) = -\frac{\mathrm{Ent}(\omega_0' \circ \tau^T|\omega_0) - \mathrm{Ent}(\omega_0'|\omega_0)}{T}.$$

The right hand side describes the mean rate at which the entropy is pumped out of the system by the perturbation V. Taking (1) into account, we make the following definition.

Definition 7 (cf. [26]) *Let the setting be as in Theorem 6. Then, the "mean EPR in the NESS* $\omega_+ \in \Sigma_+(\omega_0', \tau)$*" is defined by*

$$\mathrm{Ep}(\omega_+) = \omega_+(\sigma_V),$$

where $\sigma_V = \delta_{\omega_0}(V)$ *is called the "EPR observable".*

Remark 8 Due to the two properties of the relative entropy mentioned above, it immediately follows that, for a NESS $\omega_+ \in \Sigma_+(\omega_0, \tau)$, we have

$$\mathrm{Ep}(\omega_+) \geq 0.$$

3 Open systems

The term *open system* designates a special instance of the class of non-equilibrium systems described in Section 2 for which the C^*-algebra of observables $\mathcal{O}$ carries an additional factorization structure,

$$\mathcal{O} = \mathcal{O}_{\mathcal{S}} \otimes \mathcal{O}_{\mathcal{R}}.$$

Bringing such a structure into use is motivated by the physical situation in which a (confined) *sample* $\mathcal{S}$ is brought in contact with an (extended) *reservoir*[28] $\mathcal{R}$. Both the sample and the reservoir are described by C^*-dynamical systems $(\mathcal{O}_{\mathcal{S}}, \tau_{\mathcal{S}})$ and $(\mathcal{O}_{\mathcal{R}}, \tau_{\mathcal{R}})$, respectively, and the C^*-dynamics τ_0^t from Section 2, now called the *uncoupled* dynamics, describes the time evolution of the total uncoupled system,

$$\tau_0^t = \tau_{\mathcal{S}}^t \otimes \tau_{\mathcal{R}}^t.$$

Moreover, the reference state $\omega_0 \in \mathcal{E}(\mathcal{O}, \tau_0)$ is chosen to factorize accordingly,

$$\omega_0 = \omega_{\mathcal{S}} \otimes \omega_{\mathcal{R}}.$$

In order to be able to model the physically important situation of an environment supporting a temperature gradient which, eventually, may lead to a heat flux across the sample, we further introduce an additional subreservoir structure, i.e. we assume $\mathcal{R}$ to consist of several parts $\mathcal{R}_1, ..., \mathcal{R}_M$, cf. Figure 1. The j-th reservoir $\mathcal{R}_j$ is described by a C^*-subalgebra $\mathcal{O}_{\mathcal{R}_j} \subseteq \mathcal{O}_{\mathcal{R}}$ with the properties that

$$\tau_{\mathcal{R}}^t(\mathcal{O}_{\mathcal{R}_j}) \subseteq \mathcal{O}_{\mathcal{R}_j}, \quad \mathcal{O}_{\mathcal{R}_j} \cap \mathcal{O}_{\mathcal{R}_k} = \mathbb{C}1,$$

for all $k \neq j$, and $\mathcal{O}_{\mathcal{R}}$ is assumed to be generated by $\mathcal{O}_{\mathcal{R}_1}, ..., \mathcal{O}_{\mathcal{R}_M}$.[29] The sample $\mathcal{S}$ is coupled to the reservoir $\mathcal{R}_j$ through a junction $V_j = V_j^* \in \mathcal{O}_{\mathcal{S}} \otimes \mathcal{O}_{\mathcal{R}_j}$, and the total coupling is

$$V = \sum_j V_j.$$

[27] δ_{ω_0} is a so-called $*$-*derivation*, i.e. it is a linear operator on $\mathcal{O}$ whose domain $\mathrm{dom}\,(\delta_{\omega_0})$ is a $*$-subalgebra of $\mathcal{O}$. It has the properties $\delta_{\omega_0}(A)^* = \delta_{\omega_0}(A^*)$, $\delta_{\omega_0}(AB) = \delta_{\omega_0}(A)B + A\delta_{\omega_0}(B)$ (the *Leibniz rule*) for all $A, B \in \mathrm{dom}\,(\delta_{\omega_0})$, and

$$\sigma^t_{\omega_0} = \mathrm{e}^{t\delta_{\omega_0}}.$$

[28] Also called *environment*. From a physical point of view, we are not interested in the nature of this reservoir whose only task is to guarantee a sufficient heat (or charge or matter etc.) supply in an optimally regular way.

[29] In the sense that $\mathcal{O}_{\mathcal{R}}$ is such that it is the smallest C^*-algebra containing all the subreservoirs $\mathcal{O}_{\mathcal{R}_j}$. An often encountered special case of this set-up is the following. $\mathcal{R}_j$ is described by a C^*-dynamical system $(\mathcal{O}_{\mathcal{R}_j}, \tau^t_{\mathcal{R}_j})$ with reference state $\omega_{\mathcal{R}_j}$, and the total reservoir has the structure (cf. Section 4)

$$\mathcal{O}_{\mathcal{R}} = \otimes_j\, \mathcal{O}_{\mathcal{R}_j}, \quad \tau^t_{\mathcal{R}} = \otimes_j \tau^t_{\mathcal{R}_j}, \quad \omega_{\mathcal{R}} = \otimes_j\, \omega_{\mathcal{R}_j}.$$

Note that here, contrary to the more general case, we have $[\mathcal{O}_{\mathcal{R}_j}, \mathcal{O}_{\mathcal{R}_k}] = 0$.

Fluxes and entropy production rate

Let us assume for a moment that the sample is a finite dimensional quantum system[30] specified by the Hamiltonian $H_{\mathcal{S}} \in \mathcal{O}_{\mathcal{S}}$ which generates the time evolution $\tau_{\mathcal{S}}^t \in \mathrm{Aut}(\mathcal{O}_{\mathcal{S}})$. Since the total heat flux out of the reservoir $\mathcal{R}$ into the sample $\mathcal{S}$ produced by the coupled C^*-dynamics τ^t is given by[31]

$$\frac{\mathrm{d}}{\mathrm{d}t}\tau^t(H_{\mathcal{S}}+V) = \sum_j \tau^t(\delta_{\mathcal{R}_j}(V_j)),$$

we identify the heat flux out of $\mathcal{R}_j$ into $\mathcal{S}$ with

$$\Phi_j = \delta_{\mathcal{R}_j}(V_j).$$

In order to define the mean EPR, we assume, in addition, that the state $\omega_{\mathcal{R}} \in \mathcal{E}(\mathcal{O}_{\mathcal{R}}, \tau_{\mathcal{R}})$ is modular for some C^*-dynamics $\sigma_{\mathcal{R}}^t \in \mathrm{Aut}(\mathcal{O}_{\mathcal{R}})$ with

$$\sigma_{\mathcal{R}}^t(\mathcal{O}_{\mathcal{R}_j}) \subseteq \mathcal{O}_{\mathcal{R}_j},$$

and that $V_j \in \mathrm{dom}\,(\delta'_{\mathcal{R}_j})$.[32] Then, if $\omega_{\mathcal{S}} \in \mathcal{E}(\mathcal{O}_{\mathcal{S}}, \tau_{\mathcal{S}})$ is the unique $(\tau_{\mathcal{S}}, \beta_{\mathcal{S}} = 0)$-KMS state[33], the EPR observable reads $\sigma_V = \sum_j \delta'_{\mathcal{R}_j}(V_j)$. In particular, if we assume $\omega_{\mathcal{R}_j} \in \mathcal{E}(\mathcal{O}_{\mathcal{R}_j}, \tau_{\mathcal{R}_j})$ to be the $(\tau_{\mathcal{R}_j}, \beta_j)$-KMS state[34], then $\omega_{\mathcal{R}}$ is modular for the C^*-dynamics $\sigma_{\mathcal{R}}^t$ defined by $\sigma_{\mathcal{R}_j}^t = \tau_{\mathcal{R}_j}^{-\beta_j t}$ with generators $\delta'_{\mathcal{R}_j} = -\beta_j\,\delta_{\mathcal{R}_j}$. Hence,

$$\sigma_V = -\sum_j \beta_j \Phi_j,$$

and, for a NESS $\omega_+ \in \Sigma_+(\omega_0, \tau)$, we get the mean EPR

$$\mathrm{Ep}(\omega_+) = -\sum_j \beta_j\,\omega_+(\Phi_j). \tag{4}$$

This equation relates the mean EPR to the mean heat fluxes across the sample.[35]

[30] I.e. $\mathcal{O}_{\mathcal{S}} = \mathcal{L}(\mathcal{H}_{\mathcal{S}})$ and $\dim\,\mathcal{H}_{\mathcal{S}} < \infty$.

[31] $\delta_{\mathcal{R}_j}$ denotes the generator of the restriction $\tau_{\mathcal{R}_j}^t = \tau_{\mathcal{R}}^t\restriction_{\mathcal{O}_{\mathcal{R}_j}}$.

[32] $\delta'_{\mathcal{R}_j}$ is the generator of the restriction $\sigma_{\mathcal{R}_j}^t = \sigma_{\mathcal{R}}^t\restriction_{\mathcal{O}_{\mathcal{R}_j}}$.

[33] This is the *trace* state $\omega_{\mathcal{S}}(\cdot) = \mathrm{tr}(\cdot)/\dim\,\mathcal{H}_{\mathcal{S}}$ (also called *chaotic* state or *central* state).

[34] With $\omega_{\mathcal{R}_j} = \omega_{\mathcal{R}}\restriction_{\mathcal{O}_{\mathcal{R}_j}}$.

[35] The mean EPR is independent of $\omega_{\mathcal{S}}$ if $\omega_{\mathcal{S}}$ is faithful (cf. [27]).

Remark 9 Note that the first and second law of thermodynamics trivially hold in the foregoing set-up.

Remark 10 Later on, we will also consider matter and charge fluxes for non-finite samples in quasi-free systems (cf. Section 5).

In Section 5, using scattering theory, we will derive expressions for the mean EPR in the NESS of the XY chain and the EBB model. These NESS will be constructed in Section 4.

Linear response theory

We know from phenomenological non-equilibrium thermodynamics that the entropy production can be written as a bilinear form in the thermodynamic forces x_j and their conjugate fluxes ϕ_j,[36]

$$\mathrm{Ep} = \sum_j x_j \phi_j.$$

Since each flux can depend in a complicated way on the applied thermodynamic forces,

$$\phi_j = \phi_j(x_1, ..., x_M),$$

linear response theory restricts its focus on the regime in which the thermodynamic forces driving the system out of equilibrium are so small that the dependence of the fluxes upon the forces may be well described in linear approximation. In other words, linear response theory is first order perturbation theory w.r.t. the thermodynamic forces. If the reservoirs of the preceding subsection are in thermal equilibrium at inverse temperatures $\beta_1, ..., \beta_M$ (sufficiently close to some reference temperature β_{eq}, say), then, the thermodynamic forces may be identified with

$$x_j = \beta_{\mathrm{eq}} - \beta_j$$

generating the fluxes[37]

$$\phi_j = \omega_+(\Phi_j).$$

[36] The thermodynamic forces are also called *affinities*.

[37] This is due to the fact that, using energy conservation (cf. Remark 9), we can write $\mathrm{Ep}(\omega_+) = \sum_j (\beta_{\mathrm{eq}} - \beta_j)\,\omega_+(\Phi_j)$.

Now, the so-called *kinetic coefficients* are defined to be the coefficients of the linearization of the fluxes,

$$L_{ij} = \frac{\partial}{\partial x_j}\,\omega_+(\Phi_i)\Big|_{x=0},$$

where $x = (x_1, ..., x_n)$ denotes the collection of all thermodynamic forces. Linear response theory studies the properties of these kinetic coefficients. First, for time reversal invariant open systems[38], the *Onsager reciprocity relations* (ORR) reveal their symmetry,

$$L_{ij} = L_{ji}.$$

Second, again for open TRI systems, the *Green-Kubo fluctuation-dissipation formula* (GKF) expresses them by the integrated current-current correlations in equilibrium,

$$L_{ij} = \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}t\ \omega_{\mathrm{eq}}(\tau^t(\Phi_i)\Phi_j),$$

where $\omega_{\mathrm{eq}} \in \mathcal{E}(\mathcal{O})$ denotes the $(\tau, \beta_{\mathrm{eq}})$-KMS state (i.e. the NESS ω_+ for $x = 0$). Finally, third, the *central limit theorem* relates them to the statistics of the current fluctuations in equilibrium (cf. [25]).

In Section 6, we establish the ORR and the GFK in the EBB model.

Weak coupling theory

Since, from a physical point of view, we are interested in the properties of the sample only (see footnote 28), we can make use of the so-called *weak coupling theory* (or *van Hove theory*) which integrates out the degrees of freedom of the reservoirs by means of the projection

$$P_{\mathcal{S}}(A \otimes B) = A\,\omega_{\mathcal{R}}(B)$$

for $A \in \mathcal{O}_{\mathcal{S}}$ and $B \in \mathcal{O}_{\mathcal{R}}$. If the coupling strength is parameterized by some real λ, then, on the time scale t/λ^2, the reduced dynamics of the sample

$$T^t_\lambda(A) = P_{\mathcal{S}}(\tau_0^{-t} \circ \tau^t(A \otimes 1_{\mathcal{R}}))$$

is governed by the so-called *Davies generator* K_{H} in the Heisenberg picture (cf. [21]),

$$\lim_{\lambda\to 0} T_\lambda^{t/\lambda^2}(A) = \mathrm{e}^{tK_{\mathrm{H}}}(A).$$

Using the Davies generator K_{H}, we describe the open system in second order perturbation theory in λ. What concerns thermodynamics in the weak coupling limit[39], we have the following. Under some effective coupling and non-degeneracy conditions (cf. Section 7), there exists a unique FGR NESS $\omega_{\mathcal{S}+} \in \mathcal{E}(\mathcal{O}_{\mathcal{S}})$ which has the property that

$$\omega_{\mathcal{S}+}(A) = \lim_{t\to\infty} \omega_{\mathcal{S}}(\mathrm{e}^{tK_{\mathrm{H}}}(A)) \tag{5}$$

for any $\omega_{\mathcal{S}} \in \mathcal{E}(\mathcal{O}_{\mathcal{S}})$.[40] With the FGR heat flux observable $\Phi_{\mathrm{fgr},j} = K_{\mathrm{H},j}(H_{\mathcal{S}})$[41] and the FGR EPR observable $\sigma_{\mathrm{fgr}} = -\sum_j \beta_j \Phi_{\mathrm{fgr},j}$, the first and second law of FGR thermodynamics hold, i.e. energy is conserved, $\sum_j \omega_{\mathcal{S}+}(\Phi_{\mathrm{fgr},j}) = 0$, and the mean FGR EPR $\mathrm{Ep}_{\mathrm{fgr}}(\omega_{\mathcal{S}+}) = \omega_{\mathcal{S}+}(\sigma_{\mathrm{fgr}})$ satisfies

$$\mathrm{Ep}_{\mathrm{fgr}}(\omega_{\mathcal{S}+}) \geq 0.$$

In those models which allow for a rigorous relation of the microscopic to the FGR thermodynamics in the sense of

$$\mathrm{Ep}(\omega_+) = \lambda^2\,\mathrm{Ep}_{\mathrm{fgr}}(\omega_{\mathcal{S}+}) + \mathcal{O}(\lambda^3), \tag{6}$$

the question about the strict positivity of $\mathrm{Ep}(\omega_+)$ for sufficiently small coupling reduces to the much simpler question about the strict positivity of $\mathrm{Ep}_{\mathrm{fgr}}(\omega_{\mathcal{S}+})$.

[38] A bijective antilinear involution $\mathfrak{r}$ on $\mathcal{O}$ is called a *time reversal* iff $\mathfrak{r}(H_{\mathcal{S}}) = H_{\mathcal{S}}$, $\mathfrak{r}(V_j) = V_j$, and $\mathfrak{r} \circ \tau^t_{\mathcal{R}_j} = \tau^{-t}_{\mathcal{R}_j} \circ \mathfrak{r}$. Hence,

$$\mathfrak{r} \circ \tau_0^t = \tau_0^{-t} \circ \mathfrak{r}, \quad \mathfrak{r} \circ \tau^t = \tau^{-t} \circ \mathfrak{r}.$$

An open system with reference state ω is called *time reversal invariant* (TRI) iff there is a time reversal $\mathfrak{r}$ s.t. $\omega(\mathfrak{r}(A)) = \omega(A^*)$.

[39] We call it *Fermi Golden Rule* (FGR) thermodynamics in [7].

[40] Cf. [32] for a detailed description of all of the following.

[41] The Davies generator K_{H} can be written as

$$K_{\mathrm{H}} = \sum_j K_{\mathrm{H},j},$$

where $K_{\mathrm{H},j}$ is the Davies generator for $\mathcal{S}$ coupled to $\mathcal{R}_j$ only.

In Section 7, we establish a simple algebraic criterion which ensures the strict positivity of $\mathrm{Ep}_{\mathrm{fgr}}(\omega_{\mathcal{S}+})$. The connection (6) for the SEBB model is established in [7].[42]

4 Non-equilibrium steady states

In this section, using the time dependent C^*-scattering approach outlined in Section 2, we start off with the construction of the NESS in the motivational example of the XY chain. In a second part, we extend this consideration to the more general EBB model.

XY chain

The XY chain is a special instance of the class of Heisenberg spin models on the discrete line $\mathbb{Z}$. Let us first very briefly explain the framework of spin systems. Eventually, we will end up with quasi-free fermions. In the subsequent discussion of the EBB model, we directly proceed from the level of a quasi-free system.

The kinematic structure of the XY chain consists of a quasi-local uniformly hyperfinite algebra[43] constructed over the finite subsets of $\mathbb{Z}$, i.e. to each point $x \in \mathbb{Z}$ is associated a two-dimensional Hilbert space $\mathcal{H}_{\{x\}}$[44], to each finite subset $\Lambda \subset \mathbb{Z}$ the Hilbert space $\mathcal{H}_\Lambda = \otimes_{x\in\Lambda}\mathcal{H}_{\{x\}}$, and the C^*-algebra of local observables is defined to be $\mathfrak{S}_\Lambda = \mathcal{L}(\mathcal{H}_\Lambda)$. For a finite or infinite subset $\mathcal{Z} \subset \mathbb{Z}$, the C^*-completion of the $*$-algebra $\cup_{\Lambda\subset\mathcal{Z}}\mathfrak{S}_\Lambda$ is the infinite tensor product C^*-algebra of observables over $\mathcal{Z}$.[45]

The dynamics of the XY chain is specified by the following interaction Ψ [46] defined to be zero on all finite subsets of $\mathbb{Z}$ but on the following ones,

$$
\begin{aligned}
\Psi(\{x\}) &= 2\lambda\, \sigma_3^{(x)}, \\
\Psi(\{x, x+1\}) &= (1+\gamma)\, \sigma_1^{(x)}\sigma_1^{(x+1)} \\
&\quad +(1-\gamma)\, \sigma_2^{(x)}\sigma_2^{(x+1)},
\end{aligned}
$$

where $x \in \mathbb{Z}$.[47] The parameter $\gamma \in (-1, 1)$ denotes the *anisotropy* and $\lambda \in \mathbb{R}$ stands for the *magnetic field* in the XY chain.[48]

Remark 11 $\Psi(X)$ represents the interaction energy of the particles in X, and, since the particles are considered to be attached to the lattice sites, the total interaction energy H_Λ in Λ is the interaction energy of all subsystems.

For any finite $\Lambda \subset \mathbb{Z}$, the so-called *local XY Hamiltonian* is defined to be

$$H_\Lambda = -\frac{1}{4}\sum_{X\subseteq\Lambda}\Psi(X),$$

generating the *local dynamics*

$$\tau_\Lambda^t(A) = \mathrm{e}^{itH_\Lambda}A\mathrm{e}^{-itH_\Lambda}.$$

Since Ψ has finite range[49], the thermodynamic limit[50]

$$\tau^t(A) = \lim_{\Lambda\to\infty}\tau_\Lambda^t(A)$$

exists in norm and yields a strongly continuous one-parameter group $\tau^t \in \mathrm{Aut}(\mathfrak{S})$ (cf. [18, p.247]). The

[42] The ORR and the GKF of linear response theory in FGR thermodynamics are shown to hold in [32].

[43] Such a C^*-algebra is generated by an increasing net of C^*-subalgebras indexed by a directed set possessing an orthogonality relation (cf. [18, 40]). In applications, the index set typically consists of bounded subsets of the configuration space ordered by inclusion. An element of the net is then interpreted as the algebra of physical observables for a subsystem localized in that subset.

[44] For spins with quantum number $s = 1/2$.

[45] For the infinite tensor product of C^*-algebras, cf. [40, p.70].

[46] An *interaction* Ψ is a map from the finite subsets $X \subset \mathbb{Z}$ into the self-adjoint elements of $\mathfrak{S} = \mathfrak{S}_\mathbb{Z}$ s.t. $\Psi(X) \in \mathfrak{S}_X$.

[47] The Pauli basis of $\mathbb{C}^{2\times 2}$ is defined by $\sigma_0 = 1$, and

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

[48] Since the discovery of their ideal thermal conductivity in non-equilibrium situations as described in Section 3, such (quasi-)one-dimensional $s = 1/2$ Heisenberg systems have been intensively investigated experimentally and theoretically (cf. [41, 42] and [20, 44], respectively).

[49] Ψ has *finite range* iff there is a $d \geq 1$ s.t. $\Psi(X) = 0$ for all finite X with diameter $\sup_{x,x'\in X}|x - x'| > d$.

[50] $\Lambda \to \infty$ means that Λ eventually contains any finite $X \subset \mathbb{Z}$.

C^*-dynamical system $(\mathfrak{S}, \tau)$ describes the *infinite XY chain*.

In order to set up a non-equilibrium configuration in the sense of the paradigmatic open systems from Section 3, we couple a finite cutout $\mathbb{Z}_{\mathcal{S}}$ of $\mathbb{Z}$ between $-x_0$ and x_0 to the two remaining infinite parts $\mathbb{Z}_L$ and $\mathbb{Z}_R$ to its left and right which will act as thermal reservoirs. Using (2), we define the uncoupled C^*-dynamical system $(\mathfrak{S}, \tau_0)$, where the local perturbation is the bond-coupling

$$\begin{aligned} V &= -\frac{1}{4}\,\Psi(\{x_0, x_0+1\}) \\ &\quad -\frac{1}{4}\,\Psi(\{-(x_0+1), -x_0\}). \end{aligned} \tag{7}$$

By construction, V decouples the XY dynamics τ^t in the sense that

$$\tau_0^t = \tau_L^t \otimes \tau_{\mathcal{S}}^t \otimes \tau_R^t$$

respects the factorization

$$\mathfrak{S} = \mathfrak{S}_L \otimes \mathfrak{S}_{\mathcal{S}} \otimes \mathfrak{S}_R,$$

where $\mathfrak{S}_L = \mathfrak{S}_{\mathbb{Z}_L}$ and analogously for $\mathcal{S}$ and R. As reference state $\omega_0 \in \mathcal{E}(\mathfrak{S})$ in the construction of the NESS, we choose

$$\omega_0 = \omega_L^{\beta_L} \otimes \omega_{\mathcal{S}} \otimes \omega_R^{\beta_R}, \tag{8}$$

where $\omega_L^{\beta_L}$ is the unique (τ_L, β_L)-KMS state on $\mathfrak{S}_L$ and analogously for $\omega_R^{\beta_R}$. Moreover, $\omega_{\mathcal{S}}$ stands for the chaotic state on $\mathfrak{S}_{\mathcal{S}}$ (cf. footnote 33).

For computational convenience, we will leave the foregoing spin picture and enter the fermionic description established by the well-known Jordan-Wigner transformation (cf. [30]),[51]

$$a_x = T S^{(x)} (\sigma_1^{(x)} - i\sigma_2^{(x)})/2, \tag{9}$$

where $S^{(x)}$ is defined by $S^{(x)} = \sigma_3^{(1)} \ldots \sigma_3^{(x-1)}$ if $x \geq 2$, $S^{(1)} = 1$, and $S^{(x)} = \sigma_3^{(x)} \ldots \sigma_3^{(0)}$ if $x \leq 0$.

[51]Since we are given a two-sided infinite chain, we use the Jordan-Wigner transformation (devised for the one-sided infinite case only) in its generalized form (cf. [1] and footnote 53).

Moreover, T stems from the C^* crossed product extension by some $\mathbb{Z}_2$-action (cf. footnote 53). We denote by $\mathfrak{A}(\mathfrak{h})$ the CAR algebra[52] over $\mathfrak{h} = \ell^2(\mathbb{Z})$ generated by the Jordan-Wigner fermions a_x and a_x^*.[53]

Remark 12 The heuristic equivalence induced by the Jordan-Wigner transformation is rigorous on the even part of the corresponding algebras. However, the equivalence breaks down if one tries to extend it to the whole algebra (cf. (11) in footnote 53).[54]

After the Jordan-Wigner transformation, the interaction is quadratic in the fermions,

$$\Psi(\{x\}) = 2\lambda\,(2a_x^* a_x - 1), \tag{12}$$

$$\begin{aligned} \Psi(\{x, x+1\}) &= -2\,(a_x^* a_{x+1} + a_{x+1}^* a_x) \\ &\quad -2\gamma(a_x^* a_{x+1}^* + a_{x+1} a_x). \end{aligned} \tag{13}$$

Using the CAR (10), we can recast $\mathfrak{A}(\mathfrak{h})$ into the form of a so-called *self-dual* CAR algebra over $(\mathfrak{h}^{\oplus 2}, J)$[55]

[52]The *canonical anticommutation relations* (CAR) *algebra* $\mathfrak{A}(\mathcal{H})$ over the complex Hilbert space $\mathcal{H}$ is the completion in the unique C^*-norm of the quotient of the free $*$-algebra generated by the symbols $a^*(f)$ and $a(f)$ with $f \in \mathcal{H}$ and the identity 1, by the two-sided $*$-algebra generated by the relations $a^*(\alpha f + \beta g) = \alpha a^*(f) + \beta a^*(g)$, $a(f)^* = a^*(f)$, $\{a^*(f), a^*(g)\} = 0$, and

$$\{a(f), a(g)\} = 0, \quad \{a^*(f), a(g)\} = (g, f)1, \tag{10}$$

where $\{A, B\} = AB + BA$ is the so-called *anticommutator*. We will use the same notation for the abstract CAR algebra and its Fock representation (cf. [18, p.6]).

[53] The construction in [1] goes as follows. Let $\mathcal{O}$ be the C^*-algebra generated by $\mathfrak{S}$ and an element T satisfying $T = T^*$, $T^2 = 1$, and $TA = \theta_-(A)T$, where $\theta_- \in \mathrm{Aut}(\mathfrak{S})$ is defined by $\theta_-(\sigma_i^{(x)}) = -\sigma_i^{(x)}$ if $x \leq 0$ and $\theta_-(\sigma_i^{(x)}) = \sigma_i^{(x)}$ if $x > 0$ for $i = 1, 2$, and $\theta_-(\sigma_3^{(x)}) = \sigma_3^{(x)}$ for all $x \in \mathbb{Z}$. Moreover, define $\theta \in \mathrm{Aut}(\mathfrak{S})$ by $\theta(\sigma_i^{(x)}) = -\sigma_i^{(x)}$ for $i = 1, 2$ and $\theta(\sigma_3^{(x)}) = \sigma_3^{(x)}$ for all $x \in \mathbb{Z}$. Hence, $\mathfrak{S} = \mathfrak{S}_+ + \mathfrak{S}_-$, where $\mathfrak{S}_\pm = \{A \in \mathfrak{S} : \theta(A) = \pm A\}$, and $\mathfrak{S}_+$ is the *even* C^*-subalgebra of $\mathfrak{S}$. Defining $\theta(T) = T$, we can write $\mathfrak{A}(\mathfrak{h}) = \mathfrak{A}(\mathfrak{h})_+ + \mathfrak{A}(\mathfrak{h})_-$, and, hence,

$$\mathfrak{S}_+ = \mathfrak{A}(\mathfrak{h})_+, \quad \mathfrak{S}_- = T\mathfrak{A}(\mathfrak{h})_-. \tag{11}$$

Since $\Psi(X) \in \mathfrak{S}_+$, $\mathfrak{S}_\pm$ are invariant under τ_0^t and τ^t which implies $\omega_0(\mathfrak{S}_-) = 0$. Hence, $(\mathfrak{S}_+, \tau)$ suffices for our purposes.

[54]For an interesting consequence of this fact, cf. [34].

[55]In [2], the *self-dual CAR algebra* $\mathfrak{A}(\mathcal{H}, J)$ over the Hilbert

by using the complex linear mapping $B\colon \mathfrak{h}^{\oplus 2} \to \mathcal{L}(\mathfrak{h})$,

$$B(f) = a^*(f_1) + a(\bar{f}_2),$$

for $f = [f_1, f_2] \in \mathfrak{h}^{\oplus 2}$. Moreover, with the antiunitary involution J on $\mathfrak{h}^{\oplus 2}$ defined by

$$J[f_1, f_2] = [\bar{f}_2, \bar{f}_1],$$

these $B(f)$ satisfy the relations (14). With the help of the "self-dual second quantization" $\mathbf{B}(k) = \sum_j B(f_j)B^*(g_j)$, where $f_j, g_j \in \mathfrak{h}$ and $k = \sum_j f_j(g_j, \cdot) \in \mathcal{L}^0(\mathfrak{h})$[56], the local Hamiltonian can be expressed as $H_\Lambda = \mathbf{B}(h_\Lambda)$ with $h_\Lambda = \sum_{X\subseteq\Lambda} \psi(X) \in \mathcal{L}^0(\mathcal{H})$.[57] Since $\mathrm{e}^{\mathbf{B}(k)} B(f) \mathrm{e}^{-\mathbf{B}(k)} = B(\mathrm{e}^k f)$ in analogy to the usual second quantization[58], we arrive at $\tau_\Lambda^t(B(f)) = B(\mathrm{e}^{ith_\Lambda} f)$. In the thermodynamic limit, this leads to

$$\tau^t(B(f)) = B(\mathrm{e}^{\mathrm{i}th} f), \tag{15}$$

where the one-particle Hamiltonian h is a multiplication operator in the Fourier picture[59] which acts on $\hat{\mathfrak{h}}^{\oplus 2}$ by multiplication with the function[60]

$$h(\mathrm{e}^{\mathrm{i}\xi}) = (\cos\xi - \lambda) \otimes \sigma_3 + \gamma \sin\xi \otimes \sigma_2. \tag{16}$$

Analogously, the one-particle Hamiltonian

$$h_0 = h - v = h_L \oplus h_{\mathcal{S}} \oplus h_R \tag{17}$$

with $v = -(\psi(\{x_0, x_0{+}1\}) + \psi(\{-(x_0{+}1), -x_0\}))/4$ generates the decoupled dynamics[61]

$$\tau_0^t(B(f)) = B(\mathrm{e}^{\mathrm{i}th_0} f). \tag{18}$$

Let us now turn to the reference state ω_0 from (8). This state is an example of a so-called quasi-free state. A state $\omega \in \mathcal{E}(\mathfrak{A}(\mathfrak{h}^{\oplus 2}, J))$ is called *quasi-free* iff it vanishes on the odd polynomials in $B(f)$,

$$\omega(B(f_1) \dots B(f_{2n+1})) = 0,$$

and iff it is a Pfaffian[62] on the even polynomials,

$$\omega(B(f_1) \dots B(f_{2n})) = \mathrm{pf}\, \Omega(n), \tag{20}$$

where $\Omega(n) \in \mathbb{C}^{2n\times 2n}$ is given by

$$\Omega(n)_{kl} = \begin{cases} \omega(B(f_k)B(f_l)), & k < l \\ 0, & k = l \\ -\omega(B(f_l)B(f_k)), & k > l \end{cases}. \tag{21}$$

Hence, a quasi-free state is completely characterized by its two-point function $\omega(B^*(f)B(g))$ which, in turn, determines an operator $\varrho \in \mathcal{L}(\mathfrak{h}^{\oplus 2})$ by

$$\omega(B^*(f)B(g)) = (f, \varrho g). \tag{22}$$

Moreover, due to (14), ϱ has the properties[63]

$$0 \le \varrho = \varrho^* \le 1, \quad \varrho + J\varrho J = 1. \tag{23}$$

For any state ω (quasi-free or not), we call the operator ϱ i n (23) the *density* of ω. Since the reference state ω_0 from (8) is the product of quasi-free KMS states, it is a quasi-free state with density

$$\varrho_0 = (1 + \mathrm{e}^{-k_0})^{-1},$$

space $\mathcal{H}$ with involution J is defined similarly to footnote 52 for symbols $B(f)$ satisfying linearity and the relations

$$\{B^*(f), B(g)\} = (f, g)1, \quad B(Jf) = B^*(f). \tag{14}$$

[56] $\mathcal{L}^0(\mathcal{H})$ denotes the operators of finite rank on $\mathcal{H}$.

[57] $\psi(X)$ can be read off from (12) and (13),

$$\begin{aligned} \psi(\{x\}) &= -\lambda |x\rangle\langle x| \otimes \sigma_3, \\ \psi(\{x, x+1\}) &= c_x \otimes \sigma_3 - \gamma s_x \otimes \sigma_2, \end{aligned}$$

with $c_x = (|x\rangle\langle x+1| + |x+1\rangle\langle x|)/2$ and $s_x = (|x\rangle\langle x+1| - |x+1\rangle\langle x|)/(2i)$ (using $\mathfrak{h}^\oplus \simeq \mathfrak{h} \otimes \mathbb{C}^2$).

[58] In reality, for this relation to hold, we have to impose $Jk = -k^*J$ which is satisfied by $\psi(X)$.

[59] With convention $\hat{\varphi}(\mathrm{e}^{\mathrm{i}\xi}) = \sum_{x\in\mathbb{Z}} \varphi(x)\, \mathrm{e}^{\mathrm{i}x\xi}$ and $\hat{\mathfrak{h}} = L^2(\mathbb{T})$.

[60] Since $h(\mathrm{e}^{\mathrm{i}\xi})$ is not diagonal for $\gamma \neq 0$, the dynamics τ^t does not leave the first (and the second) factor of $\hat{\mathfrak{h}}^{\oplus 2}$ invariant. That's why the unified view in terms of a self-dual CAR algebra is useful.

[61] V in (7) is the "self-dual second quantization" of v.

[62] The Pfaffian of a matrix $A \in \mathbb{C}^{2n\times 2n}$ is defined by

$$\mathrm{pf} A = \sum_\pi \mathrm{sign}(\pi) \prod_{j=1}^n A_{\pi(2j-1),\pi(2j)}, \tag{19}$$

with the sum running over all pairings of the set $\{1, 2, ..., 2n\}$, i.e. the permutations π in the permutation group $\mathcal{S}_{2n}$ which satisfy $\pi(2j-1) < \pi(2j)$ and $\pi(2j-1) < \pi(2j+1)$.

[63] Conversely, for any $\varrho \in \mathcal{L}(\mathfrak{h}^{\oplus 2})$ satisfying (23), there is a unique quasi-free state $\omega \in \mathcal{E}(\mathfrak{A}(\mathfrak{h}^{\oplus 2}, J))$ s.t. (22) holds (cf. [2]).

where $k_0 = \beta_L h_L \oplus 0 \oplus \beta_R h_R$.[64]

Remark 13 In the EBB model described below, we start off at the point where we are now, i.e. we are directly looking at quasi-free fermionic systems.[65]

Next, as described in Section 2, our goal is to construct the Møller morphism $\gamma_+ \in \mathrm{Aut}(\mathfrak{A}(\mathfrak{h}^{\oplus 2}, J))$,

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

Since the decoupled and the coupled time evolution groups τ_0^t and τ^t, respectively, are given by Bogoliubov $*$-automorphisms [66], the problem of constructing γ_+ reduces to the question about the existence (and completeness) of the Hilbert space wave operators $W_\pm$ on the one-particle space $\mathfrak{h}^{\oplus 2}$ of the self-dual Jordan-Wigner fermions,[67]

$$W_\pm = \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}th}\mathrm{e}^{-\mathrm{i}th_0} 1_{\mathrm{ac}}(h_0). \tag{24}$$

Taking advantage of this reduction to a pure one-particle Hilbert space scattering problem, we can prove existence and uniqueness of a quasi-free NESS and identify its density with the help of the wave operators (24).

Theorem 14 (cf. [4]) *Let* $(\mathfrak{A}(\mathfrak{h}^{\oplus 2}, J), \tau_0)$ *be the* C^**-dynamical system of the uncoupled XY chain with the local bond-coupling perturbation* V *from* (7). *If the reference state* $\omega_0 \in \mathcal{E}(\mathfrak{A}(\mathfrak{h}^{\oplus 2}, J), \tau_0)$ *is given by* (8), *then there exists a unique quasi-free NESS* $\omega_+ \in \Sigma_+(\omega_0, \tau)$ *with density*

$$\varrho_+ = W_- \varrho_0 W_-^*. \tag{25}$$

Proof Since $\tau_0^t, \tau^t \in \mathrm{Aut}(\mathfrak{A}(\mathfrak{h}^{\oplus 2}, J))$ are Bogoliubov $*$-automorphisms, we have

$$\tau_0^{-t} \circ \tau^t(B(f)) = B(\mathrm{e}^{-\mathrm{i}th_0}\mathrm{e}^{\mathrm{i}th} f),$$

and therefore, since $\omega_0 \circ \tau_0^{-t} = \omega_0$,

$$\begin{aligned}\omega_0 \circ \tau^t(B^*(f)B(g)) \;&=\\ &\omega_0(B^*(\mathrm{e}^{-\mathrm{i}th_0}\mathrm{e}^{\mathrm{i}th} f)B(\mathrm{e}^{-\mathrm{i}th_0}\mathrm{e}^{\mathrm{i}th} g)).\end{aligned}$$

Hence, we are led to study the wave operator $W_- \in \mathcal{L}(\mathfrak{h}^{\oplus 2})$ from (24). In order to address this question, we appeal to scattering theory for perturbations of trace class type.[68] Indeed, the decoupling perturbation v given after (17) is of finite rank, $v \in \mathcal{L}^0(\mathfrak{h}^{\oplus 2})$, and, hence, the classical Kato-Rosenblum theorem implies that $W_\pm$ exist and are complete (cf. [43, p.193]). Moreover, due to the fact that h is given in the Fourier picture by the multiplication operator $h(\mathrm{e}^{\mathrm{i}\xi})$ from (16), its spectrum is purely absolutely continuous,[69]

$$\mathrm{spec}_{\mathrm{sc}}(h) = \emptyset, \quad \mathrm{spec}_{\mathrm{pp}}(h) = \emptyset. \tag{26}$$

Since the map $f \mapsto B(f)$ is continuous, we get

$$\gamma(B(f)) = B(W_-^* f).$$

Thus, the NESS has the asserted density,

$$\begin{aligned}\omega_+(B^*(f)B(g)) &= \omega_0 \circ \gamma_+(B^*(f)B(g))\\ &= \omega_0(B^*(W_-^* f)B(W_-^* g))\\ &= (f, W_- \varrho_0 W_-^* g).\end{aligned}$$

$\square$

Remark 15 This is the main argument which will reappear in the context of the more general EBB model below.

For the case of the XY chain, we can evaluate the density in (25). Let $\beta = (\beta_R + \beta_L)/2$ and $\delta = (\beta_R - \beta_L)/2$.

[64] More precisely, due to footnote 63, it is the restriction of ω_0 to $\mathfrak{A}(\mathfrak{h})_+ \simeq \mathfrak{A}(\mathfrak{h}^{\oplus 2}, J)_+$ which extends to the quasi-free state on $\mathfrak{A}(\mathfrak{h}^{\oplus 2}, J)$ with density ϱ_0.

[65] Up to the fact that we use the usual CAR algebra description and not the self-dual one.

[66] A $*$-automorphism on $\mathfrak{A}(\mathcal{H}, J)$ of the form

$$\tau_U(B(f)) = B(Uf),$$

where U is a unitary operator on $\mathcal{H}$ satisfying $[U, J] = 0$, is called *Bogoliubov* $*$-automorphism (cf. [2]).

[67] $1_{\mathrm{ac}}(A)$ denotes the projection onto the absolutely continuous subspace $\mathcal{H}_{\mathrm{ac}}(A)$ of the operator A on $\mathcal{H}$. For general scattering theory, cf. [43] for example.

[68] Also called *Kato-Birman theory* (cf. [43]).

[69] $\mathrm{spec}_{\mathrm{sc}}(A)$, $\mathrm{spec}_{\mathrm{ac}}(A)$, and $\mathrm{spec}_{\mathrm{pp}}(A)$ denote the spectra of the restriction of the operator A on $\mathcal{H}$ to the singular continuous, to the absolutely continuous, and to the pure point subspace, $\mathcal{H}_{\mathrm{sc}}(A)$, $\mathcal{H}_{\mathrm{ac}}(A)$, and $\mathcal{H}_{\mathrm{pp}}(A)$, respectively.

Theorem 16 (cf. [4]) *The density $\varrho_+ \in \mathcal{L}(\mathfrak{h}^{\oplus 2})$ of the NESS ω_+ looks like*

$$\varrho_+ = (1 + \mathrm{e}^{-k_+})^{-1}, \tag{27}$$

where k_+ can be expressed with the help of the asymptotic velocity v_- of the dynamics generated by h,

$$k_+ = (\beta - \delta \operatorname{sign} v_-)\, h.$$

Proof We write $W_-^* = i_L W_L^* + i_R W_R^*$, where $W_{L,R}^* = \mathrm{s} - \lim_{t\to\infty} \mathrm{e}^{-\mathrm{i}th_{L,R}} i_{L,R}^* \mathrm{e}^{\mathrm{i}th}$ are the partial wave operators which project on the left and right reservoirs. [70] Hence, since the asymptotic projections $P_{L,R} = \mathrm{s} - \lim_{t\to\infty} \mathrm{e}^{-\mathrm{i}th} i_{L,R} i_{L,R}^* \mathrm{e}^{\mathrm{i}th}$ can be written as $P_{L,R} = W_{L,R} W_{L,R}^*$, we find that ϱ_+ has the form given in (27) with[71]

$$k_+ = (\beta - \delta(P_R - P_L))h.$$

Moreover, since the asymptotic velocity $v_- = \lim_{t\to\infty} \mathrm{e}^{-ith} x \mathrm{e}^{ith}$ exists[72], we have[73]

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

Finally, using the form of h from (16), one can compute v_- explicitly. □

Remark 17 The Fourier transformed density $\hat{\varrho}_+ \in \mathcal{L}(\hat{h}^{\oplus 2})$ is an operator which acts by multiplication with the function

$$\hat{\varrho}_+(\mathrm{e}^{\mathrm{i}\xi}) = \left(1 + \mathrm{e}^{-(\beta\, h(\mathrm{e}^{\mathrm{i}\xi}) - \delta\, k(\mathrm{e}^{\mathrm{i}\xi}))}\right)^{-1}, \tag{28}$$

where

$$\begin{aligned} h(\mathrm{e}^{\mathrm{i}\xi}) &= (\cos\xi - \lambda) \otimes \sigma_3 + \gamma \sin\xi \otimes \sigma_2, \\ k(\mathrm{e}^{\mathrm{i}\xi}) &= \operatorname{sign}(\kappa(\mathrm{e}^{\mathrm{i}\xi}))\, \mu(\mathrm{e}^{\mathrm{i}\xi}) \otimes \sigma_0, \\ \kappa(\mathrm{e}^{\mathrm{i}\xi}) &= 2\lambda \sin\xi - (1-\gamma^2)\sin 2\xi, \\ \mu(\mathrm{e}^{\mathrm{i}\xi}) &= ((\cos\xi - \lambda)^2 + \gamma^2 \sin^2 \xi)^{1/2}. \end{aligned}$$

[70] $i_{L,R}$ denote the natural injections $\ell^2(\mathbb{Z}_{L,R})^{\oplus 2} \to \mathfrak{h}^{\oplus 2}$.

[71] We use basic facts from Kato-Birman theory and [22] only.

[72] In the strong resolvent sense (cf. [36, p.284]).

[73] For self-adjoint operators A and A_n, one has

$$\mathrm{s} - \lim f(A_n) = f(\mathrm{s} - \mathrm{res} - \lim A_n)$$

for f of characteristic function type (cf. [36, p.290]).

The NESS of Theorem 14 has the following properties.

Theorem 18 (cf. [4]) *The NESS ω_+ of the XY chain is*
(1) quasi-free,
(2) independent of x_0,
(3) translation invariant,
(4) modular,
(5) a factor state,
(6) and a (τ, β)-KMS state if $\beta_L = \beta_R = \beta$.

Proof *(1)* is contained in Theorem 14. Since $\hat{\varrho}_+ \in \mathcal{L}(\hat{h}^{\oplus 2})$ acts by multiplication with $\hat{\varrho}_+(\mathrm{e}^{\mathrm{i}\xi})$ of the explicit form (28), we get *(2)*, *(3)*, and

$$\mathrm{spec}_{\mathrm{pp}}(\varrho_+) = \emptyset.$$

Hence, using [2], the non-existence of the eigenvalue 0 and $1/2$ implies *(4)* and *(5)*, respectively. Finally, it has been shown in [1] that ω_+ is the unique (τ, β)-KMS state if $\beta_L = \beta_R = \beta$ which implies *(6)*. □

Remark 19 For $\beta_L \neq \beta_R$, the NESS ω_+ is not only not a KMS state w.r.t. the dynamics τ^t (for any β), but there exists no C^*-dynamics on the Pauli algebra $\mathfrak{S}$ w.r.t. which ω_+ is a KMS state (cf. [34]).

EBB model

As described in the Introduction, we now turn to models of more general type which we call the *electronic black box* (EBB) model (cf. [9]). The so-called *simple* EBB (SEBB) is a special case of the more general EBB model. For the SEBB model, explicit computations have been done in [7] (we will essentially restrict ourselves to some remarks on the SEBB model, cf. [7] for more details).

The EBB model describes a gas of noninteracting fermions which entirely fills up a spatially confined sample $\mathcal{S}$ and a finite number M of spatially extended reservoirs $\mathcal{R}_j$ to which the sample is coupled by junctions. As it has been shortly explained in the case of the XY chain in the foregoing subsection, in order to set up such an ideal system, we only have to specify the one-particle Hilbert spaces and the one-particle Hamiltonians of the sample and the reservoirs. Let $\mathfrak{h}_{\mathcal{S}}$ be the one-particle Hilbert space of the sample with Hamiltonian $h_{\mathcal{S}}$ and $\mathfrak{h}_j$ the one-particle Hilbert space of reservoir number j with Hamiltonian h_j. The kinematics of the EBB model is then given by the total one-particle Hilbert space

$$\mathfrak{h} = \mathfrak{h}_{\mathcal{S}} \oplus \mathfrak{h}_{\mathcal{R}}, \quad \mathfrak{h}_{\mathcal{R}} = \oplus_j \mathfrak{h}_j,$$

and $\mathfrak{A}(\mathfrak{h})$ denotes the C^*-algebra over $\mathfrak{h}$ containing the observables.

Remark 20 In the SEBB model, one has $\dim \mathfrak{h}_{\mathcal{S}} = 1$ (cf. [7]).

As in the XY chain, the decoupled and the coupled dynamics of the EBB model are specified to be Bogoliubov $*$-automorphisms $\tau_0^t, \tau^t \in \mathrm{Aut}(\mathfrak{A}(\mathfrak{h}))$ generated by the one-particle Hamiltonian of the decoupled system,

$$h_0 = h_{\mathcal{S}} \oplus h_{\mathcal{R}}, \quad h_{\mathcal{R}} = \oplus_j h_j,$$

and by some one-particle Hamiltonian h of the coupled system (compare with (15) and (18))[74],

$$\tau_0^t(a(f)) = a(\mathrm{e}^{\mathrm{i}th_0} f), \quad \tau^t(a(f)) = a(\mathrm{e}^{\mathrm{i}th} f).$$

In order to apply the scattering theory for perturbations of trace class type, we make the following assumptions.

Assumption 21 (cf. [9])
(H1) *h_0 and h are bounded from below*
(H2) $r^p - r_0^p \in \mathcal{L}^1(\mathfrak{h})$ *for a* $p \in \{-1\} \cup \mathbb{N}$ [75]
(H3) $\mathrm{spec}_{\mathrm{sc}}(h) = \emptyset$
(H4) $\mathrm{spec}_{\mathrm{ess}}(h_{\mathcal{S}}) = \emptyset$ [76]
(H5) $\mathrm{ran}\,(h - h_0) \subseteq \mathrm{ran}\, h_0$

[74] Note that $\tau_0^t, \tau^t \in \mathrm{Aut}(\mathfrak{A}(\mathfrak{h}))$ respect the involution $*$.

[75] $r(z) = (h-z)^{-1}$ denotes the resolvent of h (and similarly for h_0). (H2) is supposed to hold on one point in the intersection of the corresponding resolvent sets (then, it holds on all such points).

[76] $\mathrm{spec}_{\mathrm{ess}}(A)$ denotes the essential spectrum of the operator A.

For some cases we also assume time reversal invariance (cf. footnote 38).

Assumption 22 (cf. [9])
(TRI) *There is an involution* $\mathfrak{j}$ *on* $\mathfrak{h}$ *s.t.* $\mathfrak{j}h_0 = h_0\mathfrak{j}$ *and* $\mathfrak{j}h = h\mathfrak{j}$.[77]

Similarly to Theorem 14 for the XY chain, we have the following theorem for the EBB model.

Theorem 23 (cf. [9]) *Assume* (H1)–(H3), *and let* $\omega_0 \in \mathcal{E}(\mathfrak{A}(\mathfrak{h}), \tau_0)$ *be a gauge invariant*[78] *quasi-free*[79] *reference state with density* ϱ_0. *Then, there exists a unique NESS* $\omega_+ \in \Sigma_+(\mathfrak{A}(\mathfrak{h}), \tau)$ *whose restriction to* $\mathfrak{A}(\mathfrak{h}_{\mathrm{ac}}(h))$ *is the gauge invariant quasi-free state with density* $W_- \varrho_0 W_-^*$. *Moreover, if* $c \in \mathcal{L}^1(\mathfrak{h})$, *then* $\omega_+(\mathrm{d}\Gamma(c)) = \mathrm{tr}(\varrho_+ c)$ *with*[80]

$$\varrho_+ = W_- \varrho_0 W_-^* + \sum_{\varepsilon \in \mathrm{spec}_{\mathrm{pp}}(h)} 1_\varepsilon(h) \varrho_0 1_\varepsilon(h). \tag{30}$$

Proof Using (29), we write the matrix elements in $\omega_0 \circ \tau^t(a^*(g_n)...a^*(g_1)a(f_1)...a(f_n))$ as

$$(\mathrm{e}^{\mathrm{i}th}[1_{\mathrm{ac}}(h) + 1_{\mathrm{pp}}(h)]f_i, \varrho_0 \mathrm{e}^{\mathrm{i}th}[1_{\mathrm{ac}}(h) + 1_{\mathrm{pp}}(h)]g_j).$$

Whereas the ac-ac term yields the wave operator W_-^*, the two ac-pp terms do not contribute in the large time limit due to the Riemann-Lebesgue lemma. Specializing to $c = f(g, \cdot) \in \mathcal{L}^0(\mathfrak{h})$, averaging over the quasi-periodic pp-pp term (and a density argument) leads to (30). □

[77] $\mathfrak{j}$ induces a Bogoliubov $*$-automorphism on $\mathfrak{A}(\mathfrak{h})$ with the help of which one defines a state to be time reversal invariant (cf. footnote 38).

[78] A state $\omega \in \mathcal{E}(\mathfrak{A}(\mathfrak{h}))$ is *gauge invariant* iff $\omega \circ \vartheta^s = \omega$ where $\vartheta^s \in \mathrm{Aut}(\mathfrak{A}(\mathfrak{h}))$ is generated by $\mathrm{d}\Gamma(1)$.

[79] Identifying $B(F)$ and $B(JF)$ with creation and annihilation operators on a CAR algebra $\mathfrak{A}(P\mathcal{H})$ for a projection P with $JPJ + P = 1$, the C^*-algebras $\mathfrak{A}(\mathcal{H}, J)$ and $\mathfrak{A}(P\mathcal{H})$ are $*$-isomorphic. For a quasi-free state on $\mathfrak{A}(\mathfrak{h})$, we have $\omega(a^*(g)a(f)) = (f, \varrho g)$ for some $0 \leq \varrho \leq 1$, and (cf. (20))

$$\omega(a^*(g_n)...a^*(g_1)a(f_1)...a(f_m)) = \delta_{nm} \det\{(f_i, \varrho g_j)\}. \tag{29}$$

[80] $1_\varepsilon(h)$ denotes the spectral projection corresponding to $\varepsilon \in \mathrm{spec}_{\mathrm{pp}}(h)$.

Remark 24 Compared to (25) and (26) for the XY chain, there is a second term on the right hand of (30) since $\mathrm{spec}_{\mathrm{pp}}(h)$ is not assumed to be empty in general.

5 Entropy production rate

In this section, we determine the mean EPR in the XY chain by direct computation, and in the EBB model using the Landauer-Büttiker theory.

XY model

Since, in (28), we are given the explicit form of the density of the NESS ω_+ in the XY chain, the evaluation of the mean EPR proceeds by direct computation.

Theorem 25 (cf. [4]) *The mean EPR in the NESS ω_+ of the XY chain from Theorem 14 is given by*

$$\mathrm{Ep}(\omega_+) = \frac{\delta}{4}\int_0^{2\pi}\frac{\mathrm{d}\xi}{2\pi}\,|\kappa|\frac{\mathrm{sh}(\delta\mu)}{\mathrm{ch}^2(\beta\mu/2)+\mathrm{sh}^2(\beta\mu/2)}.$$

Therefore,

$$\mathrm{Ep}(\omega_+) > 0 \quad \textit{iff} \quad \beta_L \neq \beta_R.$$

Remark 26 Due to *(5)* in Theorem 18, ω_+ is a factor state. Hence, ω_+ is ω_0-singular[81] iff $\beta_L \neq \beta_R$ (cf. [7]).

EBB model

The Landauer-Büttiker theory of electronic transport describes the steady currents across the sample with the help of scattering data[82] which involves the specific structure of the sample on its one-electron level only (cf. [31, 19, 23]). In this subsection, using the Landauer-Büttiker theory, we want to derive an expression for the mean EPR making use of stationary[83] scattering theory for perturbations of trace class type. Motivated by (4) which relates the mean EPR to the mean heat fluxes across the sample, we study the rate of change of extensive thermodynamic quantities Φ_q generated by *charges* q, i.e. by self-adjoint operators on $\mathfrak{h}$ which commute with the uncoupled Hamiltonian h_0,[84]

$$\Phi_q = \mathrm{d}\Gamma(\varphi_q), \tag{31}$$

where, formally,

$$\varphi_q = -\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{\mathrm{i}th}q\mathrm{e}^{-\mathrm{i}th}\big|_{t=0} = -\mathrm{i}[h,q]. \tag{32}$$

Since, in general, the observable Φ_q describing the flux across the sample generated by the charge q is not an element of $\mathfrak{A}(\mathfrak{h})$ [85], we introduce a regularization in (32) both for the Hamiltonian h and the charge q. For so-called *tempered charges* q, i.e. charges for which $q^{(\Lambda)} = q1_{(-\infty,\Lambda]}(h_0) \in \mathcal{L}(\mathfrak{h})$ for all $\Lambda \in \mathbb{R}$, we define the mean flux in the state $\omega \in \mathcal{E}(\mathfrak{A}(\mathfrak{h}))$ with density $\varrho \in \mathcal{L}(\mathfrak{h})$ by[86]

$$\begin{aligned}\omega(\Phi_q) &= \lim_{\Lambda\to\infty}\lim_{\eta\to 0}\omega(\Phi^\eta_{q^{(\Lambda)}})\\ &= \lim_{\Lambda\to\infty}\lim_{\eta\to 0}\mathrm{tr}(\varrho\varphi^\eta_{q^{(\Lambda)}}),\end{aligned}$$

where $\Phi^\eta_{q^{(\Lambda)}} = \mathrm{d}\Gamma(\varphi^\eta_{q^{(\Lambda)}})$, and

$$\varphi^\eta_{q^{(\Lambda)}} = -i[f_\eta(h) - f_\eta(h_0), q^{(\Lambda)}] \tag{33}$$

---

[81] Let $\omega \in \mathcal{E}(\mathcal{O})$. A linear functional $\eta \in \mathcal{O}^*$ is called ω-*singular* iff $\eta \geq \omega' \geq 0$ for some $\omega' \in \mathcal{N}_\omega$ implies $\omega' = 0$.

[82] The transmission probabilities.

[83] *Stationary* scattering theory expresses the unitary evolution groups in (24) in terms of the corresponding resolvents, and the study of the large time limit is replaced by the study of the boundary values of these resolvents, the so-called *limiting absorption principle* (cf. [43, 153]).

[84] E.g. $q = h_j$ for heat fluxes or $q = 1_j$ for matter fluxes coming from reservoir $\mathcal{R}_j$ (1_j denotes the projection of $\mathfrak{h}$ onto $\mathfrak{h}_j$).

[85] Recall that the second quantization $\mathrm{d}\Gamma(c)$ is a bounded operator on the fermionic Fock space over $\mathfrak{h}$ iff $c \in \mathcal{L}^1(\mathfrak{h})$.

[86] If $\omega_\varrho \in \mathcal{E}(\mathfrak{A}(\mathfrak{h}))$ is quasi-free with density ϱ, we have

$$\omega_\varrho(\mathrm{d}\Gamma(c)) = \mathrm{tr}(\varrho c), \quad c \in \mathcal{L}^1(\mathfrak{h}).$$

for $f_\eta(\varepsilon) = \varepsilon(1+\eta\varepsilon)^{-(p+1)}$ with $\eta > 0$.[87]

Remark 27 Since $\varphi^\eta_{q^{(\Lambda)}}$ has the structure of a commutator, the mean flux $\omega_+(\Phi_q)$ in the NESS $\omega_+ \in \Sigma_+(\omega_0, \tau)$ is independent of the point spectrum contribution in (30),

$$\omega_+(\Phi^\eta_{q^{(\Lambda)}}) = \mathrm{tr}(W_- \varrho_0 W_-^* \varphi^\eta_{q^{(\Lambda)}}). \tag{34}$$

The next theorem contains the main assertion about the relation of the mean flux in the NESS ω_+ and the underlying scattering theory (the *Landauer-Büttiker theory*) expressed by the unitary *scattering operator*

$$S = W_+^* W_-.$$

Theorem 28 (cf. [9]) *Assume* (H1)-(H3). *Let ω_+ be the NESS in the EBB model from Theorem 23, and let q be a tempered charge. If* $\operatorname{ess\,sup}_{\varepsilon\in\mathrm{spec}_{\mathrm{ac}}(h_0)}(1+\varepsilon)^{p+1}\|\varrho_0(\varepsilon)\|\,\|q(\varepsilon)\| < \infty$, *then*[88]

$$\omega_+(\Phi_q) = \int_{\mathrm{spec}_{\mathrm{ac}}(h_0)} \frac{\mathrm{d}\varepsilon}{2\pi}\, \mathrm{tr}(\varrho_0[q - S^* q S]). \tag{35}$$

Proof Let $p = -1$.[89] Since, by assumption (H2), $v = h - h_0 \in \mathcal{L}^1(\mathfrak{h})$, we can write[90]

$$v = x^* y, \quad x, y \in \mathcal{L}^2(\mathfrak{h}). \tag{36}$$

Plugging (36) into the commutator (33) of (34) and passing into the spectral integral representation of h_0 on $\mathfrak{h}_{\mathrm{ac}}(h_0)$, we get the form (35) where the square bracket is written as a difference of products of the representation $Z(aW_-, \varepsilon)$ of aW_- on the ε-fiber of $\mathfrak{h}_{\mathrm{ac}}(h_0)$ for $a = x, y, xq^{(\Lambda)}, yq^{(\Lambda)}$. Now, due to (36), $Z(aW_-, \varepsilon)$ can be expressed by means of boundary values of bordered resolvents $ar_0(z)b$ for $a, b \in \mathcal{L}^2(\mathfrak{h})$.[91] Using the stationary representation of the scattering matrix $S(\varepsilon)$ (cf. [43, p.182]), we get (35), where, in the square bracket, we still have $q^{(\Lambda)}$ instead of q. With the help of the assumption $\operatorname{ess\,sup}_{\varepsilon\in\mathrm{spec}_{\mathrm{ac}}(h_0)}\|\varrho_0(\varepsilon)\|\,\|q(\varepsilon)\| < \infty$ and the estimate[92]

$$\int_{\mathrm{spec}_{\mathrm{ac}}(h_0)} \frac{\mathrm{d}\varepsilon}{2\pi}\, \|S(\varepsilon) - 1\|_1 \le \|v\|_1, \tag{37}$$

we can take the limit $\Lambda \to \infty$ which yields the assertion. □

Landauer-Büttiker formula

In order to make contact with the usual form of the Landauer-Büttiker formula, we require the sample to be confined. Using the unitarity of the scattering operator, we get the following corollary from Theorem 28.

Theorem 29 (cf. [9]) *Assume in addition* (H4), *and let the reservoir density of the reference state be of the form* $\oplus_j f_j(h_j)$.[93] *If* $q = \oplus_j g_j(h_j)$, *then* [94]

$$\omega_+(\Phi_q) = \sum_{j,k} \int \frac{\mathrm{d}\varepsilon}{2\pi}\, T_{jk}\, f_k\,(g_k - g_j). \tag{38}$$

[87] Using (H1) and (H2) in Assumption 21 and Lemma 3.1 in [9], we have $f_\eta(h) - f_\eta(h_0) \in \mathcal{L}^1(\mathfrak{h})$. Moreover, if $q \in \mathcal{L}(\mathfrak{h})$, we can drop the Λ-regularization.

[88] ϱ_0, q, and S commute with h_0. Hence, in the direct integral representation of h_0 on $\mathfrak{h}_{\mathrm{ac}}(h_0)$, they are given by some $\varrho_0(\varepsilon)$, $q(\varepsilon)$, and $S(\varepsilon)$, respectively (cf. [9]).

[89] Using Birman's *invariance principle*, the overall strategy of the proof for $p \in \mathbb{N}$ remains unchanged. The invariance principle addresses the question about the invariance of the wave operators $W_\pm$ under the transformation of h_0 and h into $\varphi(h_0)$ and $\varphi(h)$ for so-called *admissible* functions φ (cf. [43, p.86]).

[90] E.g. using the polar decomposition of v. $\mathcal{L}^2(\mathcal{H})$ denotes the Hilbert-Schmidt operators on $\mathcal{H}$.

[91] For $a, b \in \mathcal{L}^2(\mathcal{H})$, the operator-valued function

$$ar(\varepsilon \pm i\delta)b$$

has a limit in $\mathcal{L}^2(\mathcal{H})$ for $\delta \to 0$ for a.e. $\varepsilon \in \mathbb{R}$ (cf. [43, p.192]).

[92] Cf. [43, p.249]. The trace norm on the left hand side is taken over the fiber Hilbert space.

[93] Under (H4), expectations of flux observables in the NESS ω_+ are independent of the reference state of the sample, cf. [9].

[94] The *total transmission probability* is given by

$$T_{jk}(\varepsilon) = \mathrm{tr}(t_{jk}(\varepsilon) t^*_{jk}(\varepsilon)), \quad S_{jk}(\varepsilon) = \delta_{jk} + t_{jk}(\varepsilon).$$

The integration is carried out over $\mathrm{spec}_{\mathrm{ac}}(h_j) \cap \mathrm{spec}_{\mathrm{ac}}(h_k)$.

Remark 30 The mean flux in (38) can also be written in the form $\omega_+(\Phi_q) = \sum_{j,k} \int \frac{\mathrm{d}\varepsilon}{2\pi} T_{jk}\,(f_j - f_k)\, g_j$. Hence, it vanishes if all reservoirs have the same density or, from (38), if Φ_q is the total $g(h_0)$-flux entering the sample.

Let us now focus on the physically interesting NESS ω_+ in which the reservoirs are in thermal equilibrium at inverse temperatures β_j with chemical potentials μ_j. Hence, the mean EPR looks like

$$\mathrm{Ep}(\omega_+) = -\sum_j \beta_j \{\omega_+(\Phi_j^{\mathrm{h}}) - \mu_j\, \omega_+(\Phi_j^{\mathrm{c}})\},$$

where $\Phi_j^{\mathrm{h}} = \Phi_{h_j}$ and $\Phi_j^{\mathrm{c}} = \Phi_{1_j}$ (cf. (4)). Let $\xi_j(\varepsilon) = \beta_j(\varepsilon - \mu_j)$ and $F(x) = (1 + \mathrm{e}^x)^{-1}$. Then, the mean EPR has the following properties.

Theorem 31 (cf. [9]) *Assume* (H1)-(H4). *If* $f_j(\varepsilon) = (1 + \mathrm{e}^{\beta_j(\varepsilon - \mu_j)})^{-1}$, *then*[95]

$$\mathrm{Ep}(\omega_+) = \sum_{j,k} \int \frac{\mathrm{d}\varepsilon}{2\pi}\, \xi_j\, T_{jk}\,(F(\xi_j) - F(\xi_k)).$$

Moreover, $\mathrm{Ep}(\omega_+) \geq 0$, *and* $\mathrm{Ep}(\omega_+) > 0$ *if some* $\beta_j \neq \beta_k$ *or* $\mu_j \neq \mu_k$.[96]

Proof The form of the mean EPR directly follows from (38). Moreover, the unitarity of the scattering operator S allows to establish a lower bound on $\mathrm{Ep}(\omega_+)$ whose explicit structure leads to the last two assertions (cf. [9]). □

Remark 32 The Landauer-Büttiker theory has already been applied to the SEBB model in [24].

[95]The integration domain is $\mathrm{spec}_{\mathrm{ac}}(h_j) \cap \mathrm{spec}_{\mathrm{ac}}(h_k)$.

[96]More precisely, $\mathrm{Ep}(\omega_+) > 0$ if *channel* $j \to k$ *is open*, i.e. if

$$\mathfrak{L}(\{\varepsilon \in \mathrm{spec}_{\mathrm{ac}}(h_j) \cap \mathrm{spec}_{\mathrm{ac}}(h_k)\ :\ T_{jk}(\varepsilon) \neq 0\}) > 0$$

for the pair j, k (and $\mathfrak{L}(\cdot)$ is the Lebesgue measure; cf. [9]).

6 Linear response theory

EBB model

Analogously to Section 3, we denote by $x = (x_1^{\mathrm{h}}, \dots, x_n^{\mathrm{h}}, x_1^{\mathrm{c}}, \dots, x_n^{\mathrm{c}})$ the thermodynamic forces

$$x_j^{\mathrm{h}} = \beta_{\mathrm{eq}} - \beta_j, \quad x_j^{\mathrm{c}} = \beta_j \mu_j - \beta_{\mathrm{eq}} \mu_{\mathrm{eq}}$$

for some reference temperature β_{eq} and some reference chemical potential μ_{eq}. Moreover, let $f_{\mathrm{eq}}(\varepsilon) = (1 + \mathrm{e}^{\beta_{\mathrm{eq}}(\varepsilon - \mu_{\mathrm{eq}})})^{-1}$ be the density of the gauge-invariant quasi-free equilibrium state $\omega_{\mathrm{eq}} \in \mathcal{E}(\mathfrak{A}(\mathfrak{h}))$ at inverse temperature β_{eq} with chemical potential μ_{eq}. In the present context, the kinetic coefficients from Section 3 have the form

$$L_{ij}^{\mathrm{uv}} = \frac{\partial}{\partial x_j^{\mathrm{v}}}\, \omega_+(\Phi_i^{\mathrm{u}}) \Big|_{x=0},$$

where $\mathrm{u}, \mathrm{v} \in \{\mathrm{c}, \mathrm{h}\}$. In the following theorem, the first two assertions follow from Theorem 31 and (a generalization of) (37). For a proof of the GKF, cf. [9].

Theorem 33 (cf. [9]) *Assume* (H1)-(H4). *Then, the kinetic coefficients in the NESS* ω_+ *of the EBB model look like*[97]

$$L_{ij}^{\mathrm{uv}} = -\int \frac{\mathrm{d}\varepsilon}{2\pi}\, \varepsilon^{n_{\mathrm{u}} + n_{\mathrm{v}}} f_{\mathrm{eq}}(1 - f_{\mathrm{eq}})(T_{ij} - \delta_{ij} \sum_k T_{ik}).$$

If (H1)-(H4) *and* (TRI) *holds, then we have the ORR,*

$$L_{ij}^{\mathrm{hc}} = L_{ji}^{\mathrm{ch}}.$$

Finally, if (H1)-(H5) *with* $p = -1$ *and* (TRI) *holds, then we have the GKF,*

$$L_{ij}^{\mathrm{uv}} = \lim_{T \to \infty} \frac{1}{2} \int_{-T}^{T} \mathrm{d}t\ \omega_{\mathrm{eq}}(\tau^t(\Phi_i^{\mathrm{u}}) \Phi_j^{\mathrm{v}}).$$

Remark 34 In the SEBB model, the relevant actions of the wave operator can be explicitly evaluated. This, in turn, leads to explicit expressions for the kinetic coefficients, and, hence, the ORR and the GKF can be verified by direct computation (cf. [7]).

[97]With $n_{\mathrm{h}} = 1$, $n_{\mathrm{c}} = 0$. The integration domain is $\mathrm{spec}_{\mathrm{ac}}(h_0)$.

Remark 35 The ORR and the GKF have been derived axiomatically for more general classes of open systems in [29].

7 Weak coupling theory

As discussed in Section 3, we want to establish a criterion which guarantees the strict positivity of the mean FGR EPR. To this end, let us consider an open system consisting of a finite dimensional sample $\mathcal{S}$ with Hamiltonian $H_{\mathcal{S}} \in \mathcal{O}_{\mathcal{S}}$ which is coupled to reservoirs in $(\tau_{\mathcal{R}_j}, \beta_j)$-KMS states $\omega_{\mathcal{R}_j}$ by the the local perturbation λV with real coupling parameter λ, and let V be of the form $V = \sum_j V_j$ with

$$V_j = \sum_\alpha Q_j^\alpha \otimes v_j^\alpha,$$

where $Q_j^\alpha \in \mathcal{O}_{\mathcal{S}}$ and $v_j^\alpha \in \mathcal{O}_{\mathcal{R}_j}$ are self-adjoint. As discussed in Section 3, in order to establish such a criterion, we make a first assumption on the effective coupling of the sample to the reservoirs and a second one being a non-degeneracy condition for the Davies generator. The first assumption is formulated with the help of the Fourier transform of the time correlation functions of the reservoir part v_j^α of the coupling,

$$h_j^{\alpha\beta}(\varepsilon) = \int_{-\infty}^{\infty} \mathrm{d}t\ \omega_{\mathcal{R}_j}(\tau_{\mathcal{R}_j}^t(v_j^\alpha)\, v_j^\beta)\, \mathrm{e}^{-\mathrm{i}\varepsilon t},$$

whereas the second assumption involves the commutant (cf. footnote 16),

$$\mathfrak{C}_j = \{H_{\mathcal{S}}, Q_j^\alpha \text{ all } \alpha\}'.$$

Assumption 36 (cf. [5])
(E$_j$) $h_j(\varepsilon) > 0$ *for all* $\varepsilon \in \mathrm{spec}(-\mathrm{i}\delta_{\mathcal{S}})$[98]
(C$_j$) $\mathfrak{C}_j = \mathbb{C}\,1$

We can now formulate our criterion for the strict positivity of the FGR EPR. The FGR NESS $\omega_{\mathcal{S}+}$ is given in (5).

[98] We denote by $h_j(\varepsilon)$ the matrix with entries $h_j^{\alpha\beta}(\varepsilon)$. Moreover, recall that $\delta_{\mathcal{S}} = \mathrm{i}[H_{\mathcal{S}}, \cdot]$ denotes the generator of $\tau_{\mathcal{S}}^t \in \mathrm{Aut}(\mathcal{O}_{\mathcal{S}})$.

Theorem 37 (cf. [5]) *Assume* (E$_j$) *and* (C$_j$) *for all* $j = 1, ..., M$. *Then, for sufficiently small* λ, *if there are some* $\beta_i \neq \beta_j$, *the mean FGR EPR is strictly positive,*

$$\mathrm{Ep}_{\mathrm{fgr}}(\omega_{\mathcal{S}+}) > 0.$$

Proof Let us denote by K_{S} the adjoint of K_{H} w.r.t. the scalar product $(X, Y) = \mathrm{tr}(X^*Y)$ (cf. Section 3). Since

$$\mathrm{Ep}_{\mathrm{fgr}}(\omega) = \sum_j \mathrm{Ep}_{\mathrm{fgr},j}(\omega)$$

for any $\omega \in \mathcal{E}(\mathcal{O}_{\mathcal{S}})$, the total mean FGR EPR vanishes iff each nonnegative $\mathrm{Ep}_{\mathrm{fgr},j}(\omega)$ vanishes. Under the assumption (E$_j$) and (C$_j$), the only state in the kernel of $K_{\mathrm{S},j}$ is the unique $(\tau_{\mathcal{S}}, \beta_j)$-KMS state ω_{β_j} (cf. [32]). Moreover, it is the only state with vanishing mean FGR EPR (cf. [32]),

$$\mathrm{Ep}_{\mathrm{fgr},j}(\omega_{\beta_j}) = 0.$$

Since the assumption (E$_j$) and (C$_j$) also imply that the kernel of the total K_{S} is nondegenerate (cf. [32]), the assertion follows if there are some $\beta_i \neq \beta_j$. □

Remark 38 One easily constructs examples which illustrate that the conditions of Theorem 37 are sufficient but not necessary (cf. [5]).

Remark 39 As discussed at the end of Section 3, the goal is to use this algebraic criterion to prove strict positivity of the entropy production $\mathrm{Ep}(\omega_+)$ of the full microscopic model. This is achieved as soon as, for sufficiently small λ, the relation

$$\mathrm{Ep}(\omega_+) = \lambda^2\, \mathrm{Ep}_{\mathrm{fgr}}(\omega_{\mathcal{S}+}) + \mathcal{O}(\lambda^3) \tag{39}$$

is established. This has been done for a finite dimensional sample coupled to two fermionic reservoirs (cf. [28]) and for the SEBB model (cf. [7]).

Theorem 40 (cf. [5]) *If the assumptions of Theorem 37 and* (39) *hold, then, for sufficiently small* λ,

$$\mathrm{Ep}(\omega_+) > 0.$$

8 Correlations

In this last section, we will study some more correlation functions in space and time of certain types of observables in the foregoing NESS of the XY chain and in more general quasi-free states. As spatial correlations, we treat the spin-spin coupling and the emptiness formation probability, and as a correlation in time, we study the moment generating function of the Gallavotti-Cohen symmetry.

XY model

We start off with the truncated two-point function of the longitudinal[99] spin-spin correlation,

$$C_3^T(n) = \omega_+(\sigma_3^{(0)}\sigma_3^{(n)}) - \omega_+(\sigma_3^{(0)})^2,$$

where ω_+ is the unique NESS of Theorem 16 with density (27).

In contrast to the situation in thermal equilibrium, i.e. for $\beta_L = \beta_R$, where the decay is exponential (cf. [33, 35, 14]), the out of equilibrium decay in the longitudinal direction is polynomial only.

Theorem 41 (cf. [4]) *The decay of the longitudinal truncated two-point function $C_3^T(n)$ in the NESS ω_+ of the XY chain behaves like*

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

Proof With the help of the Jordan-Wigner transformation (9), the longitudinal correlation function $C_3^T(n)$ becomes a four-point function in the Jordan-Wigner fermions, and so for all n independently of their distance from the origin.[100] Hence, using the fact that ω_+ is quasi-free, the evaluation of $C_3^T(n)$ boils down to study the determinant of the inverse Fourier transform of $\hat{\varrho}_+(\mathrm{e}^{\mathrm{i}\xi})$ from (28) which, after an explicit computation, takes the form

$$C_3^T(n) = -\left(\int_0^{2\pi}\frac{\mathrm{d}\xi}{2\pi}\,\frac{\mathrm{sign}(\kappa)\,\mathrm{sh}(\delta\mu)}{\mathrm{ch}(\beta\mu)+\mathrm{ch}(\delta\mu)}\,\sin(n\xi)\right)^2 + R(n),$$

where the remainder $R(n)$ is exponentially decaying for large n. Due to the discontinuity in the integrand, the claim follows by partial integration. □

Naturally, we are also interested in the spin-spin correlation in the transversal directions. Unlike in the longitudinal correlation function $C_3^T(n)$, the number of fermionic events involved after the Jordan-Wigner transformation increases linearly in n in the transversal correlation function[101]

$$C(n) = \omega_+(\sigma_1^{(0)}\sigma_1^{(n)}).$$

This is due to the non-local nature of the Jordan-Wigner transformation (9) in the transversal direction,

$$\sigma_1^{(n)} = T\left(\prod_{k=1}^{n-1}(2a_k^*a_k - 1)\right)(a_n + a_n^*)$$

if $n \geq 2$ (cf. after (9)).[102] With the help of the Bogoliubov $*$-automorphism $\tau_x \in \mathrm{Aut}(\mathfrak{A}(\mathfrak{h}^{\oplus 2}, J))$ of translations (cf. footnote 66),

$$\tau_x(B(f)) = B(U_x f),$$

where $U_x = u_x \oplus u_x$ and $(u_x\varphi)(y) = \varphi(y-x)$ for $\varphi \in \mathfrak{h}$, we define the form factors by

$$f_{2j-1} = U_j g_0, \quad f_{2j} = U_j g_1, \tag{40}$$

where $g_0 = [-\delta_{-1}, \delta_{-1}]$ and $g_1 = [\delta_0, \delta_0]$. Hence, we can express the correlation function as[103]

$$C(n) = \mathrm{pf}\,\Omega(n). \tag{41}$$

[99] I.e. in the 3-direction. The 1,2-directions are *transversal*.

[100] The relation (9) is local in the 3-direction , i.e.

$$\sigma_3^{(n)} = 2a_n^* a_n - 1.$$

[101] We study $\sigma_1^{(0)}\sigma_1^{(n)}$, the 2-direction being analogous.

[102] Similarly, $\sigma_2^{(n)} = iTS^{(n)}(a_n - a_n^*)$.

[103] Recall that $\Omega(n)$ is the correlation matrix from (21) and pf is the Pfaffian from (19).

Since, by definition, $\Omega(n)$ is skew-symmetric, the square of the correlation becomes a determinant. Moreover, using the definitions

$$\begin{aligned}\varphi_{\alpha,\alpha'}(\mathrm{e}^{\mathrm{i}\xi}) &= \frac{\mathrm{sh}(\alpha\mu(\mathrm{e}^{\mathrm{i}\xi}))}{\mathrm{ch}(\alpha\mu(\mathrm{e}^{\mathrm{i}\xi}))+\mathrm{ch}(\alpha'\mu(\mathrm{e}^{\mathrm{i}\xi}))},\\ q(\mathrm{e}^{\mathrm{i}\xi}) &= \frac{\cos\xi-\lambda+\mathrm{i}\gamma\sin\xi}{\mu(\mathrm{e}^{\mathrm{i}\xi})}\mathrm{e}^{-\mathrm{i}\xi},\end{aligned}$$

for $\alpha,\alpha'\in\mathbb{R}$, we have the following fundamental observation.

Theorem 42 (cf. [6]) *The transversal spin-spin correlation function $C(n)^2$ in the NESS ω_+ of the XY chain is the determinant of the finite section of a Toeplitz operator $T[a]\in\mathcal{L}(\ell^2_2(\mathbb{N}))$,*[104]

$$C(n)^2=\det T_n[a],$$

where the 2×2-block symbol has the form[105]

$$a=\begin{bmatrix}-\varphi_{\delta,\beta}\,\mathrm{sign}\,\kappa & -\varphi_{\beta,\delta}\,q\\ \varphi_{\beta,\delta}\,\bar{q} & \varphi_{\delta,\beta}\,\mathrm{sign}\,\kappa\end{bmatrix}\in L^\infty_{2\times 2}(\mathbb{T}).$$

[104] An $N\times N$-block Toeplitz matrix $A\in\mathbb{C}^{Nn\times Nn}$ is a matrix whose block elements $a_{ij}\in\mathbb{C}^{N\times N}$ depend on $i-j$ only, i.e.

$$A=\begin{bmatrix}a_0 & a_{-1} & \dots & a_{-(n-1)}\\ a_1 & a_0 & \dots & a_{-(n-2)}\\ \vdots & \vdots & \ddots & \vdots\\ a_{n-1} & a_{n-2} & \dots & a_0\end{bmatrix}.$$

An infinite $N\times N$-block Toeplitz operator is defined as follows. Let $f\in\ell^2_N(\mathbb{N})$ be a $\mathbb{C}^N$-valued sequence which is square-integrable w.r.t. the Euclidean norm on $\mathbb{C}^N$, and let a_x be a sequence of complex $N\times N$-matrices. The action of a Toeplitz operator is defined by $f\mapsto\{\sum_{j=1}^\infty a_{i-j}f_j\}_{i=1}^\infty$. Due to *Toeplitz' theorem* (cf. [15]), such an operator is in $\mathcal{L}(\ell^2_N(\mathbb{N}))$ iff

$$a_x=\int_0^{2\pi}\frac{\mathrm{d}\xi}{2\pi}\,a(\mathrm{e}^{\mathrm{i}\xi})\,\mathrm{e}^{-\mathrm{i}x\xi}$$

for some $a\in L^\infty_{N\times N}(\mathbb{T})$, where $L^\infty_{N\times N}(\mathbb{T})$ denotes the $\mathbb{C}^{N\times N}$-valued functions on $\mathbb{T}$ whose components are all in $L^\infty(\mathbb{T})$. Using the projection $P_n(\{x_1,...,x_n,x_{n+1},...\})=\{x_1,...,x_n,0,0,...\}$, we define the *finite section* of $T[a]$ by $T_n[a]=P_nT[a]P_n$ on the range of P_n.

[105] A Toeplitz operator and its symbol are called *scalar* iff $N=1$ and *block* otherwise.

Proof We know from assertion *(3)* of Theorem 18 that ω_+ is translation invariant, i.e.

$$\omega_+\circ\tau_x=\omega_+.$$

Hence, due to the structure of the form factors F_j in (40), the correlation matrix $\Omega(n)$ is a 2×2-block Toeplitz matrix. Moreover, since the density $\hat{\varrho}_+$ from (28) is in $L^\infty_{2\times 2}(\mathbb{T})$, we get the assertion by invoking Toeplitz' theorem of footnote 104. □

Therefore, in order to estimate the decay rate of $C(n)$, we have to study the asymptotics of the determinant of a non-scalar Toeplitz operator. Due to the general lack of control of the spectrum of a non-regular non-scalar Toeplitz operator in the vicinity of the origin[106], we focus on an upper bound on the decay rate. The proof of the next assertion is given after Theorem 47 in the setting of more general quasi-free states.

Theorem 43 (cf. [6]) *The decay rate of the transversal correlation function in the NESS ω_+ of the XY chain has the strictly negative upper bound of the form*

$$\limsup_{n\to\infty}\frac{\log|C(n)|}{n}\le\frac{1}{2}\sum_{j=L,R}\int_0^{2\pi}\frac{\mathrm{d}\xi}{2\pi}\,\log\mathrm{th}(\beta_j\mu/2).$$

In order to learn more about the correlations out of equilibrium, we study two other types of spatial correlations in the NESS ω_+ of the XY chain, namely at the *von Neumann entropy density* and at the *emptiness formation probability* both of whose asymptotics can eventually be treated by means of Toeplitz theory. The von Neumann entropy is defined by

$$\mathrm{Ent}(n)=-\mathrm{tr}(\omega_+^{(n)}\log\omega_+^{(n)}),$$

where $\omega_+^{(n)}$ denotes the restriction of the NESS ω_+ to the subblock of n neighboring spins on the chain. Let us denote by $\eta(x)=-x\log x-(1-x)\log(1-x)$ the so-called *Shannon entropy*. Then, we have the following theorem about the asymptotics of the von Neumann entropy density.

[106] This is due to the fact that *Coburn's Lemma* has no analog in the block case (cf. [15, 186]).

Theorem 44 (cf. [8]) *The asymptotic von Neumann entropy density in the NESS ω_+ of the XY chain is strictly positive,*

$$\lim_{n\to\infty}\frac{\mathrm{Ent}(n)}{n}=\frac{1}{2}\sum_{j=L,R}\int_0^{2\pi}\frac{\mathrm{d}\xi}{2\pi}\,s(\mathrm{th}(\beta_j\mu/2)),$$

where $s(x)=\eta((1+x)/2)$.

Proof We start off by constructing the Majorana[107] correlation matrix $\Omega(n)_{ij}=\omega_+(d_id_j)$ whose imaginary part turns out to be the finite section of a 2×2-block Toeplitz operator with some symbol $a\in L^\infty_{2\times2}(\mathbb{T})$. Moreover, there exists a set of fermions c_i in the CAR algebra $\mathfrak{A}(\mathfrak{h}_n)$ over $\mathfrak{h}_n=\mathbb{C}^n$ s.t. the reduced density matrix $\omega_+^{(n)}$ has the form

$$\omega_+^{(n)}=\prod_{i=1}^{n}\left(\frac{1+\lambda_i^{(n)}}{2}c_i^*c_i+\frac{1-\lambda_i^{(n)}}{2}c_ic_i^*\right),$$

where $\pm\mathrm{i}\lambda_i^{(n)}\in\mathrm{spec}(T_n[a])$. Hence, from the spectral representation of $\omega_+^{(n)}$, we have

$$\mathrm{Ent}(n)=\sum_{i=1}^{n}s(\lambda_i^{(n)}).$$

Since $\|T_n[a]\|\le\varrho<1$ uniformly in n, Szegő's first limit theorem in the block case (cf. [15, p.202]) implies the assertion. $\square$

At the end of this subsection, we discuss the correlation function mentioned above in which the effect of the singularity of the symbol $\hat{\varrho}_+$ in (28) becomes visible (at least in the isotropic case $\gamma=0$). This is the case for the so-called *emptiness formation probability*,

$$P(n)=\omega_+(\Pi^{(1)}\Pi^{(2)}\ldots\Pi^{(n)}),$$

where $\Pi^{(j)}=(1-\sigma_3^{(j)})/2$ is the orthogonal projection onto the spin down direction. In this correlation, after casting it again into the form of a block Toeplitz determinant $\det T_n[a]$, we can extract the subleading order q in the large n asymptotics from Fisher-Hartwig theory (cf. [16, p.582]),[108]

$$\det T_n[a]\sim G[b]^{n+1}n^qF[b,t_j,\alpha_j,\delta_j].$$

Here, the Fisher-Hartwig symbol a has the form

$$a(t)=b(t)\prod_k|t-t_k|^{2\alpha_k}\varphi_{\delta_k,t_k}(t),\quad t\in\mathbb{T},$$

where t_k describes the location of singularities, $b(t)$ is sufficiently regular, and $\varphi_{\delta_i,t_i}(t)$ is the *pure Fisher-Hartwig jump* with jump phase $2\pi\delta_k$. Moreover, the function F is independent of n. [109] The following effect of the true non-equilibrium on the asymptotics of the emptiness formation probability $P(n)$ is studied in [12].

Theorem 45 (cf. [12]) *The subleading order q of the emptiness formation probability $P(n)$ in the NESS ω_+ of the isotropic XY chain is strictly positive iff $\beta_L\neq\beta_R$.*

EBB model

In this final subsection, we derive a condition on the symbol which implies exponential decay in more general quasi-free models.[110] For this purpose, we start directly in the (self-dual) quasi-free setting on the discrete line, i.e. we pick any quasi-free state $\omega\in\mathcal{E}(\mathfrak{A}(\mathfrak{h}^{\oplus2},J))$ with density $\varrho\in\mathcal{L}(\mathfrak{h}^{\oplus2})$ satisfying the conditions (23), and study the correlation $C(n)$ given by (41) under the following assumptions.

Assumption 46 (cf. [10])
(A1) *The quasi-free state ω is translation invariant.*
(A2) $f_{2j-1}=U_jg_0$ *and* $f_{2j}=U_jg_1$
(A3) $g_0=[-\delta_{-1},\delta_{-1}]$ *and* $g_1=[\delta_0,\delta_0]$

[107] $2n$ self-adjoint operators d_j on $\mathbb{C}^{2^n}$ satisfying $\{d_i,d_j\}=2\delta_{ij}$ are called *Majorana operators*.

[108] The *Fisher-Hartwig theory* describes the asymptotic behavior of Toeplitz determinants for a class of symbols whose singularity do not allow for an analysis by Szegő's theory.

[109] For the precise formulation of the conditions in the *Fisher-Hartwig theorem*, cf. [16, p.582].

[110] Cf. Remark 50 for the correlation in time mentioned above.

Due to (A1), the density ϱ is, in the Fourier picture, an operator $\hat{\varrho} \in \mathcal{L}(\hat{\mathfrak{h}}^{\oplus 2})$ which acts by multiplication with the function $\hat{\varrho}(\mathrm{e}^{\mathrm{i}\xi}) \in L^\infty_{2\times 2}(\mathbb{T})$. With the help of the spectral set

$$\mathfrak{T} = \{\xi \in [0, 2\pi) \mid 1/2 \notin \text{spec}\, \hat{\varrho}(\mathrm{e}^{\mathrm{i}\xi}) \not\subseteq \{0, 1\}\},$$

we derive the following upper bound on the decay rate $\limsup \log(|C(n)|)/n$.

Theorem 47 (cf. [10]) *Let* $\omega \in \mathcal{E}(\mathfrak{A}(\mathfrak{h}^{\oplus 2}, J))$ *be a quasi-free state with density* $\varrho \in \mathcal{L}(\mathfrak{h}^{\oplus 2})$. *Assume* (A1)-(A3), *and let* $\mathfrak{L}(\mathfrak{T}) > 0$. *Then, the decay rate of the correlation function* $C(n)$ *has a strictly negative upper bound of the form*

$$\limsup_{n\to\infty} \frac{\log |C(n)|}{n} \le \frac{1}{2} \int_{\mathfrak{T}} \frac{\mathrm{d}\xi}{2\pi} \log |\det(2\hat{\varrho}(\mathrm{e}^{\mathrm{i}\xi}) - 1)|.$$

Proof Due (A1)–(A3), the correlation $C(n)$ can be written as the determinant of the finite section of a 2×2-block Toeplitz $T[a]$ with some symbol $a \in L^\infty_{2\times 2}(\mathbb{T})$. Introducing a strictly positive and uniform gap at the origin on the set of singular values of $T_n[a]$, the Avram-Partner theorem[111] implies that the decay rate is bounded from above by

$$\int_0^{2\pi} \frac{\mathrm{d}\xi}{2\pi} \operatorname{tr} \log'(a^*(\mathrm{e}^{\mathrm{i}\xi}) a(\mathrm{e}^{\mathrm{i}\xi})),$$

where $\log'(x)$ denotes the logarithm regularized w.r.t. the gap. Using the fact that $\det a(\mathrm{e}^{\mathrm{i}\xi}) = -\det[2\hat{\varrho}(\mathrm{e}^{\mathrm{i}\xi}) - 1]$ and some basics from Toeplitz theory, we get the assertion. □

[111]The *Avram-Parter theorem* in the block case states that for a block Toeplitz operator with symbol $a \in L^\infty_{N\times N}(\mathbb{T})$ and singular values $t_j^{(n)}$, one has

$$\lim_{n\to\infty} \frac{1}{Nn} \sum_{j=1}^{Nn} g((t_j^{(n)})^2) = \frac{1}{N} \int_0^{2\pi} \frac{\mathrm{d}\xi}{2\pi} \operatorname{tr}(g(a^* a))$$

where $g \in C_0(\mathbb{R})$ (the functions of compact support; cf. [15, p.186]).

Remark 48 In the example of the XY chain out of equilibrium, Theorem 47 yields the expression already found in Theorem 43. In the case of thermal equilibrium, $\beta_L = \beta_R$, the spectral condition is still satisfied and our bound is exact. At zero temperature, the spectral condition is not fulfilled anymore. Indeed, there exists long-range order or quasi-long-range order depending on the anisotropy γ and the magnetic field λ (cf. [10]).

Remark 49 With an analogous argument, we can give a sufficient condition on the spectrum of the density ϱ which guarantees the exponential decay for the emptiness formation probability correlation from the previous subsection (cf. [12]).

Remark 50 Finally, we are interested in the *Gallavotti-Cohen* (GC) symmetry

$$e(1 - \lambda) = e(\lambda)$$

for the limit of the moment generating function

$$e(\lambda) = \lim_{t\to\infty} \frac{1}{t} \log \omega_+(\mathrm{e}^{-\lambda \int_0^t \mathrm{d}s\, \tau^s(\Phi)}),$$

where Φ is of the form (31) and (32). Using the asymptotic theory of block Wiener-Hopf determinants, $e(\lambda)$ can be expressed by the scattering operator as in Section 5. Numerical evidence is given in [13] for invalidity of the GC symmetry, a point which remains to be studied in more detail.

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