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Entropic fluctuations in XY chains and reflectionless Jacobi matrices

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Abstract. We study entropic functionals/fluctuations of the XY chain with Hamiltonian

$$\frac{1}{2}\sum_{x\in\mathbb{Z}} J_x\left(\sigma_x^{(1)}\sigma_{x+1}^{(1)}+\sigma_x^{(2)}\sigma_{x+1}^{(2)}\right)+\lambda_x\sigma_x^{(3)}$$

where initially the left ($x\leq 0$)/right ($x>0$) part of the chain is in thermal equilibrium at inverse temperature β_l/β_r. The temperature differential results in a non-trivial energy/entropy flux across the chain. The Evans-Searles (ES) entropic functional describes fluctuations of the flux observable with respect to the initial state while the Gallavotti-Cohen (GC) functional describes these fluctuations with respect to the steady state (NESS) the chain reaches in the large time limit. We also consider the full counting statistics (FCS) of the energy/entropy flux associated to a repeated measurement protocol, the variational entropic functional (VAR) that arises as the quantization of the variational characterization of the classical Evans-Searles functional and a natural class of entropic functionals that interpolate between FCS and VAR. We compute these functionals in closed form in terms of the scattering data of the Jacobi matrix $hu_x = J_x u_{x+1}+\lambda_x u_x + J_{x-1}u_{x-1}$ canonically associated to the XY chain. We show that all these functionals are identical if and only if h is reflectionless (we call this phenomenon entropic identity). If h is not reflectionless, then the ES and GC functionals remain equal but differ from the FCS, VAR and interpolating functionals. Furthermore, in the non-reflectionless case, the ES/GC functional does not vanish at $\alpha=1$ (*i.e.*, the Kawasaki identity fails) and does not have the celebrated $\alpha\leftrightarrow 1-\alpha$ symmetry. The FCS, VAR and interpolating functionals always have this symmetry. In the Schrödinger case, where $J_x=J$ for all x, the entropic identity leads to some unexpected open problems in the spectral theory of one-dimensional discrete Schrödinger operators.

1 Introduction

The XY chain is an exactly solvable model which is often used to illustrate existing theories and to test emerging theories in quantum statistical mechanics. The literature on XY chains is enormous and we mention here the mathematically rigorous works [Ar3, Ar4, AB1, AB2, AH, AP, BM, HR, Ma, Mc, OM]. It is therefore not surprising that a model of an open quantum system based on the XY chain was also a testing ground for the recent developments in non-equilibrium quantum statistical mechanics initiated in the works [JP1, JP2, Ru2]. More precisely, the first proofs of the existence of a non-equilibrium steady state (NESS) and of strict positivity of entropy production in an open quantum system were given in the papers [AH, AP] in the context of XY chains. The purpose of this paper is similar and our goal is to test the emerging theory of entropic fluctuations in non-equilibrium quantum statistical mechanics developed in [JOPP] (see also [DDM, Ku, Ro, TM] for related works) on the example of XY chains. For discussion and

references to the classical theory of entropic fluctuations (which, starting with the seminal works [CG, ES], has played a dominant role in the recent theoretical, numerical and experimental advances in classical non-equilibrium statistical mechanics) we refer the reader to the reviews [JPR, RM].

The paper is organized as follows. In Section 1.1 we describe the XY chain confined to a finite interval in $\mathbb{Z}$, introduce the finite volume and finite time entropic functionals and describe their basic properties. The thermodynamic limit of the confined XY chain and its entropic functionals is discussed in Section 1.2. The elements of spectral and scattering theory needed to state and prove our results are reviewed in Section 1.3. In Section 1.4 we review the results regarding the existence of the NESS and introduce the finite time Gallavotti-Cohen functional. Our main results are stated in Section 1.5. In Section 1.6 we briefly discuss these results and in Section 1.7 we comment on reflectionless Jacobi matrices. The proofs are given in Section 2. Some proofs are only sketched and the reader can find details and additional information in the forthcoming Master's thesis [La].

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1.1 The confined XY chain

To each $x \in \mathbb{Z}$ we associate the Hilbert space $\mathcal{H}_x = \mathbb{C}^2$ and the corresponding matrix algebra $\mathcal{O}_x = \mathrm{M}_2(\mathbb{C})$. The Pauli matrices

$$\sigma_x^{(1)} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_x^{(2)} = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}, \quad \sigma_x^{(3)} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

together with the identity matrix $\mathbb{1}_x$ form a basis of $\mathcal{O}_x$ that satisfies the relations

$$\sigma_x^{(j)}\sigma_x^{(k)} = \delta_{jk}\mathbb{1}_x + \mathrm{i}\varepsilon^{jkl}\sigma_x^{(l)}.$$

Let $\Lambda = [N, M]$ be a finite interval in $\mathbb{Z}$. The Hilbert space and the algebra of observables of the XY chain confined to Λ are

$$\mathcal{H}_\Lambda = \bigotimes_{x\in\Lambda} \mathcal{H}_x, \qquad \mathcal{O}_\Lambda = \bigotimes_{x\in\Lambda} \mathcal{O}_x.$$

The spectrum of the observable $A \in \mathcal{O}_\Lambda$ is denoted $\mathrm{sp}(A)$. If A is self-adjoint, $\mathbb{1}_E(A)$ denotes the spectral projection associated to $E \in \mathrm{sp}(A)$.

We shall identify $A_x \in \mathcal{O}_x$ with the element $(\otimes_{y\in\Lambda\setminus\{x\}}\mathbb{1}_y) \otimes A_x$ of $\mathcal{O}_\Lambda$. In a similar way we identify $\mathcal{O}_{\Lambda'}$ with the appropriate subalgebra of $\mathcal{O}_\Lambda$ for $\Lambda' \subset \Lambda$. With these notational conventions the Hamiltonian of the XY chain confined to Λ is

$$H_\Lambda = \frac{1}{2}\sum_{x\in[N,M[} J_x\left(\sigma_x^{(1)}\sigma_{x+1}^{(1)} + \sigma_x^{(2)}\sigma_{x+1}^{(2)}\right) + \frac{1}{2}\sum_{x\in[N,M]} \lambda_x\sigma_x^{(3)}.$$

Here, J_x is the nearest neighbor coupling constant and λ_x is the strength of an external magnetic field in direction (3) at the site x. Throughout the paper we shall assume that $\{J_x\}_{x\in\mathbb{Z}}$ and $\{\lambda_x\}_{x\in\mathbb{Z}}$ are bounded sequences of real numbers and that $J_x \neq 0$ for all $x \in \mathbb{Z}$.

Consider the XY chain confined to the interval $\Lambda = [-M, M]$. Its Hamiltonian can be written as

$$H_\Lambda = H_l + H_r + V,$$

where H_l is the Hamiltonian of the XY chain confined to $[-M, 0]$, H_r is the Hamiltonian of the XY chain confined to $[1, M]$, and

$$V = \frac{1}{2}J_0\left(\sigma_0^{(1)}\sigma_1^{(1)} + \sigma_0^{(2)}\sigma_1^{(2)}\right),$$

is the coupling energy. Until the end of this section $\Lambda = [-M, M]$ is fixed and we shall omit the respective subscript, *i.e.*, we write $\mathcal{H} = \mathcal{H}_\Lambda$, $\mathcal{O} = \mathcal{O}_\Lambda$, $H = H_\Lambda$, *etc.*[1]

The states of XY chain are described by density matrices on $\mathcal{H}$. The expectation value of the observable A w.r.t. the state ρ is $\rho(A) = \mathrm{tr}(\rho A)$. We set

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

In the Heisenberg/Schrödinger picture the observables/states evolve in time as

$$A_t = \tau^t(A), \qquad \rho_t = \tau^{-t}(\rho).$$

Obviously, $\rho_t(A) = \rho(A_t)$. The relative entropy of the state ρ w.r.t. the state ν is defined by

$$S(\rho|\nu) = \mathrm{tr}(\rho(\log \nu - \log \rho)).$$

We recall that $S(\rho|\nu) \leq 0$ and that $S(\rho|\nu) = 0$ iff $\rho = \nu$.[2] For additional information about the relative entropy we refer the reader to [JOPP, OP].

Following the setup of [AH], we shall consider the evolution of the XY chain with an initial state given by

$$\omega = \frac{\mathrm{e}^{-\beta_l H_l - \beta_r H_r}}{\mathrm{tr}(\mathrm{e}^{-\beta_l H_l - \beta_r H_r})}, \tag{1.1}$$

where $\beta_{l/r} > 0$. Hence, the left part of the chain is initially in thermal equilibrium at inverse temperature β_l while the right part of the chain is in thermal equilibrium at inverse temperature β_r. The XY chain is time-reversal invariant: there exists an anti-unitary involution $\theta : \mathcal{H} \to \mathcal{H}$, described in Section 2.1, such that, setting $\Theta(A) = \theta A \theta^{-1}$, one has

$$\Theta(H_{l/r}) = H_{l/r}, \qquad \Theta(V) = V, \qquad \Theta(\omega) = \omega.$$

The observables describing the heat fluxes out of the left/right chain are

$$\Phi_{l/r} = -\frac{\mathrm{d}}{\mathrm{d}t}\tau^t(H_{l/r})\Big|_{t=0} = -\mathrm{i}[H, H_{l/r}] = \mathrm{i}[H_{l/r}, V],$$

and an easy computation gives

$$\Phi_l = \frac{1}{2} J_0 J_{-1} \sigma_0^{(3)} (\sigma_1^{(1)} \sigma_{-1}^{(2)} - \sigma_1^{(2)} \sigma_{-1}^{(1)}) + \frac{1}{2} J_0 \lambda_0 (\sigma_1^{(2)} \sigma_0^{(1)} - \sigma_1^{(1)} \sigma_0^{(2)}),$$

$$\Phi_r = \frac{1}{2} J_0 J_1 \sigma_1^{(3)} (\sigma_0^{(1)} \sigma_2^{(2)} - \sigma_0^{(2)} \sigma_2^{(1)}) + \frac{1}{2} J_0 \lambda_1 (\sigma_0^{(2)} \sigma_1^{(1)} - \sigma_0^{(1)} \sigma_1^{(2)}).$$

The entropy production observable of the XY chain is

$$\sigma = -\beta_l \Phi_l - \beta_r \Phi_r.$$

Note that $\Phi_{l/r}$ and σ change sign under the time reversal:

$$\Theta(\Phi_{l/r}) = -\Phi_{l/r}, \qquad \Theta(\sigma) = -\sigma.$$

[1] One can consider a more general setup where $H_{l/r}$ is the Hamiltonian of the XY chain confined to $[-M, -N-1]/[N+1, M]$, H_c is the Hamiltonian of the XY chain confined to $[-N, N]$, and $H = H_l + H_c + H_r + V$, where

$$V = \frac{1}{2} J_{-N-1} \left(\sigma_{-N-1}^{(1)} \sigma_{-N}^{(1)} + \sigma_{-N-1}^{(2)} \sigma_{-N}^{(2)} \right) + \frac{1}{2} J_N \left(\sigma_N^{(1)} \sigma_{N+1}^{(1)} + \sigma_N^{(2)} \sigma_{N+1}^{(2)} \right).$$

In this scenario the left and the right parts of the chain are connected via the central part which is also an XY chain. In the thermodynamic limit one takes $M \to \infty$ while keeping N fixed. The central part remains finite and represents a small system (quantum dot) connecting two infinitely extended chains (thermal reservoirs). All our results and proofs extend to this setting [La]. For notational simplicity, we will discuss here only the simplest case of two directly coupled chains.

[2] $S(\rho|\nu) = -\infty$ unless $\mathrm{Ker}\, \nu \subset \mathrm{Ker}\, \rho$.

The observable describing the mean entropy production rate over the time interval $[0, t]$ is

$$\Sigma^t = \frac{1}{t}\int_0^t \sigma_s \mathrm{d}s.$$

The basic properties of this observable are summarized in:

Proposition 1.1 (1) $\log \omega_t = \log \omega + t\tau^{-t}(\Sigma^t)$.

(2) $S(\omega_t|\omega) = -t\omega(\Sigma^t)$.

(3) $\tau^t(\Sigma^{-t}) = \Sigma^t$.

(4) $\Sigma^t = -\tau^t(\Theta(\Sigma^t))$. *In particular,* $\mathrm{sp}(\Sigma^t)$ *is symmetric w.r.t. zero and* $\dim \mathbb{1}_\phi(\Sigma^t) = \dim \mathbb{1}_{-\phi}(\Sigma^t)$ *for all* $\phi \in \mathrm{sp}(\Sigma^t)$.

The proof of Proposition 1.1 is elementary and can be found in [JOPP]. Part (1) allows for the interpretation of the entropy production observable σ as the *quantum phase space contraction rate*. Part (2) implies that for all $t > 0$ the average entropy production rate over the interval $[0, t]$ is non-negative, *i.e.*,

$$\omega(\Sigma^t) = \sum_{\phi \in \mathrm{sp}(\Sigma^t)} \phi\, p^t_\phi \geq 0, \tag{1.2}$$

where

$$p^t_\phi = \omega(\mathbb{1}_\phi(\Sigma^t)),$$

is the probability that a measurement of Σ^t in the state ω will yield the value ϕ. In particular, on average heat flows from the hotter to the colder part of the chain, in accordance with the (finite time) second law of thermodynamics. By Property (4), (1.2) is equivalent to

$$\sum_{\substack{\phi \in \mathrm{sp}(\Sigma^t) \\ \phi > 0}} \phi(p^t_\phi - p^t_{-\phi}) \geq 0.$$

The finite time fluctuation relation is deeper. The direct quantization of the Evans-Searles fluctuation relation in classical non-equilibrium statistical mechanics is the identity

$$p^t_{-\phi} = \mathrm{e}^{-t\phi} p^t_\phi, \tag{1.3}$$

which should hold for all ϕ and $t > 0$. An equivalent formulation of (1.3) is that the functional

$$\mathrm{ES}_t(\alpha) = \log \omega\left(\mathrm{e}^{-\alpha t \Sigma^t}\right) = \log \sum_{\phi \in \mathrm{sp}(\Sigma^t)} \mathrm{e}^{-\alpha t \phi} p^t_\phi,$$

has the symmetry

$$\mathrm{ES}_t(\alpha) = \mathrm{ES}_t(1-\alpha), \tag{1.4}$$

that holds for all $\alpha \in \mathbb{R}$ and $t > 0$. The functional $\mathrm{ES}_t(\alpha)$ is the direct quantization of the finite time Evans-Searles functional in non-equilibrium classical statistical mechanics [JPR]. It is however easy to show that $\mathrm{ES}_t(1) > 0 = \mathrm{ES}_t(0)$ except at possibly countably many t's and so the relations (1.3) and (1.4) *cannot* hold for all $t > 0$ (see Exercise 3.3. in [JOPP]). This point is further discussed in [La].

The first class of quantum entropic functionals that satisfy the Evans-Searles fluctuation relation for all times was proposed independently by Kurchan [Ku] and Tasaki-Matsui [TM]. They involve the fundamental concept of Full Counting Statistics associated to the repeated measurement protocol of the energy/entropy flow [LL]. Consider the observable

$$\mathcal{S} = -\log \omega = \beta_l H_l + \beta_r H_r + Z,$$

where $Z = \log \mathrm{tr}(\mathrm{e}^{-\beta_l H_l - \beta_r H_r})$. Clearly, $\mathcal{S}_t = \tau^t(\mathcal{S}) = -\log \omega_{-t}$, and Properties (1) and (3) imply

$$\Sigma^t = \frac{1}{t}(\mathcal{S}_t - \mathcal{S}).$$

The probability that a measurement of $\mathcal{S}$ at time $t = 0$ (when the system is in the state ω) yields $s \in \mathrm{sp}(\mathcal{S})$ is $\omega(\mathbb{1}_s(\mathcal{S}))$. After the measurement, the system is in the reduced state

$$\frac{\omega \mathbb{1}_s(\mathcal{S})}{\omega(\mathbb{1}_s(\mathcal{S}))},$$

which evolves in time as

$$\mathrm{e}^{-\mathrm{i}tH} \frac{\omega \mathbb{1}_s(\mathcal{S})}{\omega(\mathbb{1}_s(\mathcal{S}))} \mathrm{e}^{\mathrm{i}tH}.$$

A second measurement of $\mathcal{S}$ at a later time $t > 0$ yields $s' \in \mathrm{sp}(\mathcal{S})$ with probability

$$\mathrm{tr}\left(\mathrm{e}^{-\mathrm{i}tH} \frac{\omega \mathbb{1}_s(\mathcal{S})}{\omega(\mathbb{1}_s(\mathcal{S}))} \mathrm{e}^{\mathrm{i}tH} \mathbb{1}_{s'}(\mathcal{S})\right),$$

and the joint probability of these two measurements is

$$\mathrm{tr}\left(\mathrm{e}^{-\mathrm{i}tH} \omega \mathbb{1}_s(\mathcal{S}) \mathrm{e}^{\mathrm{i}tH} \mathbb{1}_{s'}(\mathcal{S})\right).$$

The mean rate of entropy change between the two measurements is $\phi = (s' - s)/t$ and its probability distribution is

$$\mathbb{P}_t(\phi) = \sum_{s'-s=t\phi} \mathrm{tr}\left(\mathrm{e}^{-\mathrm{i}tH} \omega \mathbb{1}_s(\mathcal{S}) \mathrm{e}^{\mathrm{i}tH} \mathbb{1}_{s'}(\mathcal{S})\right).$$

The discrete probability measure $\mathbb{P}_t$ is the *Full Counting Statistics* (FCS) for the operationally defined entropy change over the time interval $[0, t]$ as specified by the above measurement protocol. Let

$$\mathrm{FCS}_t(\alpha) = \log \sum_{\phi} \mathrm{e}^{-\alpha t \phi} \mathbb{P}_t(\phi).$$

One easily verifies the identity

$$\mathrm{FCS}_t(\alpha) = \log \mathrm{tr}(\omega_t^{1-\alpha} \omega^{\alpha}), \tag{1.5}$$

and time-reversal invariance implies the fluctuation relation

$$\mathrm{FCS}_t(\alpha) = \mathrm{FCS}_t(1 - \alpha), \tag{1.6}$$

which holds for all α and t. The last relation is equivalent to

$$\mathbb{P}_t(-\phi) = \mathrm{e}^{-t\phi} \mathbb{P}_t(\phi). \tag{1.7}$$

The identities (1.6) and (1.7) provide a physically and mathematically appealing extension of the Evans-Searles fluctuation relation to the quantum domain.

Generalizations of the fluctuation relation (1.6) have been recently proposed in [JOPP]. Note that

$$\mathrm{FCS}_t(\alpha) = \log \mathrm{tr}\left(\mathrm{e}^{\frac{1-\alpha}{2}\mathcal{S}} \mathrm{e}^{\alpha \mathcal{S}_t} \mathrm{e}^{\frac{1-\alpha}{2}\mathcal{S}}\right).$$

For $p > 0$ and $\alpha \in \mathbb{R}$ we define the functionals $e_{p,t}(\alpha)$ by

$$e_{p,t}(\alpha) = \begin{cases} \log \mathrm{tr}\left(\left[\mathrm{e}^{\frac{1-\alpha}{p}\mathcal{S}} \mathrm{e}^{\frac{2\alpha}{p}\mathcal{S}_t} \mathrm{e}^{\frac{1-\alpha}{p}\mathcal{S}}\right]^{\frac{p}{2}}\right) & \text{if } 0 < p < \infty, \\ \log \mathrm{tr}\left(\mathrm{e}^{(1-\alpha)\mathcal{S} + \alpha \mathcal{S}_t}\right) & \text{if } p = \infty. \end{cases}$$

Their basic properties are summarized in:

Proposition 1.2 (1) $e_{p,t}(0) = e_{p,t}(1) = 0$.

(2) *The functions* $\mathbb{R} \ni \alpha \mapsto e_{p,t}(\alpha)$ *are real-analytic and convex.*

(3) $e_{p,t}(\alpha) = e_{p,-t}(\alpha)$.

(4) $e_{p,t}(\alpha) = e_{p,t}(1-\alpha)$.

(5) *The functions* $]0,\infty] \ni p \mapsto e_{p,t}(\alpha)$ *are continuous and decreasing.*

(6) $e'_{p,t}(0) = \mathrm{ES}'_t(0) = -e'_{p,t}(1) = -t\omega(\Sigma^t)$. *In particular, these derivatives do not depend on* p.

(7) $e_{2,t}(\alpha) = \mathrm{FCS}_t(\alpha)$ *and*

$$e''_{2,t}(0) = \mathrm{ES}''_t(0) = \int_0^t \int_0^t \omega\left((\sigma_s - \omega(\sigma_s))(\sigma_u - \omega(\sigma_u))\right) \mathrm{d}s\mathrm{d}u.$$

(8) $e_{\infty,t}(\alpha) = \max\left(S(\rho|\omega) - \alpha t \rho(\Sigma^t)\right)$, *where the maximum is taken over all states* ρ.

Remark. The variational characterization of $e_{\infty,t}(\alpha)$ in (8) is the quantization of the variational characterization of the finite time Evans-Searles functional in classical non-equilibrium statistical mechanics. Regarding the physical interpretation of $e_{p,t}(\alpha)$ for $p < \infty$, note that

$$\mathrm{tr}\left(\mathrm{e}^{\frac{1-\alpha}{p}\mathcal{S}}\mathrm{e}^{\frac{2\alpha}{p}\mathcal{S}_t}\mathrm{e}^{\frac{1-\alpha}{p}\mathcal{S}}\right)/\mathrm{tr}(\omega^{2/p}) = \int_{\mathbb{R}} \mathrm{e}^{-\alpha t\phi}\mathrm{d}\mathbb{P}_{p,t}(\phi),$$

where $\mathbb{P}_{p,t}$ is the FCS of the XY chain with scaled temperatures $2\beta_{l/r}/p$. Restoring the scaling as

$$\mathrm{tr}\left(\left[\mathrm{e}^{\frac{1-\alpha}{p}\mathcal{S}}\mathrm{e}^{\frac{2\alpha}{p}\mathcal{S}_t}\mathrm{e}^{\frac{1-\alpha}{p}\mathcal{S}}\right]^{p/2}\right),$$

distorts the connection with the FCS but links $e_{p,t}(\alpha)$ with quantized Ruelle transfer operators which provide yet another way of quantizing the classical Evans-Searles functional (see [JOPP, JOP, JP3]).

For the proof of Proposition 1.2 we refer the reader to [JOPP]. The definitions and structural relations described in this section have a simple general algebraic origin and are easily extended to any time-reversal invariant finite dimensional quantum system [JOPP]. A similar remark applies to the thermodynamic limit results described in the next section which hold for a much wider class of models than XY chains and in particular for quite general lattice quantum spin systems (for example, for the open spin systems discussed in [Ru2]). However, our study of the large time limit $t \to \infty$ critically depends on the specific properties of the XY model.

1.2 Thermodynamic limit

In this section we describe the thermodynamic limit $\Lambda = [-M, M] \nearrow \mathbb{Z}$ (for discussion of the thermodynamic limit of general spin systems we refer the reader to [BR1, BR2, I, Ru1, S]). We use the subscript M to denote the dependence of various objects on the size of Λ and write, for example, $\mathcal{H}_M$, $\mathcal{O}_M$, H_M, $e_{p,t,M}$, *etc.* The C^*-algebra $\mathcal{O}$ of observables of the extended XY chain is the uniform closure of the algebra of local observables

$$\mathcal{O}_{\mathrm{loc}} = \bigcup_M \mathcal{O}_M,$$

where we identify $\mathcal{O}_{M_1}$ with a subalgebra of $\mathcal{O}_{M_2}$ for $M_1 < M_2$. For any $A \in \mathcal{O}_{\mathrm{loc}}$ the limit

$$\tau^t(A) = \lim_{M\to\infty} \mathrm{e}^{\mathrm{i}tH_M} A \mathrm{e}^{-\mathrm{i}tH_M},$$

exists in norm and τ^t uniquely extends to a strongly continuous group of $*$-automorphisms of $\mathcal{O}$ that describes the dynamics of the extended XY chain. The physical states of the extended XY chain are

described by positive normalized linear functionals on $\mathcal{O}$. The expectation of an observable A in the state ρ is $\rho(A)$. In the Heisenberg/Schrödinger picture the observables/states evolve in time as

$$A_t = \tau^t(A), \qquad \rho_t = \rho \circ \tau^t.$$

$S(\rho|\nu)$ denotes Araki's relative entropy of the state ρ w.r.t. the state ν [Ar1, Ar2] with the notational convention of [BR2]. Let ω_M be the reference state (1.1) on $\mathcal{O}_M$. Then for all $A \in \mathcal{O}_{\rm loc}$ the limit

$$\omega(A) = \lim_{M\to\infty} \omega_M(A),$$

exists and ω uniquely extends to a state on $\mathcal{O}$ that describes the initial state of the extended XY chain. The C^* dynamical system $(\mathcal{O}, \tau^t, \omega)$ describes the extended XY chain. This quantum dynamical system is time-reversal invariant, *i.e.*, there exists an anti-linear involutive $*$-automorphism $\Theta : \mathcal{O} \to \mathcal{O}$ such that $\Theta \circ \tau^t = \tau^{-t} \circ \Theta$ for all t and $\omega(\Theta(A)) = \omega(A^*)$ for all $A \in \mathcal{O}$.

The observables $\Phi_{l/r}$ and σ are obviously in $\mathcal{O}_{\rm loc}$. Let

$$\Sigma^t = \frac{1}{t}\int_0^t \sigma_s \mathrm{d}s,$$
$$\mathrm{ES}_t(\alpha) = \log \omega(\mathrm{e}^{-\alpha t \Sigma^t}).$$

We then have

Proposition 1.3 (1)

$$\lim_{M\to\infty} \Sigma^t_M = \Sigma^t,$$

in norm and the convergence is uniform for t's in compact sets.

(2) $S(\omega_t|\omega) = -t\omega(\Sigma^t)$.

(3) $\tau^t(\Sigma^{-t}) = \Sigma^t$.

(4) $\Sigma^t = -\tau^t(\Theta(\Sigma^t))$. *In particular,* $\mathrm{sp}(\Sigma^t)$ *is symmetric with respect to the origin.*

(5)

$$\lim_{M\to\infty} \mathrm{ES}_{t,M}(\alpha) = \mathrm{ES}_t(\alpha),$$

and the convergence is uniform for t's and α's in compact sets.

Regarding the entropic functionals, we have:

Proposition 1.4 (1) *For all $\alpha \in \mathbb{R}$ and $p \in]0,\infty]$ the limits*

$$e_{p,t}(\alpha) = \lim_{M\to\infty} e_{p,t,M}(\alpha),$$

exist and are finite.

(2) $e_{p,t}(0) = e_{p,t}(1) = 0$.

(3) *The functions $\mathbb{R} \ni \alpha \mapsto e_{p,t}(\alpha)$ are real-analytic and convex.*

(4) $e_{p,t}(\alpha) = e_{p,-t}(\alpha)$.

(5) $e_{p,t}(\alpha) = e_{p,t}(1-\alpha)$.

(6) *The functions $]0,\infty] \ni p \mapsto e_{p,t}(\alpha)$ are continuous and decreasing.*

(7) $e'_{p,t}(0) = \mathrm{ES}'_t(0) = -e'_{p,t}(1) = -t\omega(\Sigma^t)$.

(8)
$$e''_{2,t}(0) = \mathrm{ES}''_t(0) = \int_0^t \int_0^t \omega\left((\sigma_s - \omega(\sigma_s))(\sigma_u - \omega(\sigma_u))\right) \mathrm{d}s\mathrm{d}u.$$

(9) *As $M \to \infty$, the sequence $\mathbb{P}_{t,M}$ converges weakly towards a Borel probability measure $\mathbb{P}_t$ on $\mathbb{R}$ and*

$$e_{2,t}(\alpha) = \log \int_{\mathbb{R}} \mathrm{e}^{-t\alpha\phi} \mathrm{d}\mathbb{P}_t(\phi).$$

All the moments of $\mathbb{P}_{t,M}$ converge to corresponding moments of $\mathbb{P}_t$. The measure $\mathbb{P}_t$ is the full counting statistics of the extended XY *chain.*

(10) $e_{\infty,t}(\alpha) = \sup\left(S(\rho|\omega) - \alpha t \rho(\Sigma^t)\right)$, *where the supremum is taken over all states ρ.*

The results of this section are easy to prove (see Section 2.3 and [La]). Also, using standard techniques [BR1, BR2, I, Ru1, S] these results are easily extended to other models in quantum statistical mechanics (general lattice quantum spin system, interacting fermionic models, Pauli-Fierz models, *etc.*). We emphasize, however, that non-trivial thermodynamical behavior only emerges in the large time limit $t \to \infty$ and that controlling the large time limit of entropic functionals in physically interesting models is typically a very hard analytic problem (see [Ro, JOPP] for existing results and discussion of this point). The advantage of models like the XY chain is that the large time limit is easy to control via trace class scattering theory and very detailed information about limiting entropic functionals is available. In the next section we review some basic results of spectral and scattering theory that we will need in this paper.

1.3 Operator theory preliminaries

Let A be a self-adjoint operator on a Hilbert space $\mathfrak{H}$. We denote by $\mathrm{sp}_{\mathrm{ac}}(A)$ the absolutely continuous spectrum of A and by $\mathfrak{H}_{\mathrm{ac}}(A)$ the corresponding spectral subspace. The projection on this subspace is denoted by $\mathbb{1}_{\mathrm{ac}}(A)$. For any $\psi_1, \psi_2 \in \mathfrak{H}$ the boundary values

$$\langle \psi_1, (A - E - \mathrm{i}0)^{-1}\psi_2\rangle = \lim_{\epsilon \downarrow 0} \langle \psi_1, (A - E - \mathrm{i}\epsilon)^{-1}\psi_2\rangle,$$

exist and are finite for Lebesgue a.e. $E \in \mathbb{R}$. In what follows, whenever we write $\langle \psi_1, (A - E - \mathrm{i}0)^{-1}\psi_2\rangle$, we will always assume that the limit exists and is finite. If $\psi_1 = \psi_2 = \psi$ then $\mathrm{Im}\,\langle \psi, (A - E - \mathrm{i}0)^{-1}\psi\rangle \geq 0$. If ν_ψ is the spectral measure of A for ψ, then its absolutely continuous component with respect to Lebesgue measure is

$$\mathrm{d}\nu_{\psi,\mathrm{ac}}(E) = \frac{1}{\pi}\mathrm{Im}\,\langle \psi, (A - E - \mathrm{i}0)^{-1}\psi\rangle \mathrm{d}E. \tag{1.8}$$

For the proofs and references regarding the above results we refer the reader to [J].

The basic tool in virtually any study of XY chains is the Jordan-Wigner transformation [JW] (see also [LSM, Ar3, AP, JOPP]). This transformation associates to our XY chain the Jacobi matrix

$$(hu)(x) = J_x u(x+1) + \lambda_x u(x) + J_{x-1} u(x-1),$$

(see Section 2.1). As an operator on the Hilbert space $\mathfrak{h} = \ell^2(\mathbb{Z})$, h is bounded and self-adjoint. Set

$$\mathfrak{h}_l = \ell^2(]-\infty, 0]), \qquad \mathfrak{h}_r = \ell^2([1, \infty[),$$

and denote $h_{l/r}$ the restrictions of h to $\mathfrak{h}_{l/r}$ with a Dirichlet boundary condition. Note that $h = h_0 + v$ where $h_0 = h_l \oplus h_r$ and

$$v = J_0\left(|\delta_l\rangle\langle\delta_r| + |\delta_r\rangle\langle\delta_l|\right), \tag{1.9}$$

$\delta_{l/r}$ being the Kronecker delta function at site $x = 0/1$. We denote by $\nu_{l/r}$ the spectral measure of $h_{l/r}$ for $\delta_{l/r}$. By (1.8),

$$\mathrm{d}\nu_{l/r,\mathrm{ac}}(E) = \frac{1}{\pi} F_{l/r}(E)\mathrm{d}E,$$

where

$$F_{l/r}(E) = \operatorname{Im} G_{l/r}(E), \qquad G_{l/r}(E) = \langle \delta_{l/r}, (h_{l/r} - E - \mathrm{i}0)^{-1} \delta_{l/r} \rangle.$$

By the spectral theorem, one can identify $\mathfrak{h}_{\mathrm{ac}}(h_0)$ with $L^2(\mathbb{R}, \mathrm{d}\nu_{l,\mathrm{ac}}) \oplus L^2(\mathbb{R}, \mathrm{d}\nu_{r,\mathrm{ac}})$ and $h_0 \restriction \mathfrak{h}_{\mathrm{ac}}(h_0)$ with the operator of multiplication by the variable $E \in \mathbb{R}$. The set $\Sigma_{l/r,\mathrm{ac}} = \{E \in \mathbb{R} \,|\, F_{l/r}(E) > 0\}$ is the essential support of the absolutely continuous spectrum of $h_{l/r}$. We set

$$\mathcal{E} = \Sigma_{l,\mathrm{ac}} \cap \Sigma_{r,\mathrm{ac}}.$$

Finally, we recall a few basic facts that follow from trace class scattering theory [RS, Y]. The wave operators

$$w_{\pm} = \mathrm{s} - \lim_{t \to \pm\infty} \mathrm{e}^{\mathrm{i}th} \mathrm{e}^{-\mathrm{i}th_0} \mathbb{1}_{\mathrm{ac}}(h_0),$$

exist. The scattering matrix

$$s = w_+^* w_- \tag{1.10}$$

is unitary on $\mathfrak{h}_{\mathrm{ac}}(h_0)$ and acts as an operator of multiplication by a unitary 2×2 matrix function (called the on-shell scattering matrix)

$$s(E) = \begin{bmatrix} s_{ll}(E) & s_{lr}(E) \\ s_{rl}(E) & s_{rr}(E) \end{bmatrix},$$

where, with $\bar{l}/\bar{r} = r/l$,

$$s_{ab}(E) = \delta_{ab} + 2\mathrm{i}J_0 \left(J_0 \langle \delta_{\bar{a}}, (h - E - \mathrm{i}0)^{-1} \delta_{\bar{b}} \rangle + \delta_{ab} - 1 \right) \sqrt{F_a(E) F_b(E)}$$

In our current setting these results can be easily proven directly (see [JKP, La]). Note that $s(E)$ is diagonal for Lebesgue a.e. $E \in \mathbb{R} \setminus \mathcal{E}$. It follows from the formula

$$\langle \delta_l, (h - E - \mathrm{i}0)^{-1} \delta_r \rangle = \langle \delta_r, (h - E - \mathrm{i}0)^{-1} \delta_l \rangle = -\frac{J_0 G_l(E) G_r(E)}{1 - J_0^2 G_l(E) G_r(E)}$$

that $s(E)$ is symmetric and not diagonal for Lebesgue a.e. $E \in \mathcal{E}$.

The Jacobi matrix h is called *reflectionless* iff $s(E)$ is off-diagonal for $E \in \mathcal{E}$. In other words, h is reflectionless if the transmission probability satisfies $|s_{lr}(E)|^2 = 1$ for $E \in \mathcal{E}$. For other equivalent definitions of reflectionless we refer the reader to Chapter 8 in [Te] (see also [La] for a discussion). For additional information and references about reflectionless Jacobi matrices we refer the reader to the recent work [Re].

1.4 The large time limit: NESS

The basic result concerning the existence of a non-equilibrium steady state (NESS) of the XY chain is:

Theorem 1.5 *Suppose that h has purely absolutely continuous spectrum. Then for all $A \in \mathcal{O}$ the limit*

$$\langle A \rangle_+ = \lim_{t \to \infty} \omega(\tau^t(A)),$$

exists. The state $\omega_+(\,\cdot\,) = \langle \cdot \rangle_+$ is called the NESS of the quantum dynamical system $(\mathcal{O}, \tau^t, \omega)$. The steady state heat fluxes are

$$\langle \Phi_l \rangle_+ = -\langle \Phi_r \rangle_+ = \frac{1}{4\pi} \int_{\mathcal{E}} E |s_{lr}(E)|^2 \frac{\sinh(\Delta\beta E/2)}{\cosh(\beta_r E/2) \cosh(\beta_l E/2)} \mathrm{d}E, \tag{1.11}$$

and the steady state entropy production is

$$\langle \sigma \rangle_+ = -\beta_l \langle \Phi_l \rangle_+ - \beta_r \langle \Phi_r \rangle_+ = \Delta\beta \langle \Phi_l \rangle_+,$$

where $\Delta\beta = \beta_r - \beta_l$.

With only notational changes the proof in [AP] extend to the proof of Theorem 1.5[3]. If in addition to its absolutely continuous spectrum h has non-empty pure point spectrum then one can show that the limit

$$\langle A\rangle_+ = \lim_{T\to\infty}\frac{1}{T}\int_0^T \omega(\tau^s(A))\mathrm{d}s,$$

exists for all $A \in \mathcal{O}$ and that the formula (1.11) remains valid (see [AJPP2]). In presence of singular continuous spectrum the existence of a NESS is not known.

If $|\mathcal{E}|$, the Lebesgue measure of $\mathcal{E}$, is zero, then obviously there is no energy transfer between the left and the right part of the chain and $\langle\sigma\rangle_+ = \langle\Phi_{l/r}\rangle_+ = 0$ for all $\beta_{l/r}$. If $|\mathcal{E}| > 0$, then $\langle\sigma\rangle_+ > 0$ iff $\beta_l \neq \beta_r$. Moreover, $\langle\Phi_l\rangle_+ > 0$ if $\beta_l < \beta_r$ and $\langle\Phi_l\rangle_+ < 0$ if $\beta_l > \beta_r$. The formula (1.11) is of course a special case of the celebrated Landauer-Büttiker formula that expresses currents in terms of the scattering data.[4]

Fluctuations of the mean entropy production rate Σ^t with respect to the NESS ω_+ are controlled by the functional

$$\mathrm{GC}_t(\alpha) = \log\omega_+(\mathrm{e}^{-\alpha t\Sigma^t}),$$

which is the direct quantization of the Gallavotti-Cohen functional in non-equilibrium classical statistical mechanics [JPR].

1.5 The large time limit: Entropic functionals

In this section we state our main results. It is convenient to introduce the following matrix notation. We let

$$k_0(E) = \begin{bmatrix} -\beta_l E & 0 \\ 0 & -\beta_r E \end{bmatrix},$$

set

$$K_\alpha(E) = \mathrm{e}^{k_0(E)/2}\mathrm{e}^{\alpha(s^*(E)k_0(E)s(E)-k_0(E))}\mathrm{e}^{k_0(E)/2}, \tag{1.12}$$

and note that $K_0(E) = \mathrm{e}^{k_0(E)}$. We further set

$$K_{\alpha,p}(E) = \left[\mathrm{e}^{k_0(E)(1-\alpha)/p}s(E)\mathrm{e}^{k_0(E)2\alpha/p}s^*(E)\mathrm{e}^{k_0(E)(1-\alpha)/p}\right]^{p/2}, \tag{1.13}$$

for $p \in]0,\infty[$, and

$$K_{\alpha,\infty}(E) = \lim_{p\to\infty}K_{\alpha,p}(E) = \mathrm{e}^{(1-\alpha)k_0(E)+\alpha s(E)k_0(E)s^*(E)}. \tag{1.14}$$

Note that $K_{0,p}(E) = K_0(E)$. Moreover, it is a simple matter to check that, for $E, \alpha \in \mathbb{R}$ and $p \in]0,\infty]$,

$$K_\alpha(E) = K_0(E) \Leftrightarrow K_{\alpha,p}(E) = K_0(E) \Leftrightarrow [s(E), k_0(E)] = 0 \Leftrightarrow \beta_l = \beta_r \text{ or } s(E) \text{ is diagonal.}$$

Recall that the last condition holds for Lebesgue a.e. $E \in \mathbb{R}\setminus\mathcal{E}$, but fails for Lebesgue a.e. $E \in \mathcal{E}$.

Theorem 1.6 *Suppose that h has purely absolutely continuous spectrum. Then the following holds:*

(1) *For $\alpha \in \mathbb{R}$ and $p \in]0,\infty]$,*

$$e_{p,+}(\alpha) = \lim_{t\to\infty}\frac{1}{t}e_{p,t}(\alpha) = \int_{\mathcal{E}}\log\left(\frac{\det(1+K_{\alpha,p}(E))}{\det(1+K_{0,p}(E))}\right)\frac{\mathrm{d}E}{2\pi},$$

$$\lim_{t\to\infty}\frac{1}{t}\mathrm{ES}_t(\alpha) = \lim_{t\to\infty}\frac{1}{t}\mathrm{GC}_t(\alpha) = e_+(\alpha) = \int_{\mathcal{E}}\log\left(\frac{\det(1+K_\alpha(E))}{\det(1+K_0(E))}\right)\frac{\mathrm{d}E}{2\pi}.$$

These functionals are identical to zero iff $|\mathcal{E}| = 0$ or $\beta_l = \beta_r$. In what follows we assume that $|\mathcal{E}| > 0$ and $\beta_l \neq \beta_r$.

[3] Alternatively, Theorem 1.5 can established by applying the results of [JKP] to the Jordan-Wigner transformed XY chain.

[4] We refer the reader to [AJPP2, N, JKP] for mathematically rigorous results regarding the Landauer-Büttiker formula and for references to the vast physical literature on the subject.

(2) *The functions* $\mathbb{R} \ni \alpha \mapsto e_{p,+}(\alpha)$ *are real-analytic and strictly convex. Moreover,* $e_{p,+}(0) = 0$, $e'_{p,+}(0) = -\langle\sigma\rangle_+$, *and*

$$e_{p,+}(\alpha) = e_{p,+}(1-\alpha).$$

(3) *The function* $\mathbb{R} \ni \alpha \mapsto e_+(\alpha)$ *is real-analytic and strictly convex. Moreover, it satisfies* $e_+(0) = 0$, $e'_+(0) = -\langle\sigma\rangle_+$, *and*

$$e''_+(0) = e''_{2,+}(0) = \lim_{T\to\infty} \frac{1}{T} \int_0^T \left\{ \frac{1}{2} \int_{-t}^{t} \langle (\sigma_s - \langle\sigma\rangle_+)(\sigma - \langle\sigma\rangle_+)\rangle_+ \, \mathrm{d}s \right\} \mathrm{d}t. \tag{1.15}$$

(4) $e_+(1) > 0$ *unless* h *is reflectionless. If* h *is reflectionless then*

$$e_+(\alpha) = \int_{\mathcal{E}} \log \left(\frac{\cosh((\beta_l(1-\alpha) + \beta_r\alpha)E/2)\cosh((\beta_r(1-\alpha) + \beta_l\alpha)E/2)}{\cosh(\beta_l E/2)\cosh(\beta_r E/2)} \right) \frac{\mathrm{d}E}{2\pi},$$

and $e_+(\alpha) = e_+(1-\alpha)$.

(5) *The function* $]0,\infty] \ni p \mapsto e_{p,+}(\alpha)$ *is continuous and decreasing. It is strictly decreasing for* $\alpha \notin \{0,1\}$ *unless* h *is reflectionless. If* h *is reflectionless, then* $e_{p,+}(\alpha)$ *does not depend on* p *and is equal to* $e_+(\alpha)$.

Remark 1. Typically, the correlation function $C(s) = \langle(\sigma_s - \langle\sigma\rangle_+)(\sigma - \langle\sigma\rangle_+)\rangle_+$ is not absolutely integrable and the Cesáro sum in (1.15) cannot be replaced by the integral of $C(s)$ over $\mathbb{R}$ without further assumptions.

Remark 2. As already noticed, time-reversal invariance implies that the on-shell scattering matrix is symmetric. It follows that one can replace $s(E)$ by $s^*(E)$ and $s^*(E)$ by $s(E)$ in (1.12)–(1.14) when inserted in the formulas of Part (1).

Remark 3. The vanishing of entropic functionals at $\alpha = 1$ is called Kawasaki's identity, see [CWWSE]. Thus, the Kawasaki identity holds for all e_p's and fails for e_+ unless h is reflectionless.

Theorem 1.6 has the following implications. To avoid discussing trivialities until the end of this section we assume that $|\mathcal{E}| > 0$ and $\beta_l \neq \beta_r$. Recall that

$$e_{2,t}(\alpha) = \mathrm{FCS}_t(\alpha) = \int_{\mathbb{R}} \mathrm{e}^{-\alpha t\phi} \mathrm{d}\mathbb{P}_t(\phi),$$

where $\mathbb{P}_t$ is the FCS measure of the extended XY chain. If $\mathbb{P}_{\mathrm{ES},t}$ and $\mathbb{P}_{\mathrm{GC},t}$ are respectively the spectral measures of Σ^t for ω and ω_+ we also have

$$\mathrm{ES}_t(\alpha) = \log \int_{\mathbb{R}} \mathrm{e}^{-\alpha t\phi} \mathrm{d}\mathbb{P}_{\mathrm{ES},t}(\phi), \qquad \mathrm{GC}_t(\alpha) = \log \int_{\mathbb{R}} \mathrm{e}^{-\alpha t\phi} \mathrm{d}\mathbb{P}_{\mathrm{GC},t}(\phi).$$

The respective large deviation rate functions are given by

$$I_{\mathrm{FCS}+}(\theta) = -\inf_{\alpha\in\mathbb{R}} (\alpha\theta + e_{2,+}(\alpha)),$$

$$I_+(\theta) = -\inf_{\alpha\in\mathbb{R}} (\alpha\theta + e_+(\alpha)).$$

The functions $I_+(\theta)$ and $I_{\mathrm{FCS}+}(\theta)$ are non-negative, real-analytic, strictly convex and vanish at the single point $\theta = \langle\sigma\rangle_+$. These two rate functions are different unless h is reflectionless. The symmetry $e_{2,+}(\alpha) = e_{2,+}(1-\alpha)$ implies

$$I_{\mathrm{FCS}+}(\theta) = I_{\mathrm{FCS}+}(-\theta) + \theta.$$

The rate function $I_+(\theta)$ satisfies this relation only if h is reflectionless. Theorem 1.6 implies:

Corollary 1.7 *Suppose that* h *has purely absolutely continuous spectrum.*

(1) *The Large Deviation Principle holds: for any open set $O \subset \mathbb{R}$,*

$$\lim_{t\to\infty} \frac{1}{t} \log \mathbb{P}_{\mathrm{ES},t}(O) = \lim_{t\to\infty} \frac{1}{t} \log \mathbb{P}_{\mathrm{GC},t}(O) = -\inf_{\theta\in O} I_+(\theta),$$

$$\lim_{t\to\infty} \frac{1}{t} \log \mathbb{P}_{\mathrm{FCS},t}(O) = -\inf_{\theta\in O} I_{\mathrm{FCS}+}(\theta).$$

(2) *The Central Limit Theorem holds: for any Borel set $B \subset \mathbb{R}$, let $B_t = \{\phi \,|\, \sqrt{t}(\phi - \langle\sigma\rangle_+) \in B\}$. Then*

$$\lim_{t\to\infty} \mathbb{P}_{\mathrm{ES},t}(B_t) = \lim_{t\to\infty} \mathbb{P}_{\mathrm{GC},t}(B_t) = \lim_{t\to\infty} \mathbb{P}_{\mathrm{FCS},t}(B_t) = \frac{1}{\sqrt{2\pi D_+}} \int_B \mathrm{e}^{-\phi^2/2D_+} \mathrm{d}\phi,$$

where the variance is $D_+ = e_+''(0)$.

1.6 Remarks

Due to non-commutativity it is natural that non-equilibrium quantum statistical mechanics has a richer mathematical structure than its classical counterpart. This is partly reflected in the emergence of novel entropic functionals. The direct quantizations of the Evans-Searles and Gallavotti-Cohen entropic functionals typically will not have the symmetries which, starting with the seminal works [CG, ES], have played a central role in recent developments in non-equilibrium classical statistical mechanics. The mathematical theory of entropic fluctuations in quantum statistical mechanics is an emerging research direction and our testing of the existing structural results on the specific example of the XY chain has lead to some surprising (at least to us) results.

If in a given model all the functionals $e_{p,+}(\alpha)$ are equal and coincide with $e_+(\alpha)$ we shall say that in this model the entropic identity holds. For the XY chain we have shown that the entropic identity holds iff the underlying Jacobi matrix is reflectionless. Note that the large time fluctuations of $\mathbb{P}_{\mathrm{ES},t}$ and $\mathbb{P}_{\mathrm{GC},t}$ are identical for all XY chains (*i.e.,* for any h) and this is not surprising—the same phenomenon generally holds in classical/quantum non-equilibrium statistical mechanics (this is the *principle of regular entropic fluctuations* of [JPR, JOP]). On the other hand, the full counting statistics of repeated measurement of entropy flux is obviously of quantum origin with no classical counterpart and in general one certainly does not expect that the large time fluctuations of $\mathbb{P}_{\mathrm{FCS},t}$ are equal to those of $\mathbb{P}_{\mathrm{ES/GC},t}$. In the same vein, one certainly expects that $e_{\infty,+}(\alpha) < e_{2,+}(\alpha)$ for $\alpha \neq 0, 1$, and more generally, that all functionals $e_{p,+}(\alpha)$ are different.

Needless to say, there are very few models for which the existence of $e_{p,+}(\alpha)$ and $e_+(\alpha)$ can be rigorously proven and the phenomenon of entropic identity, to the best of our knowledge, has not been previously discussed in mathematically rigorous literature on the subject. The XY chain is instructive since the functionals $e_{p,+}(\alpha)$ and $e_+(\alpha)$ can be computed in closed form and the entropic identity of the model can be identified with the reflectionless property of the underlying Jacobi matrix. The question whether such a physically and mathematically natural result can be extended beyond exactly solvable models like the XY chain or the Electronic Black Box Model[5] remains to be studied in the future.

1.7 Examples

Schrödinger case. If $J_x = J$ for all x then the Jacobi matrix h is the discrete Schrödinger operator

$$(hu)(x) = J(u(x+1) + u(x-1)) + \lambda_x u(x).$$

In the literature, the most commonly studied XY chains correspond to this case. The assumption that h has purely absolutely continuous spectrum plays a critical role in the formulation and the proof of Theorem 1.6. The striking fact is that the only known examples of discrete $d = 1$ Schrödinger operators with

[5] See [AJJP1, AJPP2, JKP, JOPP] for discussion of these models and references.

purely absolutely continuous spectrum are reflectionless. If the potential λ_x is constant or periodic then h has purely absolutely continuous spectrum (and is reflectionless). The only other known examples involve quasi-periodic potentials. For example, if $\lambda_x = \cos(2\pi\alpha x+\theta)$, then for $|J| > 1/2$ the operator h has purely absolutely continuous spectrum and is reflectionless (see [Av]). In this context it is an important open problem whether there exists a one-dimensional discrete Schrödinger operator h which is reflectionless and has purely absolutely continuous spectrum and therefore an XY chain with J_x constant for which the entropic identity fails .[6]

Jacobi case. If the J_x are allowed to vary, then it is easy to produce examples of h which are not reflectionless and have purely absolutely continuous spectrum (take $\lambda_x = 0$, $J_x = 1$ for $x > 0$ and $J_x = 1/2$ for $x \leq 0$). In fact, the vast majority of Jacobi matrices with purely absolutely continuous spectrum are not reflectionless. To illustrate this point, let $q : [-2, 2] \to \mathbb{C}$ be such that $|q(E)| \leq 1$ and

$$\int_{-2}^{2} \frac{\log |q(E)|}{\sqrt{2 - E^2}} \mathrm{d}E < \infty.$$

Then there exists a Jacobi matrix h such that the spectrum of h is purely absolutely continuous and equal to $[-2, 2]$, and such that $s_{lr}(E) = q(E)$ for Lebesgue a.e. $E \in [-2, 2]$ [VY]. The only reflectionless Jacobi matrix in this class is the Schrödinger operator with $J = \pm 1$ and $\lambda_x = 0$ (see [Te]). A similar result holds if the interval $[-2, 2]$ is replaced by a homogeneous set (say, a finite union of intervals or even a Cantor set of positive measure) [VY].

2 Proofs

2.1 The Jordan-Wigner transformation

Consider the XY chain confined to $\Lambda = [-M, M]$. In this subsection M is fixed and we drop the respective subscript. Let $\Lambda_l = [-M, 0]$, $\Lambda_r = [1, M]$. Set $\mathfrak{h} = \ell^2(\Lambda)$, $\mathfrak{h}_{l/r} = \ell^2(\Lambda_{l/r})$, and let h, $h_{l/r}$ be the restrictions of the Jacobi matrix to Λ, $\Lambda_{l/r}$. Whenever the meaning is clear we extend $h_{l/r}$ to $\mathfrak{h}$ by $h_l \oplus 0/0 \oplus h_r$. Let $h_0 = h_l + h_r$ and

$$h = h_0 + v,$$

where v is given by (1.9).

We shall assume that the reader is familiar with the formalism of the fermionic second quantization (see [BR2, BSZ, AJJP1] for general results and [JOPP] for a pedagogical introduction to this topic). $\mathcal{F}$ denotes the antisymmetric Fock space over $\mathfrak{h}$ and $a^*(f)/a(f)$ the creation/annihilation operator associated to $f \in \mathfrak{h}$. We write $a^*(\delta_x) = a_x^*$ *etc.* Set $S_{-M} = 1$ and

$$S_x = \prod_{y \in [-M, x[} (2a_y^* a_y - 1),$$

for $x \in]-M, M]$.

Proposition 2.1 *There exists a unitary $U_{\mathrm{JW}} : \mathcal{H} \to \mathcal{F}$, called the Jordan-Wigner transformation, such that*

$$U_{\mathrm{JW}} \sigma_x^{(1)} U_{\mathrm{JW}}^{-1} = S_x(a_x + a_x^*), \qquad U_{\mathrm{JW}} \sigma_x^{(2)} U_{\mathrm{JW}}^{-1} = \mathrm{i} S_x(a_x - a_x^*), \qquad U_{\mathrm{JW}} \sigma_x^{(3)} U_{\mathrm{JW}}^{-1} = 2a_x^* a_x - 1.$$

The Jordan-Wigner transformation goes back to [JW] and the proof of the above proposition is well-known (a pedagogical exposition can be found in [JOPP]). An immediate consequence are the identities

$$U_{\mathrm{JW}} H_{l/r} U_{\mathrm{JW}}^{-1} = \mathrm{d}\Gamma(h_{l/r}), \qquad U_{\mathrm{JW}} V U_{\mathrm{JW}}^{-1} = \mathrm{d}\Gamma(v), \qquad U_{\mathrm{JW}} H U_{\mathrm{JW}}^{-1} = \mathrm{d}\Gamma(h),$$

[6] It is believed that such an example exists. We are grateful to C. Remling and B. Simon for discussions on reflectionless Jacobi matrices.

$$U_{\mathrm{JW}}\Phi_l U_{\mathrm{JW}}^{-1} = -\mathrm{i}J_0J_{-1}\left(a_1^*a_{-1} - a_{-1}^*a_1\right) - \mathrm{i}J_0\lambda_0\left(a_1^*a_0 - a_0^*a_1\right),$$

$$U_{\mathrm{JW}}\Phi_r U_{\mathrm{JW}}^{-1} = -\mathrm{i}J_0J_1\left(a_0^*a_2 - a_2^*a_0\right) - \mathrm{i}J_0\lambda_1\left(a_0^*a_1 - a_1^*a_0\right).$$

It is also easy to see that the confined XY chain is time-reversal invariant with $\theta = U_{\mathrm{JW}}^{-1}\Gamma(j)U_{\mathrm{JW}}$, where $j\psi = \overline{\psi}$ is the standard complex conjugation on $\ell^2(\Lambda)$.

In what follows we will work only in the fermionic representation of the confined XY chain. With a slight abuse of notation we write $H_{l/r} = \mathrm{d}\Gamma(h_{l/r})$, $V = \mathrm{d}\Gamma(v)$, $H = H_l + H_r + V = \mathrm{d}\Gamma(h)$, *etc.*

2.2 Basic formulas

In this section $\Lambda = [-M, M]$ is again fixed and we drop the respective subscript. We shall make repeated use of the identity

$$\mathrm{tr}(\Gamma(A)) = \det(1 + A),$$

which holds for any linear map $A : \mathfrak{h} \to \mathfrak{h}$. Set

$$k = -\beta_l h_l - \beta_r h_r, \qquad k_t = \mathrm{e}^{\mathrm{i}th}k\mathrm{e}^{-\mathrm{i}th}.$$

The initial state of the system is described by the density matrix

$$\omega = \frac{\mathrm{e}^{-\beta_l H_l - \beta_r H_r}}{\mathrm{tr}(\mathrm{e}^{-\beta_l H_l - \beta_r H_r})} = \frac{\Gamma(\mathrm{e}^k)}{\det(1 + \mathrm{e}^k)}.$$

Since

$$\left(\omega^{(1-\alpha)/p}\omega_t^{2\alpha/p}\omega^{(1-\alpha)/p}\right)^{p/2} = \frac{\Gamma\left(\left(\mathrm{e}^{(1-\alpha)k/p}\mathrm{e}^{2\alpha k_{-t}/p}\mathrm{e}^{(1-\alpha)k/p}\right)^{p/2}\right)}{\det(1 + \mathrm{e}^k)},$$

we have

$$e_{p,t}(\alpha) = \log\frac{\det\left(1 + \left(\mathrm{e}^{(1-\alpha)k/p}\mathrm{e}^{2\alpha k_{-t}/p}\mathrm{e}^{(1-\alpha)k/p}\right)^{p/2}\right)}{\det(1 + \mathrm{e}^k)},$$

for $0 < p < \infty$. Similarly,

$$e_{\infty,t}(\alpha) = \log\frac{\det\left(1 + \mathrm{e}^{(1-\alpha)k + \alpha k_{-t}}\right)}{\det(1 + \mathrm{e}^k)},$$

and

$$\mathrm{ES}_t(\alpha) = \log\frac{\det\left(1 + \mathrm{e}^{k/2}\mathrm{e}^{\alpha(k_t - k)}\mathrm{e}^{k/2}\right)}{\det(1 + \mathrm{e}^k)}.$$

Clearly, the functions $\alpha \mapsto e_{p,t}(\alpha)$, $\alpha \mapsto \mathrm{ES}_t(\alpha)$ are real analytic. For $u \in \mathbb{R}$ and $0 < p < \infty$ set

$$\mathcal{K}_{p,t}(\alpha, u) = \frac{1}{2}\mathrm{e}^{-(1-\alpha)k_{tu}/p}\left(1 + \left(\mathrm{e}^{(1-\alpha)k_{tu}/p}\mathrm{e}^{2\alpha k_{-t(1-u)}/p}\mathrm{e}^{(1-\alpha)k_{tu}/p}\right)^{-p/2}\right)^{-1}\mathrm{e}^{(1-\alpha)k_{tu}/p} + \mathrm{h.c.}, \tag{2.16}$$

where h.c. stands for the hermitian conjugate of the first term. We also set

$$\mathcal{K}_{\infty,t}(\alpha, u) = \left(1 + \mathrm{e}^{-(1-\alpha)k_{tu} - \alpha k_{-t(1-u)}}\right)^{-1}, \tag{2.17}$$

and

$$\mathcal{K}_{\mathrm{ES},t}(\alpha, u) = -\left(1 + \mathrm{e}^{-\alpha(k_{t(1-u)} - k_{-tu})}\mathrm{e}^{-k_{-tu}}\right)^{-1}. \tag{2.18}$$

The following lemma will play the key role in the sequel.

Lemma 2.2 (1) *For* $p \in]0,\infty]$,

$$e_{p,t}(\alpha) = t\int_0^\alpha \mathrm{d}\gamma \int_0^1 \mathrm{d}u\, \mathrm{tr}\left(\mathcal{K}_{p,t}(\gamma,u)\mathrm{i}[k,h]\right). \tag{2.19}$$

(2)

$$\mathrm{ES}_t(\alpha) = t\int_0^\alpha \mathrm{d}\gamma \int_0^1 \mathrm{d}u\, \mathrm{tr}\left(\mathcal{K}_{\mathrm{ES},t}(\gamma,u)\mathrm{i}[k,h]\right). \tag{2.20}$$

To prove the lemma we need the following preliminary result (for the proof see Lemma 2.2. in [HP]):

Lemma 2.3 *Let F be a differentiable function of the real variable α taking values in Hermitian strictly positive matrices on $\mathfrak{h}$. Then for any $p \in]0,\infty[$,*

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\mathrm{tr}\log(1+F(\alpha)^p) = p\,\mathrm{tr}\left((1+F(\alpha)^{-p})^{-1}F(\alpha)^{-1}\frac{\mathrm{d}F(\alpha)}{\mathrm{d}\alpha}\right).$$

Proof of Lemma 2.2. We will derive (2.20). Relation (2.19) can be obtained in a similar way. Note that

$$\mathrm{ES}_t(\alpha) = \mathrm{tr}\log(1+F(\alpha)) - \log\det(1+\mathrm{e}^k),$$

where

$$F(\alpha) = \mathrm{e}^{k/2}\mathrm{e}^{\alpha(k_t-k)}\mathrm{e}^{k/2}.$$

Lemma 2.3 and simple algebra yield

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\mathrm{ES}_t(\alpha) = \mathrm{tr}\left(\left(1+\mathrm{e}^{-\alpha(k_t-k)}\mathrm{e}^{-k}\right)^{-1}(k_t-k)\right).$$

Since

$$k_t - k = \int_0^1 \frac{\mathrm{d}}{\mathrm{d}u}k_{tu}\,\mathrm{d}u = t\int_0^1 \mathrm{e}^{\mathrm{i}tuh}\mathrm{i}[h,k]\mathrm{e}^{-\mathrm{i}tuh}\mathrm{d}u,$$

we have

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\mathrm{ES}_t(\alpha) = -t\int_0^1 \mathrm{tr}\left(\mathrm{e}^{-\mathrm{i}tuh}\left(1+\mathrm{e}^{-\alpha(k_t-k)}\mathrm{e}^{-k}\right)^{-1}\mathrm{e}^{\mathrm{i}uth}\mathrm{i}[k,h]\right)\mathrm{d}u.$$

Using $\mathrm{ES}_t(0) = 0$, integration yields Relation (2.20). □

2.3 Thermodynamic limit

The proof of Proposition 1.3 is standard and we shall omit it (see [La]). To prove Proposition 1.4, we consider h_M as an operator on $\mathfrak{h} = \ell^2(\mathbb{Z})$ (h_M acts as zero on the orthogonal complement of $\mathfrak{h}_\Lambda$ in $\mathfrak{h}$). Clearly, $h_M \to h$ strongly and so the strong limits

$$\mathrm{s}-\lim_{M\to\infty}\mathcal{K}_{p,t,M}(\alpha,u) = \mathcal{K}_{p,t}(\alpha,u), \qquad \mathrm{s}-\lim_{M\to\infty}\mathcal{K}_{\mathrm{ES},t,M}(\alpha,u) = \mathcal{K}_{\mathrm{ES},t}(\alpha,u),$$

exist. Moreover, $\mathcal{K}_{p,t}(\alpha,u)$ and $\mathcal{K}_{\mathrm{ES},t}(\alpha,u)$ are given by the formulas (2.16), (2.17), (2.18) and hence are norm continuous functions of (p,t,α,u). Since $\mathrm{i}[k_M,h_M] = \mathrm{i}[k,h]$ does not depend on M and is a finite rank operator, an application of dominated convergence yields

$$e_{\#,t}(\alpha) = \lim_{M\to\infty} e_{\#,t,M}(\alpha) = t\int_0^\alpha \mathrm{d}\gamma \int_0^1 \mathrm{d}u\, \mathrm{tr}\left(\mathcal{K}_{\#,t}(\gamma,u)\mathrm{i}[k,h]\right), \tag{2.21}$$

where # stands for p or ES and $e_{\mathrm{ES},t}(\alpha) = \mathrm{ES}_t(\alpha)$. The functions $\mathrm{e}_{\#,t}(\alpha)$ are jointly continuous in (p,t,α) and real-analytic in α. The Trotter product formula yields

$$\lim_{p\to\infty} e_{p,t}(\alpha) = e_{\infty,t}(\alpha),$$

and Parts (1)–(6) of Proposition 1.4 follow. To prove (7) and (8), note that for given $\#$ in $\{p, \mathrm{ES}\}$ and t there is an $\epsilon > 0$ such that $e_{\#,t,M}(\alpha)$ extends analytically to the ball $|\alpha| < \epsilon$ in $\mathbb{C}$ and satisfies $\sup_{M>0,|\alpha|<\epsilon} |e_{\#,t,M}(\alpha)| < \infty$. This observation, Parts (6) and (7) of Proposition 1.2 and Vitali's convergence theorem (see, for example, Appendix B in [JOPP]) imply (7) and (8). To prove (9), we note that the function

$$\alpha \mapsto \int \mathrm{e}^{-\alpha t\phi}\, \mathrm{d}\mathbb{P}_{t,M}(\phi) = \mathrm{e}^{e_{2,t,M}(\alpha)} = \frac{\det\left(1 + \mathrm{e}^{(1-\alpha)k_M}\mathrm{e}^{-\mathrm{i}th_M}\mathrm{e}^{\alpha k_M}\mathrm{e}^{\mathrm{i}th_M}\right)}{\det(1+\mathrm{e}^{k_M})}$$
$$= \det\left(1 + (1+\mathrm{e}^{-k_M})^{-1}(\mathrm{e}^{-\alpha k_M}\mathrm{e}^{-\mathrm{i}th_M}\mathrm{e}^{\alpha k_M}\mathrm{e}^{\mathrm{i}th_M} - 1)\right),$$

is entire analytic. The bound $|\det(1+A)| \leq \mathrm{e}^{\|A\|_1}$, where $\|A\|_1$ denotes the trace norm of A, together with the formula

$$\mathrm{e}^{-\alpha k_M}\mathrm{e}^{-\mathrm{i}th_M}\mathrm{e}^{\alpha k_M}\mathrm{e}^{\mathrm{i}th_M} - 1 = \int_0^t \mathrm{e}^{-\alpha k_M}\mathrm{e}^{-\mathrm{i}sh_M}\mathrm{i}[\mathrm{e}^{\alpha k_M}, v]\mathrm{e}^{\mathrm{i}sh_M}\, \mathrm{d}s,$$

(where v is finite rank) imply that for any bounded set $B \subset \mathbb{C}$,

$$\sup_{\alpha\in B, M>0} \left|\mathrm{e}^{e_{2,t,M}(\alpha)}\right| < \infty.$$

By Vitali's convergence theorem the sequence of characteristic functions of the measures $\mathbb{P}_{t,M}$ converges locally uniformly towards an entire analytic function. The existence of the weak limit $\mathbb{P}_t$ follows (see e.g., Corollary 1 to Theorem 26.3 in [Bi]) and the convergence of the moments is a direct consequence of Vitali's theorem. Finally, (10) is a general fact which follows from Araki's perturbation theory of modular structure, see [JOP] for the proof and additional information. We shall not make use of (10) in this paper.

2.4 The Gallavotti-Cohen functional

Note that

$$\mathrm{GC}_t(\alpha) = \lim_{s\to\infty}\lim_{M\to\infty} \log \omega_{s,M}\left(\mathrm{e}^{-\alpha t\Sigma_M^t}\right).$$

Since

$$\omega_{s,M}\left(\mathrm{e}^{-\alpha t\Sigma_M^t}\right) = \frac{\det(1 + \mathrm{e}^{k_{-s,M}/2}\mathrm{e}^{\alpha(k_{t,M}-k_M)}\mathrm{e}^{k_{-s,M}/2})}{\det(1+\mathrm{e}^k)},$$

the arguments of the last two sections yield

$$\lim_{M\to\infty} \log \omega_{s,M}\left(\mathrm{e}^{-\alpha t\Sigma_M^t}\right) = -t\int_0^\alpha \mathrm{d}\gamma \int_0^1 \mathrm{d}u\, \mathrm{tr}\left(\left(1 + \mathrm{e}^{-\gamma(k_{t(1-u)}-k_{-tu})}\mathrm{e}^{-k_{-(s+tu)}}\right)^{-1}\mathrm{i}[k,h]\right).$$

The operator k is bounded, commutes with h_0 and $\mathrm{Ran}\,(k) \subset \mathfrak{h}_{\mathrm{ac}}(h_0)$. It follows that

$$\mathrm{s}-\lim_{s\to\pm\infty} k_s = \mathrm{s}-\lim_{s\to\pm\infty} \mathrm{e}^{\mathrm{i}sh}\mathrm{e}^{-\mathrm{i}sh_0}k\mathrm{e}^{\mathrm{i}sh_0}\mathrm{e}^{-\mathrm{i}sh} = w_\pm k w_\pm^* = k_\pm, \tag{2.22}$$

and the dominated convergence theorem yields

$$\mathrm{GC}_t(\alpha) = t\int_0^\alpha \mathrm{d}\gamma \int_0^1 \mathrm{d}u\, \mathrm{tr}\left(\mathcal{K}_{\mathrm{GC},t}(\gamma,u)\mathrm{i}[k,h]\right), \tag{2.23}$$

where

$$\mathcal{K}_{\mathrm{GC},t}(\alpha,u) = -\left(1 + \mathrm{e}^{-\alpha(k_{t(1-u)}-k_{-tu})}\mathrm{e}^{-k_-}\right)^{-1}. \tag{2.24}$$

2.5 Main results

Proof of Theorem 1.6. It follows from (2.18), (2.24) and (2.22) that for $u \in]0,1[$,

$$\mathcal{K}_+(\alpha) = \mathrm{s}-\lim_{t\to\infty} \mathcal{K}_{\mathrm{ES},t}(\alpha,u) = \mathrm{s}-\lim_{t\to\infty} \mathcal{K}_{\mathrm{GC},t}(\alpha,u) = -\left(1+\mathrm{e}^{-\alpha(k_+-k_-)}\mathrm{e}^{-k_-}\right)^{-1}.$$

Hence, by dominated convergence,

$$e_+(\alpha) = \lim_{t\to\infty}\frac{1}{t}\mathrm{ES}_t(\alpha) = \lim_{t\to\infty}\frac{1}{t}\mathrm{GC}_t(\alpha) = \int_0^\alpha \mathrm{tr}(\mathcal{K}_+(\gamma)\mathrm{i}[k,h])\mathrm{d}\gamma.$$

It follows from (1.10) and Theorem 4.1 in [AJPP2] that

$$\begin{aligned}\mathrm{tr}\left(\mathcal{K}_+(\gamma)\mathrm{i}[k,h]\right) &= -\mathrm{tr}\left(\left(1+\mathrm{e}^{-\gamma(s^*ks-k)}\mathrm{e}^{-k}\right)^{-1} w_-^*\mathrm{i}[k,h]w_-\right)\\ &= \int_{\mathcal{E}} \mathrm{tr}\left(\left(1+\mathrm{e}^{-\gamma(s^*(E)k_0(E)s(E)-k_0(E))}\mathrm{e}^{-k_0(E)}\right)^{-1}(s^*(E)k_0(E)s(E)-k_0(E))\right)\frac{\mathrm{d}E}{2\pi}.\end{aligned}$$

Theorem 4.1 in [AJPP2] is quite general and in the special case considered here the above formula can be also checked by an explicit computation [La]. By Lemma 2.3,

$$\begin{aligned}&\mathrm{tr}\left(\left(1+\mathrm{e}^{-\gamma(s^*(E)k_0(E)s(E)-k_0(E))}\mathrm{e}^{-k_0(E)}\right)^{-1}(s^*(E)k_0(E)s(E)-k_0(E))\right)\\ &\quad= \frac{\mathrm{d}}{\mathrm{d}\gamma}\mathrm{tr}\log\left(1+\mathrm{e}^{k_0(E)/2}\mathrm{e}^{\gamma(s^*(E)k_0(E)s(E)-k_0(E))}\mathrm{e}^{k_0(E)/2}\right),\end{aligned}$$

and so, Fubini's theorem yields

$$\begin{aligned}e_+(\alpha) &= \int_0^\alpha \mathrm{tr}(\mathcal{K}_+(\gamma)\mathrm{i}[k,h])\mathrm{d}\gamma\\ &= \int_{\mathcal{E}}\left[\int_0^\alpha \frac{\mathrm{d}}{\mathrm{d}\gamma}\mathrm{tr}\log\left(1+\mathrm{e}^{k_0(E)/2}\mathrm{e}^{\gamma(s^*(E)k_0(E)s(E)-k_0(E))}\mathrm{e}^{k_0(E)/2}\right)\mathrm{d}\gamma\right]\frac{\mathrm{d}E}{2\pi}\\ &= \int_{\mathcal{E}}\log\frac{\det\left(1+\mathrm{e}^{k_0(E)/2}\mathrm{e}^{\alpha(s^*(E)k_0(E)s(E)-k_0(E))}\mathrm{e}^{k_0(E)/2}\right)}{\det(1+\mathrm{e}^{k_0(E)})}\frac{\mathrm{d}E}{2\pi}.\end{aligned}$$

The formula for $e_{p,+}(\alpha)$ is derived in the same way, starting with

$$\begin{aligned}\mathcal{K}_{p,+}(\alpha) &= \mathrm{s}-\lim_{t\to\infty}\mathcal{K}_{p,t}(\alpha,u)\\ &= \frac{1}{2}\mathrm{e}^{-(1-\alpha)k_+/p}\left(1+\left(\mathrm{e}^{(1-\alpha)k_+/p}\mathrm{e}^{2\alpha k_-/p}\mathrm{e}^{(1-\alpha)k_+/p}\right)^{-p/2}\right)^{-1}\mathrm{e}^{(1-\alpha)k_+/p}+\mathrm{h.c.},\end{aligned}$$

for $p \in]0,\infty[$, and

$$\mathcal{K}_{\infty,+} = \mathrm{s}-\lim_{t\to\infty}\mathcal{K}_{\infty,t}(\alpha,u) = \left(1+\mathrm{e}^{-(1-\alpha)k_+-\alpha k_-}\right)^{-1}.$$

This, together with the remark preceding Theorem 1.6, prove Part (1).

The formulas derived in Part (1) clearly show that $e_{p,+}$ and e_+ are real analytic functions of α satisfying $e_{p,+}(0) = e_+(0) = 0$. As limits of convex functions they are also convex and hence have non-negative second derivatives. Thus, these derivatives either vanish identically or have an isolated set of real zeros. It follows that $e_{p,+}$ and e_+ are either linear or strictly convex . The symmetry $e_{p,+}(\alpha) = e_{p,+}(1-\alpha)$, a consequence of Proposition 1.2 (4), implies $e_{p,+}(1) = 0$ and hence $e_{p,+}$ is strictly convex if it

doesn't vanish identically. Regarding e_+, an explicit calculation (see [La]) shows that if it doesn't vanish identically, then $e''_+(\alpha) > 0$ for all $\alpha \in \mathbb{R}$.

It follows from (2.21), (2.23) that there exists $\epsilon > 0$ such that the functions $e_{2,t}(\alpha)/t$, $\mathrm{ES}_t(\alpha)/t$ and $\mathrm{GC}_t(\alpha)/t$ have analytic extensions to the complex disc $|\alpha| < \epsilon$ and are uniformly bounded on this disc for $t > 0$. Vitali's convergence theorem, Proposition 1.4 (7) and the fact that $\mathrm{GC}'_t(0) = -t\langle\sigma\rangle_+$ imply

$$e'_{p,+}(0) = \lim_{t\to\infty} \frac{1}{t} e'_{p,t}(0) = \lim_{t\to\infty} \frac{1}{t} \mathrm{ES}'_t(0) = e'_+(0) = \lim_{t\to\infty} \frac{1}{t} \mathrm{GC}'_t(0) = -\langle\sigma\rangle_+.$$

Moreover,

$$e''_+(0) = \lim_{t\to\infty} \frac{1}{t} \mathrm{ES}''_t(0) = \lim_{t\to\infty} \frac{1}{t} \mathrm{GC}''_t(0), \qquad e''_{2,+}(0) = \lim_{t\to\infty} \frac{1}{t} e''_{2,t}(0),$$

and since $e''_{2,t}(0) = \mathrm{ES}''_t(0)$ by Proposition 1.4 (8), we derive that $e''_{2,+}(0) = e''_+(0)$. Using that ω_+ is τ^t-invariant, one easily derives

$$\begin{aligned}\frac{1}{t}\mathrm{GC}''_t(0) &= \frac{1}{2}\int_{-t}^{t} \langle(\sigma_s - \langle\sigma\rangle_+)(\sigma - \langle\sigma\rangle_+)\rangle_+ \left(1 - \frac{|s|}{t}\right) \mathrm{d}s \\ &= \frac{1}{t}\int_0^t \left[\frac{1}{2}\int_{-s}^{s} \langle(\sigma_u - \langle\sigma\rangle_+)(\sigma - \langle\sigma\rangle_+)\rangle_+ \,\mathrm{d}u\right] \mathrm{d}s.\end{aligned}$$

This completes the proof of Parts (2) and (3).

To prove (4), we compare $e_+(1)$ and $e_{\infty,+}(1)$. Since $\det(1 + A) = 1 + \mathrm{tr}(A) + \det(A)$ for any 2×2 matrix A and $\det(K_\alpha(E)) = \det(K_{\alpha,\infty}(E))$, we have, taking into account Remark 2 after Theorem 1.6,

$$\det\left(1 + K_\alpha(E)\right) - \det\left(1 + K_{\alpha,\infty}(E)\right) = \mathrm{tr}\left(\mathrm{e}^{k_0(E)}\mathrm{e}^{\alpha\Delta(E)}\right) - \mathrm{tr}\left(\mathrm{e}^{k_0(E)+\alpha\Delta(E)}\right),$$

with $\Delta(E) = s^*(E)k_0(E)s(E) - k_0(E)$. By the Golden-Thompson inequality (see Corollary 2.3 and Exercise 2.8 in [JOPP]), the above difference of traces is strictly positive unless

$$[k_0(E), \Delta(E)] = [k_0(E), s^*(E)k_0(E)s(E)] = 0. \tag{2.25}$$

One easily verifies that for $E \neq 0$ this happens if and only if $s(E)$ is either diagonal or off-diagonal. It follows that

$$e_+(1) > e_{\infty,+}(1) = 0,$$

unless h is reflectionless.

To prove Part (5), note that

$$\det(1 + K_{\alpha,p}(E)) - \det(1 + K_{\alpha,q}(E)) = \mathrm{tr}(K_{\alpha,p}(E)) - \mathrm{tr}(K_{\alpha,q}(E)).$$

The Araki-Lieb-Thirring inequality ([Ar5, LT], see also Theorem 2.2. and Exercise 2.8 in [JOPP]) implies that the function

$$]0,\infty] \ni p \mapsto \mathrm{tr}(K_{\alpha,p}(E)) = \mathrm{tr}\left(\left[\mathrm{e}^{(1-\alpha)k_0(E)/p}\mathrm{e}^{2\alpha s(E)k_0(E)s^*(E)/p}\mathrm{e}^{(1-\alpha)k_0(E)/p}\right]^{p/2}\right),$$

is strictly decreasing unless (2.25) holds, in which case this function is constant. Part (5) follows. □

Proof of Corollary 1.7. Part (1) follows from Theorem 1.6 and the Gärtner-Ellis theorem (see Appendix A.2 in [JOPP] or any book on large deviation theory). The analyticity argument used in the proof of Part (3) of Theorem 1.6 and Bryc lemma (see [Br] and Appendix A.4. in [JOPP]) yield Part (2). □

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