On the emptiness formation probability in quasi-free states

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Abstract

We study the behavior of the emptiness formation probability for large spin strings in translation invariant quasi-free states on the CAR algebra on the discrete line and establish a simple criterion on the one-particle density matrix of the quasi-free state which ensures exponential decay. As an illustration, we treat the example of the XY spin chain out of equilibrium, in thermal equilibrium, in the ground state, and in the chaotic state.

Dedicated to Jean-Michel Combes on the occasion of his sixtyfifth birthday

1 Introduction

Low-dimensional magnetic systems are being studied intensively for many different reasons. For instance, the discovery of the ideal thermal conductivity in quasi-one-dimensional Heisenberg spin-$1/2$ systems has triggered an ongoing experimental and theoretical activity, see for example [17, 18] and [14, 21, 22]. Not only this highly unusual transport property motivates the further study of such non-equilibrium models, but also these models, and in particular the XY chain, are a useful means to get a clearer picture about the general concepts in rigorous non-equilibrium quantum statistical mechanics.
With this motivation in mind, we propose to study the decay of a special correlation function, the so-called emptiness formation probability (EFP) in the non-equilibrium steady state (NESS) of the XY chain constructed in [10] (and already in [6] in lesser generality). Since, due to the fact that this NESS turned out to be a translation invariant quasi-free state on the canonical anticommutation relations (CAR) algebra over the discrete line $\mathbb{Z}$

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(by using the Jordan-Wigner transformation which maps the spins to fermions, see (2) below), we are naturally led to study the decay of the EFP directly in this more general setting of quasi-free states. The EFP $P(n)$ describes the probability that a ferromagnetic string of length n is formed in the translation invariant quasi-free state ω,

$$P(n) = \omega\big(\Pi^{(1)}\Pi^{(2)} \dots \Pi^{(n)}\big) \tag{1}$$

with $\Pi^{(j)} = (1 - \sigma_3^{(j)})/2$ (given in (8) in terms of Jordan-Wigner fermions), i.e. the probability that the first n spins of the chain are all aligned downwards.

The EFP in the XY chain has already been studied at vanishing and nonvanishing temperature. In both cases, $P(n)$ can be written as the determinant of the n-dimensional section of a Toeplitz operator with scalar symbol (there are also other methods for the treatment of $P(n)$, as, for example, the Fredholm determinant method and the method of multiple integrals, see [16] and references therein).
Since the higher order asymptotics of a Toeplitz determinant is highly sensitive to the regularity of the symbol of the Toeplitz operator (in the sense of the zeroes and the singularities of the symbol), the asymptotic behavior of $P(n)$ at vanishing temperature is qualitatively different in the non-critical and the critical regimes defined by the values of the anisotropy γ and the exterior magnetic field λ (see (18)). It has been found that the EFP decays like a Gaussian in one of the critical regimes (with some additional explicit numerical prefactor and some power-law prefactor, see [16] and references therein). In a second critical regime and in all the noncritical regimes, $P(n)$ decays exponentially (in contrast to the non-critical regime, there is an additional power-law prefactor in the second critical regime whose exponent differs from the one in the first critical regime, see [1, 15]). These results have been derived by using well-known theorems of Szegö, Widom, and Fisher-Hartwig, and the (yet unproven) Basor-Tracy conjecture (and some extension), see [20, 11, 12]. At non-vanishing temperature, using a theorem of Szegö, the EFP decays again exponentially, see for example [16, 15].
In contrast, out of equilibrium, the EFP is a (2×2)-block Toeplitz determinant. Due to the lack of control of the higher order determinant asymptotics in the Toeplitz theory with nontrivial block symbols, we study bounds on the leading asymptotic order for a class of general (2×2)-block Toeplitz determinants. We ask the question whether there is a simple criterion on a general translation invariant quasi-free state ω on the CAR algebra on the discrete line for the EFP to be exponentially decaying. It turns out that suitable basic spectral information about the one-particle density matrix specifying the quasi-free state is sufficient to ensure exponential decay of the EFP (see [8] for the study of the decay of spin-spin correlations in quasi-free states by the same strategy). We compare our bounds to the available asymptotic rates in the scalar Toeplitz determinant cases, and they turn out to be exact.

Section 2 contains the setting and Section 3 our main assertion. Section 4 is devoted to the examples of the XY chain out of equilibrium, in thermal equilibrium at non-vanishing temperature, at vanishing temperature, and at infinite temperature.

2 The setting

To study the large n asymptotics of the EFP $P(n)$ defined in (1), we will make use of the Jordan-Wigner transformation which allows us to pass from the spin picture to the more convenient fermionic picture. The Jordan-Wigner transformation is defined as follows. For the site x on the discrete line $\mathbb{Z}$, let $\varrho^{(x)} = \sigma_3^{(1)} \dots \sigma_3^{(x-1)}$ if $x > 1$, $\varrho^{(1)} = 1$, and $\varrho^{(x)} = \sigma_3^{(x)} \dots \sigma_3^{(0)}$ if $x < 1$. Then,

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

defines the annihilation operator $a_x \equiv a(\delta_x)$ in the CAR algebra $\mathcal{A}$ over the Hilbert space $\ell^2(\mathbb{Z})$ (see [2, 13] for example). Here, $\sigma_j^{(x)}$ stands for the spin in the j-direction at site x, $j = 1, 2, 3$, the matrices $\sigma_0, \dots, \sigma_3$ denote the elements of the Pauli basis of $\mathbb{C}^{2\times 2}$,

$$\sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{3}$$

and $\delta_x \in \ell^2(\mathbb{Z})$ is the Kronecker function. Moreover, T has the properties $T^* = T$, $T^2 = 1$, and $T\sigma_j^{(x)}T = \theta_-(\sigma_j^{(x)})$, where, for $j = 1, 2$, the $*$-automorphism θ_- on the spin algebra is defined by $\theta_-(\sigma_j^{(x)}) = -\sigma_j^{(x)}$ if $x \le 0$ and $\theta_-(\sigma_j^{(x)}) = \sigma_j^{(x)}$ if $x \ge 1$ (the element T stems from Araki's C^* crossed product extension for the CAR algebra on the two-sided chain, see [4] for details). Next, let us define the complex linear mapping

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

where $F \in \ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z})$ is written as $F = [f_1, f_2]$. Moreover, let J be the antiunitary involution on $\ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z})$ defined by $J[f_1, f_2] = [\bar{f}_2, \bar{f}_1]$ (where $\bar{f}$ denotes the complex conjugate of $f \in \ell^2(\mathbb{Z})$). Hence, the adjoint of $B(F)$ is implemented as

$$B^*(F) = B(JF), \tag{4}$$

and using the CAR for the annihilation and creation operators $a(f)$ and $a^*(f)$, we get the generalized relations

$$\{B^*(F), B(G)\} = (F, G), \tag{5}$$

where $\{A, B\} = AB + BA$ denotes the anticommutator of A and B, and (F, G) is the scalar product of $F, G \in \ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z})$.

Remark 1 The algebra generated by the $B(F)$ (which is $*$-isomorphic to $\mathcal{A}$) is a special case of a so-called self-dual CAR algebra, a concept introduced in [2] (see also [3]). Self-dual CAR algebras turned out, among other things, to be convenient for the description of correlation functions in spin models using the Jordan-Wigner transformation, see for example [4, 9, 10].

As discussed in the Introduction, we want to study a correlation function of the form $\omega(B(F_1)...B(F_{2n}))$ with ω a translation invariant quasi-free state (and with the observables from (8)). A state ω on $\mathcal{A}$ is called quasi-free if it vanishes on the odd polynomials in $B(F)$,

$$\omega(B(F_1)...B(F_{2n-1})) = 0,$$

and if it factorizes on the even polynomials in $B(F)$ as

$$\omega(B(F_1)...B(F_{2n})) = \sum_\pi \mathrm{sign}(\pi) \prod_{j=1}^{n} \omega(B(F_{\pi(2j-1)})B(F_{\pi(2j)})) \tag{6}$$

for any $F_j \in \ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z})$ with $j = 1, ..., 2n$, and for all $n \in \mathbb{N}$. The sum in (6) runs over all pairings of the set $\{1, 2, ..., 2n\}$, i.e. over all those permutations π in the permutation group $\mathcal{S}_{2n}$ which satisfy $\pi(2j-1) < \pi(2j+1)$ and $\pi(2j-1) < \pi(2j)$. Let us define the correlation matrix $\Omega(n) \in \mathbb{C}^{2n\times 2n}$ by

$$\Omega(n)_{kl} = \begin{cases} \omega(B(F_k)B(F_l)), & k < l \\ 0, & k = l \\ -\omega(B(F_l)B(F_k)), & k > l \end{cases},$$

for $k, l = 1, ..., 2n$. Then, we not only have

$$\omega(B(F_1)...B(F_{2n})) = \mathrm{pf}\ \Omega(n)$$

due to (6) (the expression $\mathrm{pf}\ A = \sum_\pi \mathrm{sign}(\pi) \prod_{j=1}^n A_{\pi(2j-1),\pi(2j)}$ with the sum running over all pairings of the set $\{1, 2, ..., 2n\}$ is exactly the so-called Pfaffian of $A \in \mathbb{C}^{2n\times 2n}$), but also, since $\Omega(n)$ is skew-symmetric, i.e. $\Omega(n)^t = -\Omega(n)$ (where A^t is the transpose of A), the square of the correlation function can be expressed as a determinant,

$$\omega(B(F_1)...B(F_{2n}))^2 = \det \Omega(n), \tag{7}$$

which is due to the well-known property $(\mathrm{pf}\ A)^2 = \det A$ for skew-symmetric matrices A (see for example [19]). Hence, the study of the correlation function $\omega(B(F_1)...B(F_{2n}))^2$ with quasi-free state ω amounts to analyze the determinant of the $(2n \times 2n)$-matrix $\Omega(n)$.

In the following, we formulate an assumption under which $\Omega(n)$ becomes the finite section of a Toeplitz operator with the symbol corresponding to the EFP observable in (1) (the reader not familiar with Toeplitz theory may consult Appendix A for the definitions and the basic facts). To this end, we define the translation $*$-automorphism group τ_x on the CAR algebra $\mathcal{A}$ by

$$\tau_x(B(F)) = B(U_x F), \quad U_x = u_x \oplus u_x,$$

where u_x is the usual translation operator on $\ell^2(\mathbb{Z})$ of the form $(u_x f)(y) = f(y-x)$ for $x, y \in \mathbb{Z}$. A state ω is called translation invariant if it is invariant under the $*$-automorphism group τ_x, i.e. if $\omega \circ \tau_x = \omega$.

Assumption 1 *The quasi-free state ω is translation invariant. Moreover, the form factors F_j, $j \in \mathbb{N}$, are given by*

$$F_{2j-1} = U_j G_0, \; F_{2j} = U_j G_1 \quad \textit{with} \quad G_0 = JG_1 = [0, \delta_0],$$

and δ_0 is the Kronecker function localized at $x = 0$.

Hence, under Assumption 1, and using the Jordan-Wigner transformation (2), the EFP observable in (1) projects on a string of length n without Jordan-Wigner fermions,

$$\Pi^{(1)} \ldots \Pi^{(n)} = a_1 a_1^* \ldots a_n a_n^* = B(F_1) \ldots B(F_{2n}). \tag{8}$$

We then straightforwardly get the following lemma.

Lemma 2 *Let ω be a quasi-free state, and let Assumption 1 hold. Then, the correlation matrix $\Omega(n)$ is a (2×2)-block Toeplitz matrix.*

Finally, we want to relate the (2×2)-block symbol a of the Toeplitz operator with finite section $\Omega(n)$ to the quasi-free state ω. A quasi-free state ω is completely characterized by its two-point function $\omega(B^*(F)B(G))$ which, in turn, defines an operator S on $\ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z})$ through

$$\omega(B^*(F)B(G)) = (F, SG). \tag{9}$$

Due to the positivity of the state ω and (4) and (5), the operator S has the properties

$$0 \leq S^* = S \leq 1, \tag{10}$$

$$JSJ = 1 - S. \tag{11}$$

Conversely, to any bounded operator S on $\ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z})$ satisfying (10) and (11), there exists a unique quasi-free state with two-point function (9) which we denote by ω_S (see [3]). The operator S is called the one-particle density matrix of the quasi-free state ω_S.

Since $\omega_S(\tau_x(B^*(F)B(G))) = (F, U_x^* S U_x G)$, the quasi-free state ω_S is translation invariant, if and only if its one-particle density matrix S commutes with U_x,

$$SU_x = U_x S. \tag{12}$$

In the next lemma, we switch to the Fourier picture and write $s = \mathcal{F} S \mathcal{F}^*$, where $\mathcal{F} = \hat{} \oplus \hat{}$ is the direct sum of the Fourier transform $\hat{} : \ell^2(\mathbb{Z}) \to L^2(\mathbb{T})$ of the form $\hat{\varphi}(e^{i\xi}) = \sum_{x \in \mathbb{Z}} \varphi(x) e^{ix\xi}$ (with $\mathbb{T} = \{t \in \mathbb{C} \,|\, |t| = 1\}$). The spaces ℓ_2^2, $L^\infty_{2\times 2}$, and the operator P_n below are defined in (28), (29), and (30), respectively. Moreover, we use the natural identification of $\ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z})$ with $\ell^2(\mathbb{Z}, \mathbb{C}^2)$, and $(\cdot, \cdot)_{\mathbb{C}^2}$ stands for the Euclidean scalar product on $\mathbb{C}^2$.

Remark 2 We write the Fourier transformation of the one-particle density matrix S on $\ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z})$ as $s = \mathcal{F} S \mathcal{F}^*$ on $L^2(\mathbb{T}) \oplus L^2(\mathbb{T})$ with

$$s = \begin{bmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{bmatrix}, \quad s_{ij} : L^2(\mathbb{T}) \to L^2(\mathbb{T}).$$

Due to (10), the operator s_{ij} is bounded, and, due to (12), it is translation invariant, i.e. $s_{ij}e^{ix\xi} = e^{ix\xi}s_{ij}$. Therefore, s_{ij} acts through multiplication by a function in $L^\infty(\mathbb{T})$ (see [12, p.45] for example). We denote this function again by s_{ij}, and hence

$$s = s(e^{i\xi}).$$

As in (1), let us define $\Pi = (1-\sigma_3)/2$, and let the infinite matrix Ω stand for the matrix $\Omega(n)$ with arbitrary large n. Then, the (2×2)-block symbol a of the Toeplitz operator with finite section $\Omega(n)$ relates to the one-particle density matrix of the quasi-free state ω as follows (see [8] for details).

Lemma 3 *Let ω_S be the quasi-free state characterized by the one-particle density matrix S. If Assumption 1 holds, then Ω defines a bounded Toeplitz operator $T[a]$ on ℓ_2^2 with symbol*

$$a = (s-\Pi)\sigma_1 \in L^\infty_{2\times 2}, \tag{13}$$

and the correlation matrix $\Omega(n)$ is the finite section of $T[a]$, i.e. $\Omega(n) = T_n[a]$.

Therefore, using (7) and (8), the square of the EFP (1) can be expressed as the determinant of the finite section of the Toeplitz operator with the (2×2)-block symbol a from (13),

$$P(n)^2 = \det T_n[a]. \tag{14}$$

Hence, the study of the decay of the EFP boils down to the analysis of the determinant of a large truncated Toeplitz operator.

3 The decay of the emptiness formation probability

In our main assertion, Theorem 4 below, we establish a criterion for exponential decay of the EFP making use of the set

$$\mathfrak{S} = \{\xi \in [0,2\pi) \mid |\det[s(e^{i\xi})-\Pi]| \not\subseteq \{0,1\}\}. \tag{15}$$

The proof of Theorem 4 is analogous to the proof in [8]. For the sake of completeness, we repeat it here. In the following, we denote by $\mathfrak{L}(M)$ the Lebesgue measure of the subset M of $\mathbb{R}$.

Theorem 4 *Let ω_S be the quasi-free state characterized by the one-particle density matrix S. If Assumption 1 holds, and if $\mathfrak{L}(\mathfrak{S}) > 0$, then the decay rate is bounded from above by*

$$\limsup_{n\to\infty} \frac{1}{n}\log|P(n)| \leq \frac{1}{2}\int_{\mathfrak{S}} \frac{d\xi}{2\pi}\, \log|\det[s(e^{i\xi})-\Pi]| < 0.$$

Proof Since $|P(n)|^2 = |\det T_n[a]|$ due to (14), we estimate the singular values

$$0 \le t_1^{(n)} \le t_2^{(n)} \le \ldots \le t_{2n}^{(n)} = \|T_n[a]\|$$

of the Toeplitz matrix $T_n[a]$. Let $N_{\varepsilon,n}$ be the number of those singular values whose square is contained in $[0,\varepsilon]$ for $\varepsilon > 0$ (to be chosen sufficiently small in the following). Then, using the singular value decomposition (see for example [11, p.84]), we have

$$|P(n)|^4 = |\det T_n[a]|^2 = \prod_{j=1}^{2n} (t_j^{(n)})^2 \le \varepsilon^{N_{\varepsilon,n}} \prod_{j=N_{\varepsilon,n}+1}^{2n} (t_j^{(n)})^2.$$

In order to treat the gap of size ε at the origin, we pick a continuous characteristic function $\chi_\varepsilon : \mathbb{R} \to [0,1]$ with $\chi_\varepsilon(x) = 0$ if $x \in (-\infty, \varepsilon] \cup [\|T[a]\|^2 + 1 + \varepsilon, \infty)$, and $\chi_\varepsilon(x) = 1$ if $x \in [2\varepsilon, \|T[a]\|^2 + 1]$. Moreover, let us define the function $g_\varepsilon : \mathbb{R} \to \mathbb{R}$ by $g_\varepsilon(x) = 0$ if $x \le 0$ and $g_\varepsilon(x) = \chi_\varepsilon(x) \log x$ if $x > 0$. Then,

$$\log |P(n)|^4 \le \sum_{j=N_{\varepsilon,n}+1}^{2n} \log((t_j^{(n)})^2) \le \sum_{j=1}^{2n} g_\varepsilon((t_j^{(n)})^2).$$

Since $g_\varepsilon \in C_0(\mathbb{R})$ and $a \in L^\infty_{2\times 2}$, the Avram-Parter theorem (32) yields

$$\limsup_{n\to\infty} \frac{1}{n} \log |P(n)| \le \frac{1}{4} \int_0^{2\pi} \frac{d\xi}{2\pi} \operatorname{tr} g_\varepsilon(a^*(e^{i\xi}) a(e^{i\xi})). \tag{16}$$

In order to estimate the right hand side of (16) from above, we define the following subsets of $\mathfrak{S}$ (spec$A$ denotes the spectrum of the operator A),

$$\begin{aligned} \mathfrak{S}_\alpha &= \{\xi \in [0,2\pi) \mid |\det[s(e^{i\xi}) - \Pi]| \ne \alpha\}, \quad \alpha = 0, 1, \\ \mathfrak{R}_\delta &= \{\xi \in [0,2\pi) \mid \operatorname{spec} a^*(e^{i\xi}) a(e^{i\xi}) \subseteq (\delta, \|a\|_\infty^2]\}, \quad \delta > 0. \end{aligned}$$

Since, due to (13),

$$\det a(e^{i\xi}) = -\det[s(e^{i\xi}) - \Pi],$$

we have $\mathfrak{S}_0 = \{\xi \in [0,2\pi) \mid \operatorname{spec} a^*(e^{i\xi}) a(e^{i\xi}) \subseteq (0, \|a\|_\infty^2]\}$. Hence, since $\mathfrak{L}(\mathfrak{S}_0) \ge \mathfrak{L}(\mathfrak{S}_0 \cap \mathfrak{S}_1) = \mathfrak{L}(\mathfrak{S}) > 0$ by assumption, and since $\mathfrak{L}(\mathfrak{S}_0 \setminus \mathfrak{R}_\delta)$ tends to zero for $\delta \to 0$, we have $\mathfrak{L}(\mathfrak{R}_\delta) > 0$ for sufficiently small δ. Therefore, writing the integration domain as $[0,2\pi) = \mathfrak{R}_\delta \cup ([0,2\pi) \setminus \mathfrak{R}_\delta)$ on the right hand side of (16), and choosing $\delta = 2\varepsilon$ small enough, we have

$$\frac{1}{4} \int_0^{2\pi} \frac{d\xi}{2\pi} \operatorname{tr} g_\varepsilon(a^*(e^{i\xi}) a(e^{i\xi})) \le \frac{1}{2} \int_{\mathfrak{R}_{2\varepsilon}} \frac{d\xi}{2\pi} \log |\det a(e^{i\xi})|,$$

where we used $\|T[a]\| = \|a\|_\infty$ from (31). Moreover, property (10) implies $|\det a(e^{i\xi})| \le 1$. Hence, since $\mathfrak{S}_1 = \{\xi \in [0,2\pi) \mid |\det a(e^{i\xi})| \ne 1\}$ and since $\mathfrak{L}(\mathfrak{S}_1 \cap \mathfrak{R}_{2\varepsilon}) > 0$,

$$\frac{1}{2} \int_{\mathfrak{R}_{2\varepsilon}} \frac{d\xi}{2\pi} \log |\det a(e^{i\xi})| = \frac{1}{2} \int_{\mathfrak{S}_1 \cap \mathfrak{R}_{2\varepsilon}} \frac{d\xi}{2\pi} \log |\det[s(e^{i\xi}) - \Pi]| < 0.$$

This brings the proof of Theorem 4 to an end. □

Remark 3 We do not exclude that the bound is $-\infty$ (but see the examples in Section 4).

Remark 4 Note that in the case $\|a\|_\infty < 1$, exponential decay follows because

$$|P(n)|^2 = |\det T_n[a]| \leq \|T_n[a]\|^{2n} \leq \|T[a]\|^{2n} = \|a\|_\infty^{2n}, \tag{17}$$

where the last equality stems from (31). Making again use of conditions (10) and (11) in their Fourier transformed form,

$$0 \leq s^*(e^{i\xi}) = s(e^{i\xi}) \leq 1, \quad \sigma_1 \overline{s}(e^{-i\xi})\sigma_1 = 1 - s(e^{i\xi}),$$

a straightforward computation yields

$$\|a(e^{i\xi})\|_{\mathcal{L}(\mathbb{C}^2)} = \frac{1}{2}\left(\lambda(e^{i\xi})^2 + \lambda(e^{-i\xi})^2 + |\lambda(e^{i\xi})^2 - \lambda(e^{-i\xi})^2|\right),$$

where $\lambda(e^{i\xi})$ is any of the two eigenvalues of $s(e^{i\xi}) - \Pi$. If we choose, for example, a continuous $\lambda(e^{i\xi})$ with values in $(0, 1)$ for $\xi \in (0, 2\pi)$ and with $\lambda(1) = 1$, we have

$$\|a\|_\infty = \operatorname*{ess\,sup}_{\xi \in [0,2\pi)} \|a(e^{i\xi})\|_{\mathcal{L}(\mathbb{C}^2)} = 1.$$

However, Theorem 4 still applies and yields a nontrivial decay rate. Finally, note that, due to $0 \leq \lambda(e^{i\xi}) \leq 1$, it is not possible that $\|a\|_\infty > 1$.

Remark 5 For the case $\mathfrak{L}(\mathfrak{S}) = 2\pi$, we note that the bound (17) is weaker than the one from Theorem 4,

$$\frac{1}{2}\int_0^{2\pi} \frac{d\xi}{2\pi} \log|\det a(e^{i\xi})| \leq \frac{1}{2}\int_0^{2\pi} \frac{d\xi}{2\pi} \log\left[\|a(e^{i\xi})\|^2_{\mathcal{L}(\mathbb{C}^2)}\right] \leq \log\,\|a\|_\infty.$$

4 Examples

In this section, we illustrate the foregoing considerations with the examples of the EFP in the XY chain out of equilibrium, in thermal equilibrium, in the ground state, and in the chaotic state.

Example 1 *Decay rate out of equilibrium*

The NESS ω_+ of the XY chain with the formal Hamiltonian

$$H = -\frac{1}{4}\sum_{x \in \mathbb{Z}} \left\{(1+\gamma)\,\sigma_1^{(x)}\sigma_1^{(x+1)} + (1-\gamma)\,\sigma_2^{(x)}\sigma_2^{(x+1)} + 2\lambda\,\sigma_3^{(x)}\right\} \tag{18}$$

has been constructed in [10] (and already in [6] for $\gamma = \lambda = 0$) by coupling a finite cutout of the XY chain to the two infinite parts to its left and right acting as thermal reservoirs at different inverse temperatures β_L and β_R. Here, $\gamma \in (-1, 1)$ denotes the anisotropy and $\lambda \in \mathbb{R}$ the external magnetic field of the XY chain. It has been shown in [10] that ω_+ is a translation invariant quasi-free state whose one-particle density matrix in the Fourier picture looks like

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

Here, $\beta = (\beta_R + \beta_L)/2$ and $\delta = (\beta_R - \beta_L)/2 > 0$,

$$\begin{aligned} h(e^{i\xi}) &= (\cos\xi - \lambda) \otimes \sigma_3 + \gamma \sin\xi \otimes \sigma_2, & (19)\\ k(e^{i\xi}) &= \operatorname{sign}(\kappa(e^{i\xi}))\, \mu(e^{i\xi}) \otimes \sigma_0, \\ \kappa(e^{i\xi}) &= 2\lambda \sin\xi - (1-\gamma^2) \sin 2\xi, \\ \mu(e^{i\xi}) &= \sqrt{(\cos\xi - \lambda)^2 + \gamma^2 \sin^2\xi}. & (20) \end{aligned}$$

Expanding $s(e^{i\xi})$ with respect to the Pauli basis $\sigma_0, ..., \sigma_3$ of $\mathbb{C}^{2\times 2}$ from (3), we find the components of $s(e^{i\xi}) = s_0(e^{i\xi}) \otimes \sigma_0 + \sum_{k=1}^{3} s_k(e^{i\xi}) \otimes \sigma_k$ to look like

$$\begin{aligned} s_0(e^{i\xi}) &= \frac{1}{2} - \frac{1}{2}\, \varphi_{\delta,\beta}(e^{i\xi}) \operatorname{sign} \kappa(e^{i\xi}), & (21)\\ s_k(e^{i\xi}) &= \frac{1}{2}\, \varphi_{\beta,\delta}(e^{i\xi})\, r_k(e^{i\xi}), \quad k = 1, 2, 3, & (22) \end{aligned}$$

where we used the definitions

$$\begin{aligned} r(e^{i\xi}) &= \frac{1}{\mu(e^{i\xi})}\, (0, \gamma \sin\xi, \cos\xi - \lambda), \\ \varphi_{\alpha,\alpha'}(e^{i\xi}) &= \frac{\operatorname{sh}(\alpha\mu(e^{i\xi}))}{\operatorname{ch}(\alpha\mu(e^{i\xi})) + \operatorname{ch}(\alpha'\mu(e^{i\xi}))}, \quad \alpha, \alpha' \in \mathbb{R}. \end{aligned}$$

Hence, the argument of the logarithm in the integrand of the bound on the decay rate in Theorem 4 becomes

$$\begin{aligned} |\det[s(e^{i\xi}) - \Pi]| = \frac{1}{4} \Bigg(& 1 + \operatorname{th}\Big(\beta_L \frac{\mu(e^{i\xi})}{2}\Big) \operatorname{th}\Big(\beta_R \frac{\mu(e^{i\xi})}{2}\Big) \\ & + \left[\operatorname{th}\Big(\beta_L \frac{\mu(e^{i\xi})}{2}\Big) + \operatorname{th}\Big(\beta_R \frac{\mu(e^{i\xi})}{2}\Big)\right] \frac{\cos\xi - \lambda}{\mu(e^{i\xi})} \Bigg). \quad (23) \end{aligned}$$

Let us denote by $\mathcal{H}$ the set of the so-called critical parameters $(\lambda, \gamma) \in \mathbb{R} \times (-1, 1)$ for which $\mu(e^{i\xi})$ vanishes. From (20), it immediatly follows that

$$\mathcal{H} = (-1, 1) \times \{0\} \cup \{-1, 1\} \times (-1, 1), \quad (24)$$

which is depicted in Figure 1. Both in the noncritical case, $(\lambda, \gamma) \notin \mathcal{H}$, and in the critical case, $(\lambda, \gamma) \in \mathcal{H}$, the determinant $|\det[s(e^{i\xi}) - \Pi]|$ from (23) is strictly bounded away from 0 and 1 for all $\xi \in [0, 2\pi)$. This implies

$$\mathfrak{L}(\mathfrak{S}) = 2\pi,$$

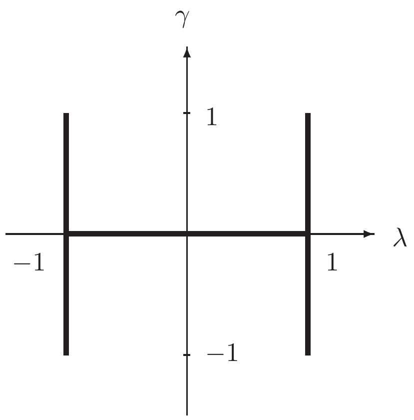

Figure 1: The set of critical parameters $\mathcal{H}$.

and, thus, Theorem 4 holds with (23).

Remark 6 The zeroes of the function $\mu(e^{i\xi})$ determine the critical and the non-critical regimes. If $(\lambda, \gamma) \in (-1,1) \times \{0\}$, it has exactly the two zeroes at $\xi = \pi/2$ and at $\xi = 3\pi/2$. If $(\lambda, \gamma) \in \{-1\} \times (-1,1)$, it has exactly one zero at $\xi = \pi$, and if $(\lambda, \gamma) \in \{1\} \times (-1,1)$, it has exactly one zero at $\xi = 0$. If $(\lambda, \gamma) \in \mathbb{R} \times (-1,1) \setminus \mathcal{H}$, it has no zeroes at all.

Remark 7 In the isotropic case, $\gamma = 0$, the structure of the symbol (13) allows the EFP to be expressed by means of scalar Toeplitz determinants. Using Szegö's first limit theorem for the leading order contribution to the asymptotics (see [11, p.139] for example), we can compute the decay rate, and, it turns out, that our bound is exact. The subleading contributions to the asymptotics will be studied elsewhere [7].

Example 2 *Decay rate in thermal equilibrium*

For $\beta_L = \beta_R \equiv \beta$, i.e. $\delta = 0$, we recover the bound on the decay rate in thermal equilibrium from Example 1. In this case, the one-particle density matrix in the Fourier picture reads

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

where the one-particle Hamiltonian h is specified in (19). Hence,

$$|\det[s(e^{i\xi}) - \Pi]| = \frac{1}{4}\left(1 + \mathrm{th}^2\Big(\beta\,\frac{\mu(e^{i\xi})}{2}\Big) + 2\,\mathrm{th}\Big(\beta\,\frac{\mu(e^{i\xi})}{2}\Big)\,\frac{\cos\xi - \lambda}{\mu(e^{i\xi})}\right). \tag{25}$$

and, of course, we again have

$$\mathfrak{L}(\mathfrak{S}) = 2\pi.$$

Theorem 4 thus holds with (25).

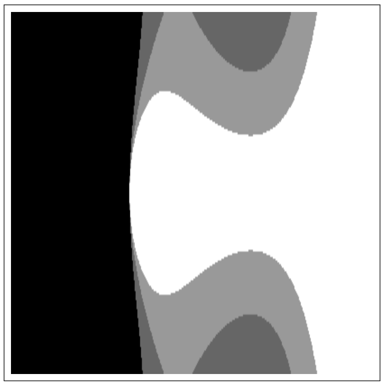

Figure 2: The ordering of the bounds on the decay rate in and out of equilibrium (Remark 11). The magnetic field on the abscissa runs from $\lambda = -2$ to $\lambda = 2$ and the anisotropy on the ordinate from $\gamma = -1$ to $\gamma = 1$.

Remark 8 In thermal equilibrium, i.e. if $\delta = 0$ (and also in the ground state from Example 3 for $\beta = \infty$), the (2×2)-block Toeplitz matrix $T_n[a]$ can be unitarily transformed such that its determinant can be expressed by means of a scalar Toeplitz determinant (see [16, 1] for example). Hence, in contrast to the case of general block Toeplitz determinants, Fisher-Hartwig type theorems are at one's disposal (see also Remark 7).

Remark 9 In [16], using a theorem of Szegö (see [12, 11]), the decay rate for the isotropic XY chain (i.e. $\gamma = 0$ in (18)) is shown to be an affine function of the free energy per site (see also [15] for the anisotropic case $\gamma \neq 0$). Our bound is exact in this case.

Remark 10 Again in [16], a low temperature expansion of the decay rate ($\equiv$ negative of the inverse correlation length) is given. It is shown that it diverges for $T \to 0$ if $\gamma = 0$ and $|\lambda| < 1$ which signals a crossover from the exponential decay to a stronger decay at $T = 0$. It turned out that this decay is Gaussian, see Example 3.

Remark 11 For fixed β_L and β_L, let us denote by $\varrho(\beta_L, \beta_R)$ the bound on the decay rate from Theorem 4 with (23) being the argument of the logarithm. The ordering of the bounds on the decay rate in and out of equilibrium depends sensitively on $(\lambda, \gamma) \in \mathbb{R} \times (-1, 1)$, see Figure 2: For $\beta_L = 2$ and $\beta_L = 4$, we have $\varrho(\beta_L, \beta_L) < \varrho(\beta_L, \beta_R) < \varrho(\beta_R, \beta_R)$ in the black regime, $\varrho(\beta_L, \beta_R) < \varrho(\beta_L, \beta_L) < \varrho(\beta_R, \beta_R)$ in the dark grey regime, $\varrho(\beta_L, \beta_R) < \varrho(\beta_R, \beta_R) < \varrho(\beta_L, \beta_L)$ in the light grey regime, and $\varrho(\beta_R, \beta_R) < \varrho(\beta_L, \beta_R) < \varrho(\beta_L, \beta_L)$ in the white regime . The complexity of the diagram increases with decreasing temperatures.

Example 3 *Decay rate in the ground state*

The ground state of the XY chain on the transversal spin-spin observable can be described by the one-particle density matrix of Example 1 by setting $\delta = 0$ and $\beta = \infty$ in (21) and

(22). This yields

$$s(e^{i\xi}) = \frac{1}{2}\left(1 + \frac{1}{\mu(e^{i\xi})}\begin{bmatrix} \cos\xi - \lambda & -i\gamma\sin\xi \\ i\gamma\sin\xi & -(\cos\xi - \lambda) \end{bmatrix}\right), \tag{26}$$

and hence (compare with (25)),

$$|\det[s(e^{i\xi}) - \Pi]| = \frac{1}{2}\left(1 + \frac{\cos\xi - \lambda}{\mu(e^{i\xi})}\right). \tag{27}$$

Remark 12 The phase diagram for the ground states of the infinite XY model has been completely determined in [5]. For the parameters $(\lambda, \gamma) \in \mathbb{R} \times (-1, 1)$ which we consider here, there is a unique pure ground state for $(\lambda, \gamma) \in \mathcal{H}$ and two pure ground states for $(\lambda, \gamma) \notin \mathcal{H}$, see Figure 1. On the EFP observable (8) they coincide with the quasi-free state specified by the one-particle density matrix (26).

Let us discuss (27) in the different regimes of $\mathcal{H}$ from (24), see Figure 1. For this purpose, we restrict ourselves to the two cases $0 < \gamma < 1$ and $\gamma = 0$ (the discussion for negative γ is identical, see (18)). Moreover, we denote by $f(e^{i\xi})$ the right hand side of (27).
Let us first consider the anisotropic case $0 < \gamma < 1$. If the magnetic field $\lambda < -1$, we have $1/2 < f(e^{i\xi}) < 1$ for all $\xi \in [0, 2\pi)$, whereas $1/2 < f(e^{i\xi}) < 1$ for all $\xi \in [0, 2\pi) \setminus \{0, \pi\}$ and $f(1) = 1$, $f(-1) = 1/2$ if $\lambda = -1$. Moreover, $0 < f(e^{i\xi}) < 1$ for all $\xi \in [0, 2\pi)$ if $-1 < \lambda < 1$. Analogously, if $1 < \lambda$, we have $0 < f(e^{i\xi}) < 1/2$ for all $\xi \in [0, 2\pi)$, whereas $0 < f(e^{i\xi}) < 1/2$ for all $\xi \in [0, 2\pi) \setminus \{0, \pi\}$ and $f(1) = 1/2$, $f(-1) = 0$ if $\lambda = 1$. Hence, in the case of nonvanishing anisotropy γ, the assumption of Theorem 4 is satisfied,

$$\mathfrak{L}(\mathfrak{S}) = 2\pi \quad \text{if} \quad 0 < |\gamma| < 1.$$

Remark 13 In [16, 1], the bound on the decay rate in the ground state has been computed using theorems of Szegö and Fisher-Hartwig, and the Basor-Tracy conjecture (and some extension), see [12, 11]. If $0 < |\gamma| < 1$, it is valid both in the noncritical and in the critical regime. Again, our bound from Theorem 4 turns out to be exact.

Next, we consider the isotropic case $\gamma = 0$. If $\lambda \leq -1$, we have $f(e^{i\xi}) = 1$ for all $\xi \in [0, 2\pi)$, whereas $f(e^{i\xi}) \in \{0, 1\}$ for all $\xi \in [0, 2\pi)$ if $-1 < \lambda < 1$. Analogously, $f(e^{i\xi}) = 0$ for all $\xi \in [0, 2\pi)$ if $\lambda \geq 1$. Therefore, in the isotropic case, Theorem 4 is not applicable because

$$\mathfrak{L}(\mathfrak{S}) = 0 \quad \text{if} \quad \gamma = 0.$$

Remark 14 In [16], using a theorem of Widom (see [20]), the EFP for $\gamma = 0$ is shown to decay like a Gaussian for $|\lambda| < 1$ (with a power-law and a numerical prefactor; the latter diverges if the magnetic field approaches the critical value $\lambda = -1$). On the other hand, using (14), (13), and (26), we have $P(n) = 0$ if $\lambda \geq 1$ and $P(n) = 1$ if $\lambda \leq -1$ for all n (note that the ground state is completely polarized in the direction of the positive and negative 3-axis, respectively).

Example 4 *Decay in the chaotic state*

In the chaotic ($\equiv$ central) state at infinite temperature, i.e. for $\delta = \beta = 0$, we get from (21) and (22),

$$s(e^{i\xi}) = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

and hence (compare with (25)),

$$|\det[s(e^{i\xi}) - \Pi]| = \frac{1}{4}.$$

Remark 15 Our bound from Theorem 4 coincides with the exact rate obtained in the high temperature limit in [16].

Remark 16 The reason for the use of the Avram-Parter theorem (32) lies in the fact that the symbol a is block and, in general, not sufficiently regular. The exactness of our bounds in the cases where the symbol can be reduced to a scalar one suggests the bounds to be exact in general. This point remains to be studied in more detail.

A Toeplitz operators

Toeplitz operators [11, p.185]
The space ℓ^2_N of all $\mathbb{C}^N$-valued sequences $f = \{f_i\}_{i=1}^\infty$, $f_i \in \mathbb{C}^N$, $N \in \mathbb{N}$, is defined by

$$\ell^2_N = \{f : \mathbb{N} \to \mathbb{C}^N \mid \|f\| < \infty\}, \quad \|f\| = \left(\sum_{i=1}^\infty \|f_i\|^2_{\mathbb{C}^N}\right)^{1/2}, \tag{28}$$

where $\|\cdot\|_{\mathbb{C}^N}$ denotes the Euclidean norm on $\mathbb{C}^N$ (we write $\ell^2 \equiv \ell^2_1$). 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 $a \in L^\infty_{N\times N}$, where

$$L^\infty_{N\times N} = \{\phi : \mathbb{T} \to \mathbb{C}^{N\times N} \mid \phi_{ij} \in L^\infty(\mathbb{T}), i, j = 1, ..., N\}, \tag{29}$$

and $\mathbb{T} = \{t \in \mathbb{C} \mid |t| = 1\}$ (this is Toeplitz' theorem from which these operators got their name, see [11, p.186]). In this case, we write the Toeplitz operator as

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

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 of the form

$$P_n(\{x_1, ..., x_n, x_{n+1}, ...\}) = \{x_1, ..., x_n, 0, 0, ...\}. \tag{30}$$

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

$$T_n[a] = P_n T[a] P_n|_{\operatorname{ran} P_n},$$

where ran$A$ denotes the range of the operator A.

Norm of Toeplitz operators [11, p.186]
The norm of a Toeplitz operator is related to its symbol by

$$\|T[a]\| = \|a\|_\infty, \tag{31}$$

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 $a \in L^\infty_{N\times N}$. From [12, p.101],

$$\|a\|_\infty = \operatorname*{ess\,sup}_{t\in\mathbb{T}} \|a(t)\|_{\mathcal{L}(\mathbb{C}^N)},$$

where $\|\cdot\|_{\mathcal{L}(\mathbb{C}^N)}$ is the operator norm induced by the Euclidean norm on $\mathbb{C}^N$.

Avram-Parter theorem [11, p.203]
Let $t_1^{(n)}, ..., t_{Nn}^{(n)}$ be the singular values of the truncated Toeplitz operator $T_n[a]$ with block symbol $a \in L^\infty_{N\times N}$, and let g be a continuous function with compact support, $g \in C_0(\mathbb{R})$. Then, we have

$$\lim_{n\to\infty} \frac{1}{Nn} \sum_{j=1}^{Nn} g((t_j^{(n)})^2) = \frac{1}{N} \int_0^{2\pi} \frac{d\xi}{2\pi} \operatorname{tr} g(a^*(e^{i\xi}) a(e^{i\xi})), \tag{32}$$

where $\operatorname{tr}A$ is the trace of the matrix A.

References

[1] Abanov G A and Franchini F 2003 Emptiness formation probability for the anisotropic XY spin chain in a magnetic field *Phys. Lett. A* **316** 342–9

[2] Araki H 1968 On the diagonalization of a bilinear Hamiltonian by a Bogoliubov transformation *Publ. RIMS Kyoto Univ.* **6** 385–442

[3] Araki H 1971 On quasifree states of CAR and Bogoliubov automorphisms *Publ. RIMS Kyoto Univ.* **6** 385–442

[4] Araki H 1984 On the XY-model on two-sided infinite chain *Publ. RIMS Kyoto Univ.* **20** 277–96

[5] Araki H and Matsui T 1985 Ground states of the XY-model *Commun. Math. Phys.* **101** 213–45

[6] Araki H and Ho T G 2000 Asymptotic time evolution of a partitioned infinite two-sided isotropic XY-chain *Proc. Steklov Inst. Math.* **228** 191–204

[7] Aschbacher W H, in preparation

[8] Aschbacher W H and Barbaroux J M 2006 On the decay of spin-spin correlations in quasi-free states, submitted

[9] Aschbacher W H and Barbaroux J M 2006 Out of equilibrium correlations in the XY chain *Lett. Math. Phys.* **77** 11–20

[10] Aschbacher W H and Pillet C A 2003 Non-equilibrium steady states of the XY chain *J. Stat. Phys.* **112** 1153–75

[11] Böttcher A and Silbermann B 1999 *Introduction to large truncated Toeplitz matrices* (New York: Springer)

[12] Böttcher A and Silbermann B 2006 *Analysis of Toeplitz operators* (Berlin: Springer)

[13] Bratteli O and Robinson D W *Operator algebras and quantum statistical mechanics 2* (Berlin: Springer)

[14] Castella H, Zotos X, and Prelovšek P. (1995) Integrability and ideal conductance at finite temperatures *Phys. Rev. Lett.* **74** 972–5

[15] Franchini F and Abanov A G 2005 Asymptotics of Toeplitz determinants and the emptiness formation probability for the XY spin chain *J. Phys. A: Math. Gen.* **38** 5069–95

[16] Shiroishi M, Takahashi M, and Nishiyama Y 2001 Emptiness formation probability for the one-dimensional isotropic XY model *J. Phys. Soc. Jap.* **70** 3535–43

[17] Sologubenko A V, Felder E, Giannò K, Ott H R, Vietkine A, and Revcolevschi A 2000 Thermal conductivity and specific heat of the linear chain cuprate Sr_2CuO_3: Evidence for the thermal transport via spinons *Phys. Rev. B* **62** R6108–11

[18] Sologubenko A V, Giannò K, Ott H R, Vietkine A, and Revcolevschi A 2001 Heat transport by lattice and spin excitations in the spin-chain compounds $SrCuO_2$ and Sr_2CuO_3 *Phys. Rev. B* **64** 054412-1–11

[19] Vein R and Dale P 1999 *Determinants and their applications in mathematical physics* Applied Mathematical Sciences, Vol. 134 (New York: Springer)

[20] Widom H 1971 The strong Szegö limit theorem for circular arcs *Ind. Univ. Math. J.* **21** 277–83

[21] Zotos X 1999 Finite temperature Drude weight of the one-dimensional spin-$1/2$ Heisenberg model *Phys. Rev. Lett.* **82** 1764–7

[22] Zotos X, Naef F, and Prelovšek P 1997 Transport and conservation laws *Phys. Rev. B* **55** 11029–32