Non-zero entropy density in the XY chain out of equilibrium

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Abstract

The von Neumann entropy density of a block of \( n \) spins is proved to be non-zero for large \( n \) in the non-equilibrium steady state of the XY chain constructed by coupling a finite cutout of the chain to the two infinite parts to its left and right which act as thermal reservoirs at different temperatures. Moreover, the non-equilibrium density is shown to be strictly greater than the density in thermal equilibrium.

Mathematics Subject Classifications (2000). 46L60, 47B35, 82C10, 82C23.

Key words. Non-equilibrium steady state, XY chain, von Neumann entropy, Toeplitz operators.

1 Introduction

In this letter, we study the large \( n \) asymptotic behavior of the von Neumann entropy

\[
S^{(n)} = -\text{tr} \left( \rho^{(n)} \log \rho^{(n)} \right)
\]

of the reduced density matrix \( \rho^{(n)} \) which is the restriction to a subblock of \( n \) neighboring spins of the non-equilibrium steady state \( \omega_\pm \) from [7] on the anisotropic XY chain in an external magnetic field whose formal Hamiltonian is specified by

\[
H = -\frac{1}{4} \sum_{x \in \mathbb{Z}} \left\{ (1 + \gamma) \sigma_1^{(x)} \sigma_1^{(x+1)} + (1 - \gamma) \sigma_2^{(x)} \sigma_2^{(x+1)} + 2\lambda \sigma_3^{(x)} \right\}.
\]

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Here, $\sigma_j^{(x)}$, $j = 1, 2, 3$, denote the Pauli matrices at site $x \in \mathbb{Z}$ (see (5) below), the parameter $\gamma \in (-1, 1)$ describes the anisotropy of the spin-spin coupling, and $\lambda \in \mathbb{R}$ stands for the external magnetic field. In [17] (and, for $\gamma = \lambda = 0$, already in [4] by a different method), the non-equilibrium steady state $\omega_+$ has been constructed in a setting which has become to serve as paradigm in non-equilibrium quantum statistical mechanics: a finite cutout of the chain, the "small" system, is coupled to the two infinite parts to its left and right acting as thermal reservoirs at different temperatures (see Section 4 for a more detailed description).

Since the discovery of their ideal thermal conductivity in such states, quasi-one-dimensional Heisenberg spin-$1/2$ systems, made from different materials, have been intensively investigated experimentally (see for example [23, 24]; the materials SrCuO$_2$ and Sr$_2$CuO$_3$ are considered to be among the best physical realizations of one-dimensional XYZ Heisenberg models) and theoretically (see for example [12, 27, 28]). Not only this highly unusual transport property motivates the theoretical study of correlations in such non-equilibrium models, but the XY chain also represents one of the simplest non-trivial testing grounds for the development of general ideas in rigorous non-equilibrium quantum statistical mechanics.

With this motivation in mind, we construct the reduced density matrix $\rho^{(n)}$ of $\omega_+$ as in [20, 26, 18] and prove that the von Neumann entropy (1) is asymptotically linear for large block size $n$. Moreover, we show that its non-equilibrium limit density is strictly greater than the limit density in thermal equilibrium.

For further applications of the von Neumann entropy, see Remark 7.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1}
\caption{The block of $n$ neighboring spins in (1).}
\end{figure}

\section{The non-equilibrium setting for the XY chain}

In this section, we give a brief informal description of our non-equilibrium setting for the XY spin model on $\mathbb{Z}$. We refer to [6, 7, 17] for a precise formulation within the framework of $C^*$ algebraic quantum statistical mechanics (see also Remark 1 below).

Consider the XY chain described by the Hamiltonian (2) and remove the bonds at any two sites. Doing so, the initial spin chain divides into a compound of three noninteracting subsystems, a left infinite chain $\mathbb{Z}_L$, a finite piece $\mathbb{Z}_\Box$, and a right infinite chain $\mathbb{Z}_R$. This configuration is what we call the free system whose Hamiltonian

\[ H_0 = H_L + H_\Box + H_R \]
is built on the parts $\mathbb{Z}_L$, $\mathbb{Z}_C$, and $\mathbb{Z}_R$ according to (2). The infinite pieces $\mathbb{Z}_L$ and $\mathbb{Z}_R$ will play the role of thermal reservoirs to which the finite system $\mathbb{Z}_C$ is coupled by means of the perturbation $H - H_0$. In contrast, the configuration described by $H$, i.e. the original XY chain on the whole of $\mathbb{Z}$, is considered to be the perturbed system. In order to construct a non-equilibrium steady state $\omega_+$ in the sense of [21], we choose the initial state $\omega_0$ to be composed of thermal equilibrium states on the spins on $\mathbb{Z}_L$, $\mathbb{Z}_C$, and $\mathbb{Z}_R$, with inverse temperatures $\beta_L$, $\beta_C$, and $\beta_R$, respectively.

It is well-known that the XY spin model can be described in terms of a model of free fermions with annihilation and creation operators $b_x, b^*_x, x \in \mathbb{Z}$, satisfying the canonical anticommutation relations (CAR),

$$\{b_x, b_y\} = 0, \quad \{b^*_x, b_y\} = \delta_{xy},$$

where $\{A, B\} = AB + BA$, the operator $b^*_x$ is the adjoint of $b_x$, and $\delta_{xy}$ is the Kronecker symbol. This description is achieved with the help of the Jordan-Wigner transformation [19],

$$b_x = T \pi(x) (\sigma_1^{(x)} - i \sigma_2^{(x)})/2,$$

where $\pi(x) = \sigma_3^{(x)} \ldots \sigma_3^{(x-1)}$ for $x > 1$, $\pi^{(1)} = 1$, and $\pi(x) = \sigma_3^{(x)} \ldots \sigma_3^{(0)}$ for $x < 1$ (the spin $\sigma_j^{(x)}$ at site $x, j = 1, 2, 3$, is given by $... \otimes 1_2 \otimes 1_2 \otimes \sigma_j \otimes 1_2 \otimes 1_2 \ldots$, and $1 = ... \otimes 1_2 \otimes 1_2 \otimes ...$; $1_m$ denotes the identity matrix on $\mathbb{C}^m$). Here, $\sigma_0, ..., \sigma_3$ is the Pauli basis of $\mathbb{C}^{2 \times 2}$,

$$\sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Moreover, $T$ has the properties $T^* = T$, $T^2 = 1$, and $T \sigma_j^{(x)} T = \theta_-(\sigma_j^{(x)})$, where, for $j = 1, 2$, $\theta_-$ is defined by $\theta_-(\sigma_j^{(x)}) = -\sigma_j^{(x)}$ if $x \leq 0$ and $\theta_-(\sigma_j^{(x)}) = \sigma_j^{(x)}$ if $x \geq 1$.

Remark 1 The element $T$ stems from the $C^*$ crossed product extension by $\mathbb{Z}_2$ of the $C^*$ algebra $\mathcal{S}$ of the spins on $\mathbb{Z}$ for the two-sided chain (see [15] [7]; for the one-sided chain, $T$ can be dropped): The $C^*$ algebra $\mathcal{O}$ generated by $\mathcal{S}$ and the element $T$ contains the CAR algebra $\mathcal{A}$ generated by the fermions $b_x, b^*_x$ on $\mathbb{Z}$ as a $C^*$ subalgebra. The extension to $\mathcal{O}$ of the $^*$-automorphisms $\theta$ on $\mathcal{S}$, defined as the rotation of the spins about the $z$-axis with angle $\pi$, $\theta(\sigma_j^{(x)}) = -\sigma_j^{(x)}$ for $j = 1, 2$ and $\theta(\sigma_3^{(x)}) = \sigma_3^{(x)}$, yields the decomposition of $\mathcal{S}$ and $\mathcal{A}$ into even and odd parts with respect to parity, $\theta(A) = \pm A$, $A \in \mathcal{O}$. The even parts coincide, $\mathcal{S}_+ = \mathcal{A}_+$, and form a $C^*$ algebra (for the odd parts one has $\mathcal{S}_- = TA_-$ and $\mathcal{S}_-$ is merely a Banach subspace). Since the extension to $\mathcal{O}$ of the $^*$-automorphism groups $\tau_0$ and $\tau$ generated by $H_0$ and $H$ leave the even parts invariant, and since the unique KMS states on $\mathcal{S}$ and $\mathcal{A}$ coincide on $\mathcal{S}_+ = \mathcal{A}_+$, the even parts only are of importance in the construction of the non-equilibrium steady state $\omega_+$ in [7].

Using Kato-Birman scattering theory for the construction of the wave operators on the 1-particle Hilbert space of the Jordan-Wigner fermions [4], the non-equilibrium steady state $\omega_+$ with
respect to the initial state $\omega_0$ and the time evolution $\tau^t$ generated by $H$ has been constructed in \cite{7} as the limit

$$\omega_+(b_x) = \lim_{t \to +\infty} \omega_0(\tau^t(b_x)) = \omega_0 \circ \gamma_+(b_x),$$

where $\gamma_+$ denotes the algebraic analogon of the wave operator on Hilbert space, the so-called Møller morphism on $\mathcal{A}$. Moreover, it has been shown in \cite{7} that $\omega_+$ is a quasi-free state characterized by its 2-point operator $S$ (see Appendix A).

$$\omega_+(B^*(f)B(g)) = (f, Sg),$$

(6)

where, with $h = l^2(\mathbb{Z})$, $f, g \in h \oplus h \simeq h \otimes \mathbb{C}^2$ (and $(f, g)$ denotes the scalar product in $h \oplus h$). Here, $B$ is the linear mapping

$$f = (f_+, f_-) \mapsto B(f) = \sum_{x \in \mathbb{Z}} (f_+(x) b_x^* + f_-(x) b_x)$$

(7)

introduced in \cite{2} in the framework of self-dual CAR algebras (see Appendix A). It has the properties

$$\{B^*(f), B(g)\} = (f, g), \quad B^*(f) = B(Jf),$$

(8)

where $J$ is the antiunitary involution defined by $(f_+, f_-) \mapsto (\bar{f}_-, \bar{f}_+)$ (the bar denotes complex conjugation). Finally, $S$ has been explicitly computed in \cite{7}. In the Fourier picture, $l^2(\mathbb{Z}) \otimes \mathbb{C}^2 \simeq L^2(\mathbb{T}) \otimes \mathbb{C}^2$ (with $\mathbb{T} = \{z \in \mathbb{C} \mid |z| = 1\}$), $S$ reads

$$s(\xi) = (1 + e^{\beta h(\xi) + \delta k(\xi)})^{-1},$$

with the temperature parameters $\beta$ and $\delta$ given by

$$\beta = \frac{1}{2} (\beta_R + \beta_L), \quad \delta = \frac{1}{2} (\beta_R - \beta_L).$$

(9)

The 1-particle operators $h$ and $k$ have the form

$$h(\xi) = (\cos \xi - \lambda) \otimes \sigma_3 - \gamma \sin \xi \otimes \sigma_2, \quad k(\xi) = \text{sign}(\kappa(\xi)) \mu(\xi) \otimes \sigma_0,$$

where the functions $\kappa(\xi)$ and $\mu(\xi)$ are defined by

$$\kappa(\xi) = 2\lambda \sin \xi - (1 - \gamma^2) \sin 2\xi, \quad \mu(\xi) = \left((\cos \xi - \lambda)^2 + \gamma^2 \sin^2 \xi\right)^{1/2}.$$

Expanding $s(\xi)$ with respect to $\sigma_0, ..., \sigma_3$ from \cite{5}, we find the 0-th component of $s(\xi) = s_0(\xi) \otimes \sigma_0 + \sum_{k=1}^3 s_k(\xi) \otimes \sigma_k$ to look like

$$s_0(\xi) = \frac{1}{2} - \frac{1}{2} \varphi_{\delta, \beta}(\xi) \text{sign}(\kappa(\xi)).$$

(10)
whereas $s_k(\xi), \, k = 1, 2, 3,$ has the form

$$s_k(\xi) = \frac{1}{2} \varphi_{\beta,\delta}(\xi) r_k(\xi), \quad r(\xi) = \frac{1}{\mu(\xi)} \left(0, -\gamma \sin \xi, \cos \xi - \lambda\right). \quad (11)$$

Here, we used the definition

$$\varphi_{\alpha,\alpha'}(\xi) = \frac{\text{sh}(\alpha \mu(\xi))}{\text{ch}(\alpha \mu(\xi)) + \text{ch}(\alpha' \mu(\xi))}, \quad \alpha, \alpha' \in \mathbb{R}. \quad (12)$$

In order to study the von Neumann entropy (11), we restrict $\omega_+$ to spins on the finite configuration subset $\Lambda_n = \{1, \ldots, n\}, \, n \in \mathbb{N},$ of the entire spin chain on $\mathbb{Z}$. Due to the Jordan-Wigner transformation (4), this is equivalent to restricting $\omega_+$ to the fermions $b_i, b_i^*$ at the same sites $\Lambda_n$ (on the even part of the algebra, see Remark 1). Let $\mathfrak{h}_n = l^2(\Lambda_n) \simeq \mathbb{C}^n$ be the state space over $\Lambda_n$ (where here and in the following, $\mathfrak{h}_n$ is considered as a subspace of $\mathfrak{h}$ by the trivial injection). Since the Fock space $\mathfrak{F}(\mathfrak{h}_n)$ over the $n$-dimensional state space $\mathfrak{h}_n$ is $2^n$-dimensional, the CAR algebra $\mathcal{A}_n \equiv \mathcal{A}(\mathfrak{h}_n)$ over $\mathfrak{h}_n$ is $2^{2n}$-dimensional, $\mathcal{A}_n \simeq \mathcal{L}(\mathfrak{F}(\mathfrak{h}_n)) \simeq \mathbb{C}^{2^n \times 2^n}$ (see for example [6] or [10, p.15]); we denote by $\mathcal{L}(\mathcal{H})$ the bounded operators on the Hilbert space $\mathcal{H})$. Therefore, the restriction of $\omega_+$ to the spins on $\Lambda_n$ is described by a density matrix $\rho^{(n)} \in \mathcal{L}(\mathfrak{F}(\mathfrak{h}_n))$ (see for example [10, p.267]),

$$\omega_+(A) = \text{tr}(\rho^{(n)} A), \quad A \in \mathcal{A}_n. \quad (13)$$

### 3  The asymptotics of the von Neumann entropy

In Theorem 3 our main result, we prove that the large $n$ asymptotics of the von Neumann entropy $S^{(n)}$ from (11) in the non-equilibrium steady state $\omega_+$ is, to leading order in $n$, proportional to the volume of the spin block, and we derive an explicit expression for the non-vanishing proportionality constant. To do so, we express $S^{(n)}$ with the help of the eigenvalues of a Toeplitz matrix which we will construct next. Let us first define the Majorana correlation matrix $\Omega_n \in \mathbb{C}^{2n \times 2n}$ by

$$(\Omega_n)_{kl} = \omega_+(B(w^{(k)})B(w^{(l)})), \quad k, l = 1, \ldots, 2n, \quad (14)$$

where $B(f)$ is given in (7), and $w^{(k)} = (w_+^{(k)}, w_-^{(k)}) \in \mathfrak{h}_n \oplus \mathfrak{h}_n$ is specified, for $j = 1, \ldots, n$, by

$$w_+^{(k)}(j) = (\oplus_1^n \tau)_{k, 2j} = \delta_{k, 2j-1} - i\delta_{k, 2j},$$

$$w_-^{(k)}(j) = (\oplus_1^n \tau)_{k, 2j-1} = \delta_{k, 2j-1} + i\delta_{k, 2j}.$$ 

Moreover, the matrix $\tau \in \mathbb{C}^{2 \times 2}$ reads

$$\tau = \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix}. \quad (15)$$
**Remark 2** By virtue of (5), the $2n$ operators $d_k = B(w^{(k)})$ are Majorana operators, i.e.

\[ d_k^* = d_k, \quad \{d_k, d_l\} = 2\delta_{kl}. \]

In the following, we define a suitable block Toeplitz matrix $T_n[a]$. The reader not familiar with Toeplitz theory may consult Appendix [B] where the notation and the relevant facts are given. Moreover, in the proofs below, we will refer to Appendix [A] for an elementary construction of a suitable fermionic basis.

**Lemma 1** The imaginary part of the Majorana correlation matrix $\Omega_n$ from (14) is a skew-symmetric $2 \times 2$ block Toeplitz matrix $T_n[a]$ with symbol $a \in L^\infty_{2 \times 2}$,

\[ \Omega_n = 1_{2n} + iT_n[a], \quad a(\xi) = \frac{2}{i} \left[ \begin{array}{cc} s_0(\xi) - \frac{1}{2} & s_2(\xi) - is_3(\xi) \\ s_2(\xi) + is_3(\xi) & s_0(\xi) - \frac{1}{2} \end{array} \right], \]

where the functions $s_0, ..., s_3$ are defined in (10) and (11).

**Proof** With the Fourier transform $F : l^2(\mathbb{Z}) \rightarrow L^2(\mathbb{T})$ in the form $Ff(\xi) = \sum_{x \in \mathbb{Z}} f(x) e^{ix\xi}$, we have $Fw_x^{(2k-1)} = e_k, Fw_x^{(2k)} = T e_k$, and $S = F^* \otimes 1_{2} s F \otimes 1_{2}$, where we define $e_k(\xi) = e^{ix\xi}$. Hence, with $\eta_x = (1, \pm 1) \in \mathbb{C}^2$, we compute

\[ (\Omega_n)_{2j-1,2k-1} = \omega_+ (B(w^{(2j-1)})) (B(w^{(2k-1)})) = (w_x^{(2j-1)}, w_x^{(2k-1)}) = \sum_{\alpha=0}^{3} (e_j \otimes \eta_+, s_\alpha e_k \otimes \sigma_\alpha \eta_+) = 2 (e_j, (s_0 + s_1) e_k) = \delta_{jk} - \int_0^{2\pi} \frac{d\xi}{2\pi} \varphi_{\delta, \beta}(\xi) \text{sign}(\xi) e^{-i(k-j)\xi}. \]

In the last equality only, we used the explicit expressions of $s_0$ and $s_1$ from (10) and (11) (the function $\varphi_{\delta, \beta}$ is defined in (12)). In the same way, we obtain

\[ (\Omega_n)_{2j,2k} = 2 (e_j, (s_2 - is_3) e_k) = - \int_0^{2\pi} \frac{d\xi}{2\pi} \frac{q(\xi)}{\mu(\xi)} \varphi_{\delta, \beta}(\xi) e^{-i(k-j)\xi}, \]

\[ (\Omega_n)_{2j,2k-1} = 2 (e_j, (s_2 + is_3) e_k), \]

\[ (\Omega_n)_{2j,2k} = 2 (e_j, (s_0 - s_1) e_k), \]

where we define

\[ q(\xi) = -\gamma \sin \xi - i (\cos \xi - \lambda). \]
Hence, the matrix $T_n[a] = (\Omega_n - 1_{2n})/i$ is a block Toeplitz matrix with $2 \times 2$ blocks, i.e. $(\Omega_n)_{k+2i,l+2i} = (\Omega_n)_{kl}$. Its symbol $a \in L^\infty_{2 \times 2}$ can be read off from (18) and (19),

$$
T_n[a] \in \mathbb{R}^{2n \times 2n}, \quad T_n[a]^t = -T_n[a].
$$

This is the claim of Lemma 1.

In the next lemma, we choose a special set of fermions in $\mathcal{A}_n$ stemming from the block diagonalization of $T_n[a]$ by means of real orthogonal transformation $V \in O(2n) = \{ V \in \mathbb{R}^{2n \times 2n} | V V^t = 1_{2n} \}$.

**Lemma 2** There exists a set of fermions $c_i \equiv c_i(n) \in \mathcal{A}_n$, and numbers $\lambda_i(n) \in \mathbb{R}, i = 1, ..., n$, such that the reduced density matrix $\rho(n)$ from (13) has the form

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

**Proof** Let $c_i, i = 1, ..., n$, be arbitrary fermions in $\mathcal{A}_n$ and define operators $e^{(i)}_{\alpha \beta}, i = 1, ..., n, \alpha, \beta = 1, 2$, by

$$
e^{(i)}_{11} = c_i^* c_i, \quad e^{(i)}_{12} = c_i^*, \quad e^{(i)}_{21} = c_i, \quad e^{(i)}_{22} = c_i c_i^*.
$$

Since Lemma 6 in Appendix A states that the $2^2n$ operators $\prod_{i=1}^n e^{(i)}_{\alpha_i \beta_i}, \alpha_1, \beta_1, ..., \alpha_n, \beta_n = 1, 2$, constitute an orthonormal basis in $\mathcal{L}(\mathfrak{H}_n)$, we can write $\rho(n) \in \mathcal{L}(\mathfrak{H}_n)$ as

$$
\rho(n) = \sum_{\alpha_1, \beta_1, ..., \alpha_n, \beta_n=1, 2} \omega_+ \left( \prod_{i=1}^n e^{(i)}_{\alpha_i \beta_i} \right)^* \prod_{j=1}^n e^{(j)}_{\alpha_j \beta_j}.
$$

The goal of the following is to make a special choice for the fermions $c_i$ such that the density matrix $\rho(n)$ from (22) can be written in the form (20). For this purpose, let $V \in O(2n)$ be any real orthogonal $2n \times 2n$ matrix and choose

$$
c_i = B(v^{(i)}), \quad i = 1, ..., n,
$$

where $v^{(i)}$ is an arbitrary $2n$-vector.

Non-zero entropy density in the XY chain out of equilibrium
where $v^{(i)} = (v_+^{(i)}, v_-^{(i)}) \in h_n \oplus h_n$ is specified, for $j = 1, ..., n$, by

$$
v_+^{(i)}(j) = \left((\oplus V_1^n) V (\oplus V_1^n)\right)_{2i-1,2j};
$$

$$
v_-^{(i)}(j) = \left((\oplus V_1^n) V (\oplus V_1^n)\right)_{2i-1,2j-1},
$$

and $\tau$ is defined in (15) (note that for the choice $V = 1_{2n}$ we recover the Jordan-Wigner fermions $b_i$ from (4)). Using

$$
c_i = \sum_{k=1}^{2n} \left((\oplus V_1^n) V\right)_{2i-1,k} d_k,
$$

the Majorana relations (16), the fact that $V \in O(2n)$, and the properties of $\tau$, we see that the operators $c_i$ are fermionic,

$$
\{c_i, c_j\} = 2 \left((\oplus V_1^n) V V^* (\oplus V_1^n)\right)_{2j-1,2i-1} = (\oplus V_1^n \sigma_1)_{2j-1,2i-1} = 0,
$$

$$
\{c_i^*, c_j\} = 2 \left((\oplus V_1^n) V V^* (\oplus V_1^n)\right)_{2j-1,2i-1} = (\oplus V_1^n \sigma_0)_{2j-1,2i-1} = \delta_{ij}
$$

(note that, in general, the CAR are not satisfied if we choose $V$ to be complex unitary or complex orthogonal). Next, let us make a special choice for $V$. Since we know from Lemma 1 that $T_n[a]$ is real and skew-symmetric, there exists a matrix $Q \in O(2n)$ which transforms $T_n[a]$ into its real canonical form (see for example [16, p.107]),

$$
Q T_n[a] Q^T = \oplus_{j=1}^n (\lambda_j^{(n)} i \sigma_2) = \text{diag} (\lambda_1^{(n)}, ..., \lambda_n^{(n)}) \otimes i \sigma_2,
$$

where $\pm i \lambda_j^{(n)} \in \mathbb{R}$, are the eigenvalues of $T_n[a]$. Hence, setting $V = Q$ in (24), and using (25) and (26), we find, similarly as for the CAR above,

$$
\omega_+ (c_i c_j) = \frac{1}{2} \left((\oplus V_1^n) (\sigma_1 - \lambda_k i \sigma_2)\right)_{2i-1,2j-1} = 0,
$$

$$
\omega_+ (c_i^* c_j) = \frac{1}{2} \left((\oplus V_1^n) (\sigma_0 + \lambda_k \sigma_3)\right)_{2i-1,2j-1} = \delta_{ij} \frac{1 + \lambda_i^{(n)}}{2}.
$$

Now, let us write $\rho^{(n)}$ from (22) with the help of this special choice of fermions. Since (27) and (28) hold, we have, from Lemma 5 in Appendix A that

$$
\omega_+ \left( \prod_{i=1}^n c_{\alpha_i \beta_i}^{(i)} \right)^* = \prod_{i=1}^n \delta_{\alpha_i \beta_i} \omega_+ (c_{\alpha_i \alpha_i}^{(i)}).
$$

Therefore, plugging (29) into (22) and using (24), (27), and (28), we find that the reduced density matrix $\rho^{(n)}$ takes the form

$$
\rho^{(n)} = \prod_{i=1}^n \left( \omega_+ (c_i^* c_i) c_i^* c_i + \omega_+ (c_i^* c_i^*) c_i c_i^* \right) = \prod_{i=1}^n \left( \frac{1 + \lambda_i^{(n)}}{2} c_i^* c_i + \frac{1 - \lambda_i^{(n)}}{2} c_i c_i^* \right),
$$
which is (20). □

Next, we formulate our main assertion about the asymptotic behavior of the von Neumann entropy $S^{(n)} = - \text{tr} (\rho^{(n)} \log \rho^{(n)})$ in the non-equilibrium steady state $\omega_+$ characterized by (6) with its reduced density matrix $\rho^{(n)}$ from (13). The temperatures $\beta$ and $\delta$ are defined in (9).

**Theorem 3** Let $\omega_+$ be the non-equilibrium steady state of the XY chain with reduced density matrix $\rho^{(n)}$. Then, for the temperatures $0 \leq \delta < \beta < \infty$, the anisotropy $\gamma \in (-1, 1)$, and the magnetic field $\lambda \in \mathbb{R}$, the von Neumann entropy $S^{(n)}$ is asymptotically linear for $n \to \infty$,

$$S^{(n)} = C n + o(n) \quad \text{with} \quad C \equiv C_{\beta, \delta, \gamma, \lambda} > 0,$$

and $C$ is given in (34).

**Remark 3** The existence of the limit $\lim_{n \to \infty} S^{(n)}/n$ for translation invariant states of spin systems follows from the strong subadditivity property of the mapping $[1, \ldots, n] \to S^{(n)}$, see for example [10, p.287]. In (34), we derive an explicit expression for this limit and show that it is strictly positive.

**Proof** The properties (47) and (48) from Appendix B imply that the spectral radius of the Toeplitz matrix $T_n[a]$ is bounded by

$$\|T_n[a]\| \leq \text{ess sup}_{\xi \in [0, 2\pi]} \|a(\xi)\|_{\mathcal{L}(\mathbb{C}^2)} = \text{ess sup}_{\xi \in [0, 2\pi]} (\varphi_{\beta, \delta}(\xi) + \varphi_{\delta, \beta}(\xi)) = \varrho,$$

where, due to the finiteness of the temperatures, $\varrho$ is strictly smaller than 1,

$$\varrho = \text{th}(\beta R (1 + |\lambda|)/2) < 1. \quad (31)$$

The form (20) immediately yields the spectral representation of $\rho^{(n)}$ with the $2^n$ eigenvalues

$$\lambda_{\epsilon_1, \ldots, \epsilon_n} = \prod_{i=1}^{n} \frac{1 + (-1)^{\epsilon_i} \lambda^{(n)}_i}{2}, \quad \epsilon_1, \ldots, \epsilon_n \in \{0, 1\}. \quad (32)$$

Due to (30) and (31), we have $0 < \lambda_{\epsilon_1, \ldots, \epsilon_n} < 1$. Using (32), $\text{tr} \rho^{(n)} = 1$, and the entropy function $h : (-1, 1) \to \mathbb{R}^+$ (for which $h(x) = \eta((1 + x)/2)$ with $\eta(x) = -x \log x - (1 - x) \log(1 - x)$ the Shannon entropy; see Figure 2 for $h(x)$),

$$h(x) = -\frac{1 + x}{2} \log \left(\frac{1 + x}{2}\right) - \frac{1 - x}{2} \log \left(\frac{1 - x}{2}\right), \quad (33)$$

$$\varrho = \text{th}(\beta R (1 + |\lambda|)/2) < 1. \quad (31)$$
the von Neumann entropy $S^{(n)} = -\text{tr}(\rho^{(n)} \log \rho^{(n)})$ can be written in the form

$$S^{(n)} = - \sum_{\epsilon_1, \ldots, \epsilon_n \in \{0, 1\}} \lambda_{\epsilon_1, \ldots, \epsilon_n} \log \lambda_{\epsilon_1, \ldots, \epsilon_n} = \sum_{i=1}^{n} h(\lambda_i^{(n)}).$$

To determine the asymptotic behavior of $S^{(n)}$, we want to make use of Szegö’s first limit theorem for the case of block Toeplitz matrices (see [9, p.202] and (49) in Appendix B). To do so, we note that the symbol $ia \in L^\infty_{2 \times 2}$ is self-adjoint (with $a$ from (17)) and that $\pm \lambda_j \in (-\varrho, \varrho)$ are the eigenvalues of the self-adjoint Toeplitz matrix $iT_n[a] = T_n[ia]$ (see (26)). Moreover, with the definition $\tilde{h}(x) = h(x)$ for $x \in (-1, 1)$ and $\tilde{h}(x) = 0$ for $x \in \mathbb{R} \setminus (-1, 1)$, we have $\tilde{h} \in C_0(\mathbb{R})$ (the continuous functions with compact support) and hence, due to $h(-x) = h(x)$, Szegö’s first limit theorem (49) implies

$$C_{\beta, \delta, \gamma, \lambda} = \lim_{n \to \infty} \frac{S^{(n)}}{n} = \frac{1}{2} \int_{0}^{2\pi} \frac{d\xi}{2\pi} \text{tr} \tilde{h}(ia(\xi)) = \frac{1}{2} \int_{0}^{2\pi} \frac{d\xi}{2\pi} (h(\varphi_{\beta, \delta}(\xi) + \varphi_{\delta, \beta}(\xi)) + h(\varphi_{\beta, \delta}(\xi) - \varphi_{\delta, \beta}(\xi))) \geq h(\varrho) > 0. \quad (34)$$

This proves our theorem. \qed

**Remark 4** Contrary to what one would expect naively, the singular nature of the symbol does not affect the leading order of the asymptotics of the entropy density: As soon as there is a strictly positive temperature in the system, the spectral radius of the Toeplitz operator contracts to a value strictly less than 1. The same phenomenon has been observed for the transversal spin-spin correlations in this model, see [5].

**Remark 5** In the case $\delta = 0$, the symbol of the Toeplitz operator becomes smooth. Then, second order trace formulas imply that the subleading term has the form $o(n) = \text{const} + o(1)$, see [9, p.133, 207].
Remark 6 Note that for $\beta \to \infty$, the right hand side of (34) vanishes in agreement with the findings in the literature. In this case, the logarithmic behavior of the entropy density has been derived using the asymptotics of Toeplitz operators with Fisher-Hartwig symbols, see [18].

Remark 7 The von Neumann entropy $S^{(n)}$ is widely being used as a measure of entanglement in the ground state of a variety of quantum mechanical systems. In [20] [26] [18] for example, it has been shown that the entanglement entropy tends to a finite saturation value, whereas at a quantum phase transition (see [22]), it grows logarithmically with the size $n$ of the subsystem. These results can be related to conformal field theory computations of the geometric entropy, see, for example, [25] [11] [14] [15].

Corollary 4 For large $n$, the non-equilibrium entropy density is strictly greater than the entropy density in thermal equilibrium, i.e. $C_{\beta,\delta,\gamma,\lambda} > C_{\beta,0,\gamma,\lambda}$.

Proof From (34) we have

$$C_{\beta,\delta,\gamma,\lambda} = \frac{1}{2} \int_0^{2\pi} d\xi \frac{d\xi}{2\pi} \left( h(\text{th}(\beta R\mu(\xi)/2)) + h(\text{th}(\beta R\mu(\xi)/2 - \delta \mu(\xi))) \right) > C_{\beta,0,\gamma,\lambda}. \quad \square$$

Remark 8 In [13], following [1], a non-equilibrium steady state has been constructed by imposing a current on the system (these states differ in general from the non-equilibrium steady states in the sense of [21], see also [6]). The content of the corollary is in agreement with [13] in the sense that the von Neumann entropy increases in the current carrying state (by doubling the prefactor of the asymptotically logarithmic behavior).

A Quasi-free states on self-dual CAR algebras

Quasi-free states on self-dual CAR algebras have been introduced in [2]. We briefly review these notions. A self-dual CAR algebra over a Hilbert space $\mathcal{K}$ with scalar product $(\cdot, \cdot)$ and antiunitary involution $J$ is a $C^*$ completed $^*$-algebra generated by $B(f), f \in \mathcal{K}, B^*(f)$, and an identity $1$ which satisfy

$$\{B^*(f), B(g)\} = (f, g), \quad B^*(f) = B(Jf), \quad (35)$$

and $B(f)$ is linear in $f$. A quasi-free state on a self-dual CAR algebra is defined by

$$\omega(B(f^{(1)})...B(f^{(2m-1)})) = 0, \quad (36)$$

$$\omega(B(f^{(1)})...B(f^{(2m)})) = \sum_\pi \text{sign} \pi \prod_{i=1}^m \omega(B(f^{(\pi(2i-1)})B(f^{(\pi(2i))})), \quad (37)$$
for $m \in \mathbb{N}$, and the sum runs over all permutations $\pi$ in the permutation group $S_{2m}$ with signature $\text{sign} \pi$ which satisfy $\pi(2i - 1) < \pi(2i), \pi(2i + 1)$ (the pairings of $\{1, \ldots, 2m\}$). Such a state is characterized through

$$\omega(B^*(f)B(g)) = (f, Sg)$$

by its 2-point operator $S$ on $\mathcal{K}$ with the properties (see [2])

$$0 \leq S \leq 1, \quad S + JSJ = 1.$$

**Remark 9** The definition of $B(f)$ in (1) and of $J$ after (3), with $f \in \mathcal{K} = \mathfrak{h} \oplus \mathfrak{h}$, is a special case of a self-dual CAR algebra, and the non-equilibrium steady state $\omega_+$ from (6) is a quasifree state in the sense (36), (37), see [7].

Let $c_i, i = 1, \ldots, n$, be any fermions in $\mathcal{A}_n \simeq \mathcal{L}(\mathfrak{h}) \simeq \mathbb{C}^{2n \times 2n},$

$$\{c_i, c_j\} = 0, \quad \{c_i^*, c_j\} = \delta_{ij},$$

(38)

and define operators $e_{\alpha \beta}^{(i)}$, $i = 1, \ldots, n, \alpha, \beta = 1, 2$, by

$$e_{11}^{(i)} = c_i^* c_i, \quad e_{12}^{(i)} = c_i^*, \quad e_{21}^{(i)} = c_i, \quad e_{22}^{(i)} = c_i c_i^*.$$  

(39)

It follows from the CAR (38) that the operators $e_{\alpha \beta}^{(i)}$ have the properties

$$e_{\alpha \beta}^{(i)} e_{\gamma \delta}^{(j)} = (-1)^{(\alpha + \beta)(\gamma + \delta)} e_{\gamma \delta}^{(j)} e_{\alpha \beta}^{(i)}, \quad \text{for} \quad i \neq j,$$

(40)

$$e_{\alpha \beta}^{(i)} e_{\alpha \beta}^{(i)} = \delta_{\beta \gamma} e_{\alpha \beta}^{(i)}.$$  

(41)

**Remark 10** Note that, due to (35), the operators $c_i = B(f^{(i)})$ are fermions (38), if and only if $(Jf^{(i)}, f^{(j)}) = 0$ and $(f^{(i)}, f^{(j)}) = \delta_{ij}$. In the case at hand, the fermions are given in (23) (there is a *-isomorphism between the CAR algebra $\mathcal{A}$ over $\mathfrak{h}$ and the self-dual CAR algebra over $\mathfrak{h} \oplus \mathfrak{h}$, see [2]).

**Lemma 5** Let $e_{\alpha \beta}^{(i)}$ be defined by (39) for fermions $c_i = B(f^{(i)})$, and let $\omega$ be a quasi-free state on $\mathcal{A}_n$ which satisfies

$$\omega(c_i c_j) = 0, \quad \omega(c_i^* c_j) = \delta_{ij} \omega(c_i^* c_i), \quad i, j = 1, \ldots, n.$$

(42)

Then, $\omega$ factorizes on $\prod_{i=1}^n e_{\alpha_i \beta_i}^{(i)}$ as

$$\omega \left( \prod_{i=1}^n e_{\alpha_i \beta_i}^{(i)} \right) = \prod_{i=1}^n \delta_{\alpha_i \beta_i} \omega(e_{\alpha_i \alpha_i}^{(i)}).$$

(43)
Proof Assume first that the number of $B(\cdot)$ in $\prod_{i=1}^{n} e_{\alpha_{i} \beta_{i}}^{(i)}$ is odd. Then, there exists an $i \in \{1, \ldots, n\}$ such that $\alpha_{i} \neq \beta_{i}$ and, hence, due to (36), (43) holds. Now, let the number of $B(\cdot)$ in $\prod_{i=1}^{n} e_{\alpha_{i} \beta_{i}}^{(i)}$ be even. If $\alpha_{i} \neq \beta_{i}$ for some $i \in \{1, \ldots, n\}$, then every term in the sum (37) contains a factor of the form $\omega(B(J^{e_{i}} f^{(i)}) B(J^{e_{j}} f^{(j)}))$ with $i \neq j$ and some $e_{i}, e_{j} \in \{0, 1\}$. Therefore, due to (42), we have

$$\omega\left(\prod_{i=1}^{n} e_{\alpha_{i} \beta_{i}}^{(i)}\right) = \prod_{i=1}^{n} \delta_{\alpha_{i} \beta_{i}} \omega\left(\prod_{j=1}^{n} e_{\alpha_{j} \beta_{j}}^{(j)}\right).$$

(44)

For the same reason, applying (37) to the right hand side of (44), the only nonvanishing term is the one for which $\pi$ is the identity permutation. This implies (43).

Figure 3: The pairings of the right hand side of (44) for $n = 2$.

Lemma 6 Let $e_{\alpha \beta}^{(i)}$ be defined by (39) for fermions $c_{i} = B(f^{(i)})$. Then, the set of operators $\prod_{i=1}^{n} e_{\alpha_{i} \beta_{i}}$ with $\alpha_{1}, \beta_{1}, \ldots, \alpha_{n}, \beta_{n} = 1, 2$, is an orthonormal basis of the Hilbert space $A_{n}$ with scalar product $(A, B) \mapsto \text{tr}(A^{\ast} B)$.

Proof We show that the $2^{2n}$ vectors $\prod_{i=1}^{n} e_{\alpha_{i} \beta_{i}}$ with $\alpha_{1}, \beta_{1}, \ldots, \alpha_{n}, \beta_{n} = 1, 2$, are orthonormal with respect to the scalar product $A_{n} \times A_{n} \supset (A, B) \mapsto \text{tr}(A^{\ast} B)$ by proving

$$\text{tr} \left( \prod_{i=1}^{n} e_{\alpha_{i} \beta_{i}}^{(i)} \prod_{j=1}^{n} e_{\gamma_{j} \delta_{j}}^{(j)} \right) = \prod_{i=1}^{n} \delta_{\alpha_{i} \gamma_{i}} \delta_{\beta_{i} \delta_{i}}.$$  

(45)

For this purpose, we push the $j$-th term in the second product on the left hand side of (45) to the left using (41) until it it hits the $j$-th term in the first product and apply (41) (note that $e_{\gamma_{j} \delta_{j}}^{(j)} = \epsilon_{\delta_{j}^{j}}^{(j)}$). Doing so, from $j = n$ until $j = 1$, we arrive at

$$\prod_{i=1}^{n} e_{\alpha_{i} \beta_{i}}^{(i)} \left( \prod_{j=1}^{n} e_{\gamma_{j} \delta_{j}}^{(j)} \right)^{*} = \prod_{i=1}^{n} \delta_{\beta_{i} \gamma_{i}} \prod_{j=1}^{n-1} (-1)^{\gamma_{j} + \delta_{j}} \sum_{k_{j}=1}^{n} (\alpha_{k_{j}} + \delta_{k_{j}}) \prod_{l=1}^{n} e_{\alpha_{l} \delta_{l}}.$$  

(46)

Since $\text{tr}(\cdot)/2^{n}$ is a quasi-free state on $A_{n}$ (see for example [2]) which, due to the CAR (38) and the cyclicity of the trace, satisfies (42), we have, using (43) and (46),

$$\text{tr} \left( \prod_{i=1}^{n} e_{\alpha_{i} \beta_{i}}^{(i)} \prod_{j=1}^{n} e_{\gamma_{j} \delta_{j}}^{(j)} \right)^{*} = \prod_{i=1}^{n} \delta_{\beta_{i} \gamma_{i}} \prod_{j=1}^{n-1} (-1)^{\gamma_{j} + \delta_{j}} \sum_{k_{j}=1}^{n} (\alpha_{k_{j}} + \delta_{k_{j}}) \prod_{l=1}^{n} \delta_{\alpha_{l} \delta_{l}} \text{tr}(e^{(l)}_{\alpha_{l} \beta_{l}}).$$
(of course, (43) can easily be verified directly for $\text{tr}(-)/2^n$). Finally, using again the CAR (38) and the cyclicity of the trace, we have $\text{tr}(e_{\alpha(\alpha)})/2^n = 1/2$ and (45) follows. $\square$

**B  Toeplitz operators**

**Toeplitz operators** [9, p.185] Let $N \in \mathbb{N}$. We define the space $l_2^N$ of all $\mathbb{C}^N$-valued sequences $f = \{f_i\}_{i=1}^\infty$, $f_i \in \mathbb{C}^N$, by

$$l_2^N = \{ f : \mathbb{N} \to \mathbb{C}^N \mid \| f \| < \infty \}, \quad \| f \| = \left( \sum_{i=1}^\infty \| f_i \|_2^2 \right)^{1/2},$$

where $\| \cdot \|_2$ denotes the Euclidean norm on $\mathbb{C}^N$. For $N = 1$ we write $l_2^1 \equiv l_2^2$.

Let $\{a_x\}_{x \in \mathbb{Z}}$ be a sequence of $N \times N$ matrices, $a_x \in \mathbb{C}^{N \times N}$. The Toeplitz operator defined through its action on elements of $l_2^N$ by $f \mapsto \{ \sum_{j=1}^\infty a_{i-j} f_j \}_{i=1}^\infty$ is a bounded operator on $l_2^N$, if and only if

$$a_x = \int_0^{2\pi} \frac{d\xi}{2\pi} a(\xi) e^{-ix\xi}$$

for some $a \in L_\infty^{N \times N}$ (see [9, p.186]), where we define (with $\mathbb{T} = \{ z \in \mathbb{C} \mid |z| = 1 \}$)

$$L_\infty^{N \times N} = \{ \phi : \mathbb{T} \to \mathbb{C}^{N \times N} \mid \phi_{ij} \in L_\infty(\mathbb{T}), i, j = 1, \ldots, N \}.$$

In this case, we write the Toeplitz operator as

$$T[a] = \begin{bmatrix} a_0 & a_{-1} & a_{-2} & \ldots \\ a_1 & a_0 & a_{-1} & \ldots \\ a_2 & a_1 & a_0 & \ldots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}.$$  

The function $a \in L_\infty^{N \times N}$ is called the symbol of $T[a]$. If $N = 1$ the symbol $a \in L_\infty \equiv L_\infty^{1 \times 1}$ and the Toeplitz operator $T[a]$ are called scalar, whereas for $N > 1$ they are called block.

For $n \in \mathbb{N}$, let $P_n$ be the projections on $l_2^N$,

$$P_n(\{ f_1, \ldots, f_n, f_{n+1}, \ldots \}) = \{ f_1, \ldots, f_n, 0, 0, \ldots \}.$$  

With the help of these $P_n$, we define the truncated $Nn \times Nn$ Toeplitz matrices as

$$T_n[a] = P_n T[a] P_n \mid_{\text{ran} P_n},$$

where $\text{ran} A$ denotes the range of the operator $A$. 

Norm of Toeplitz operators [9, p.186] The norm of a Toeplitz operator is related to its symbol,
\[
\|T[a]\| = \|a\|_\infty,
\]
where \(\|a\|_\infty\) is defined to be the operator norm of the multiplication operator acting on \(\oplus_1^N L^2(\mathbb{T})\) by multiplication with the matrix function \(a \in L^\infty_{N \times N}\). We have
\[
\|a\|_\infty = \text{ess sup}_{\xi \in [0, 2\pi]} \|a(\xi)\|_{L(C^N)},
\]
where \(\| \cdot \|_{L(C^N)}\) is the operator norm induced by the \(l^2\) norm on \(C^N\), see also [8, p.101].

Szegö’s first limit theorem in the block case [9, p.202] Let \(a \in L^\infty_{N \times N}\) be self-adjoint, \(a^* = a\), and let \(\lambda_1^{(n)}, \ldots, \lambda_N^{(n)}\) be the eigenvalues of the block Toeplitz matrix \(T_n[a]\). Then, for any continuous function \(f\) with compact support, \(f \in C_0(\mathbb{R})\), we have
\[
\lim_{n \to \infty} \frac{1}{Nn} \sum_{k=1}^{Nn} f(\lambda_k^{(n)}) = \frac{1}{N} \int_0^{2\pi} \frac{d\xi}{2\pi} \text{tr} f(a(\xi)).
\]

Acknowledgements It is a great pleasure to thank Herbert Spohn for his interesting comments. Moreover, I am grateful to the referee for his constructive remarks.

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