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# A REMARK ON THE SUBLEADING ORDER IN THE ASYMPTOTICS OF THE NONEQUILIBRIUM EMPTINESS FORMATION PROBABILITY

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We study the asymptotic behavior of the emptiness formation probability for large spin strings in a translation invariant quasifree nonequilibrium steady state of the isotropic XY chain. Besides the overall exponential decay, we prove that, out of equilibrium, the exponent of the subleading power law contribution to the asymptotics is nonvanishing and strictly positive due to the singularities in the density of the steady state.

*Keywords*: Nonequilibrium steady state; emptiness formation probability; Toeplitz theory.

AMS Subject Classification: 46L60, 47B35, 82C10, 82C23

## 1. Introduction

In this note, we propose to enlarge upon the study started in Aschbacher [6] of the asymptotic behavior of a special and important correlator, the so-called emptiness formation probability (EFP). Written down in the framework of a spin system over the two-sided discrete line, the EFP observable is given by

$$A_n = \prod_{i=1}^{n} p_i, \tag{1.1}$$

where $p_i$ denotes the projection $p := (1 - \sigma_3)/2$ at site $i$ onto the spin down configuration of the spin $\sigma_3$ in the 3-direction. For a given state $\omega$ of the spin system, the probability that a ferromagnetic string of length $n$ is formed in this state is thus expressed by

$$\mathrm{P}(n) = \omega(A_n). \tag{1.2}$$

Due to the existence of the Jordan–Wigner transformation which maps, in a certain sense, spins onto fermions, the EFP has been heavily studied for states of the XY chain whose formal Hamiltonian is given in Remark 2.1 below. As a matter of fact, this model becomes a gas of independent fermions under the Jordan–Wigner transformation, and it is thus ideally suited for rigorous analysis.[a]

The large $n$ behavior of the EFP in the XY chain has already been analyzed for the cases where the state $\omega$ is a ground state or a thermal equilibrium state at positive temperature. In both cases, the EFP can be written as the determinant of the section of a Toeplitz operator with scalar symbol. Since the higher order asymptotics of a Toeplitz determinant is highly sensitive to the regularity of the symbol of the Toeplitz operator, the asymptotic behavior of the ground state EFP is qualitatively different in the so-called critical and noncritical regimes corresponding to certain values of the anisotropy and the exterior magnetic field of the XY chain.[b] It has been found in Shiroishi *et al.* [16] that the EFP decays like a Gaussian in one of the critical regimes.[c] In a second critical regime and in all noncritical regimes, the EFP decays exponentially.[d] These results have been derived by using well-known theorems of Szegő, Widom, and Fisher-Hartwig, and the yet unproven Basor–Tracy conjecture and some of its extensions, see Widom [19] and Böttcher and Silbermann [11, 12]. On the other hand, in thermal equilibrium at positive temperature, the EFP can again be shown to decay exponentially by using a theorem of Szegő, see for example Shiroishi *et al.* [16] and Franchini and Abanov [13].

In contrast, for the case where $\omega$ is the nonequilibrium steady state (NESS) constructed in Aschbacher and Pillet [9],[e] the EFP can still be written as a Toeplitz determinant, but now, the symbol is, in general, no longer scalar. Due to the lack of control of higher order determinant asymptotics in Toeplitz theory with nontrivial irregular block symbols, we started off by studying bounds on the leading asymptotic order for a class of general block Toeplitz determinants in Aschbacher [6]. It turned out that suitable basic spectral information on the density of the state is sufficient to derive a bound on the rate of the exponential decay of the EFP in general translation invariant fermionic quasifree states. This bound proved to be exact not only for the decay rates of the EFP in the ground states and the equilibrium states at positive temperature treated in Abanov and Franchini [1, 13] and Shiroishi *et al.* [16], but it will also do so for the nonequilibrium situation treated here exhibiting the so-called left mover-right mover structure already found in Aschbacher [7] and Aschbacher and Barbaroux [8] for nonequilibrium expectations of different correlation observables.[f] Hence, given this exponential decay in

[a] Low-dimensional magnetic systems are also heavily studied experimentally, see for example Sologubenko *et al.* [17].

[b] I.e., in (2.13) below, the parameters $\gamma$ and $\lambda$, respectively.

[c] With some additional explicit numerical prefactor and some power law prefactor, see Shiroishi *et al.* [16] and references therein.

[d] In contrast to the noncritical 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 Abanov and Franchini [1, 13].

[e] And in Araki and Ho [5] for $\gamma = \lambda = 0$.

[f] This has already been noted in Aschbacher [6].

leading order which parallels qualitatively the behavior in thermal equilibrium at positive temperature, one may wonder whether there is some characteristic signature of the nonequilibrium left at some lower order of the EFP asymptotics. It turns out, and this is the main result of this note, that, in contradistinction to the leading order contribution, the subleading power law contribution to the large $n$ asymptotics of the EFP in Fisher–Hartwig theory is sensitive to the singularity of the symbol of the underlying Toeplitz operator, and it has a strictly positive exponent if and only if the system is truly out of equilibrium. This may be interpreted as the manifestation, in subleading order, of the long-range nature of the underlying formal effective Hamiltonian of the NESS.[g] This connection is not made precise here, though, but it is left to be studied in greater detail elsewhere.

Section 2 contains the setting and Sec. 3 the main assertion. The reader not familiar with quasifree states on CAR algebras and/or with Toeplitz theory may consult the Appendix where definitions and basic facts are collected.

## 2. Nonequilibrium Setting

In this section, we shortly summarize the setting for the system out of equilibrium used in Aschbacher and Pillet [9]. In contradistinction to the presentation there, we will skip the formulation of the two-sided XY chain as a spin system and rather focus directly on the underlying $C^*$-dynamical system structure in terms of Bogoliubov automorphisms on a selfdual CAR algebra as introduced by Araki [4].[h]

For some $N \in \{0\} \cup \mathbb{N}$, the nonequilibrium configuration is set up by cutting the finite piece

$$\mathbb{Z}_{\mathcal{S}} := \{x \in \mathbb{Z} \,|\, -N \leq x \leq N\} \tag{2.1}$$

out of the two-sided discrete line $\mathbb{Z}$. This piece will play the role of the confined sample, whereas the remaining parts,

$$\mathbb{Z}_L := \{x \in \mathbb{Z} \,|\, x \leq -(N+1)\}, \tag{2.2}$$

$$\mathbb{Z}_R := \{x \in \mathbb{Z} \,|\, x \geq N+1\}, \tag{2.3}$$

will act as infinitely extended thermal reservoirs at different temperatures to which the sample will be suitably coupled.

We first specify the observables contained in the system to be considered.

[g]See Remark 3 in Aschbacher and Pillet [9]. This effective Hamiltonian is to be understood on a formal level only. It has been shown by Matsui and Ogata [14] that there exists no dynamics on the Pauli spin algebra w.r.t. which this NESS is a KMS state.
[h]For an introduction to the algebraic approach to open quantum systems, see also for example Aschbacher *et al.* [10].

**Definition 2.1.** (Observables) Let $\mathfrak{F}(\mathfrak{h})$ denote the fermionic Fock space built over the one-particle Hilbert space of wave functions on the discrete line,

$$\mathfrak{h} := \ell^2(\mathbb{Z}). \tag{2.4}$$

With the help of the usual creation and annihilation operators $a^*(f), a(f) \in \mathcal{L}(\mathfrak{F}(\mathfrak{h}))$ for any $f \in \mathfrak{h}$,[i] the complex linear mapping $B : \mathfrak{h}^{\oplus 2} \to \mathcal{L}(\mathfrak{F}(\mathfrak{h}))$ is defined, for $F := [f_1, f_2] \in \mathfrak{h}^{\oplus 2}$, by

$$B(F) := a^*(f_1) + a(\bar{f}_2). \tag{2.5}$$

Moreover, the antiunitary involution $J : \mathfrak{h}^{\oplus 2} \to \mathfrak{h}^{\oplus 2}$ is given, for all $f_1, f_2 \in \mathfrak{h}$, by

$$J[f_1, f_2] := [\bar{f}_2, \bar{f}_1]. \tag{2.6}$$

The observables are described by the selfdual CAR algebra over $\mathfrak{h}^{\oplus 2}$ with involution $J$ generated by the operators $B(F) \in \mathcal{L}(\mathfrak{F}(\mathfrak{h}))$ for all $F \in \mathfrak{h}^{\oplus 2}$. We denote this algebra by $\mathfrak{A} := \mathfrak{A}(\mathfrak{h}^{\oplus 2}, J)$.[j]

The time evolution is generated as follows.

**Definition 2.2.** (Dynamics) Let $\lambda \in \mathbb{R}$, and let $u \in \mathcal{L}(\mathfrak{h})$ be the translation operator defined by $(uf)(x) := f(x-1)$ for all $f \in \mathfrak{h}$ and all $x \in \mathbb{Z}$. The coupled and the decoupled one-particle Hamiltonians $h, h_0 \in \mathcal{L}(\mathfrak{h})$ are defined by

$$h := \mathrm{Re}(u) + \lambda, \tag{2.7}$$

$$h_0 := h - (v_L + v_R), \tag{2.8}$$

respectively, where the decoupling operators $v_L, v_R \in \mathcal{L}^0(\mathfrak{h})$ have the form

$$v_L := \mathrm{Re}(u^{-(N+1)} p_0 u^N), \tag{2.9}$$

$$v_R := \mathrm{Re}(u^N p_0 u^{-(N+1)}), \tag{2.10}$$

and the projection $p_0 \in \mathcal{L}^0(\mathfrak{h})$ is given by $p_0 f := (\delta_0, f)\delta_0$ for all $f \in \mathfrak{h}$.[k] For all $t \in \mathbb{R}$, the coupled and the decoupled time evolutions are the Bogoliubov $*$-automorphisms $\tau^t, \tau_0^t \in \mathrm{Aut}(\mathfrak{A})$ defined on the generators $B(F) \in \mathfrak{A}$ with $F \in \mathfrak{h}^{\oplus 2}$ by

$$\tau^t(B(F)) := B(\mathrm{e}^{\mathrm{i}t(h \oplus -h)} F), \tag{2.11}$$

$$\tau_0^t(B(F)) := B(\mathrm{e}^{\mathrm{i}t(h_0 \oplus -h_0)} F). \tag{2.12}$$

[i] The bounded operators on the Hilbert space $\mathcal{H}$ are denoted by $\mathcal{L}(\mathcal{H})$.
[j] The concept of a selfdual CAR algebra has been introduced and developed by Araki [2,3]. Here, it is just a convenient way of working with the linear combination (2.5).
[k] We write $\mathcal{L}^0(\mathcal{H})$ for the finite rank operators on the Hilbert space $\mathcal{H}$. Moreover, $\delta_x \in \mathfrak{h}$ for $x \in \mathbb{Z}$ denotes the Kronecker function. Finally, for an operator $A \in \mathcal{L}(\mathcal{H})$, the real part is $\mathrm{Re}(A) := (A + A^*)/2$.

**Remark 2.1.** As mentioned above, this model has its origin in the XY spin chain whose formal Hamiltonian is given by

$$H = -\frac{1}{4}\sum_{x\in\mathbb{Z}}\{(1+\gamma)\,\sigma_1^{(x)}\sigma_1^{(x+1)} + (1-\gamma)\,\sigma_2^{(x)}\sigma_2^{(x+1)} + 2\lambda\,\sigma_3^{(x)}\}, \tag{2.13}$$

where $\gamma \in (-1,1)$ denotes the anisotropy, $\lambda \in \mathbb{R}$ the external magnetic field, and the Pauli basis of $\mathbb{C}^{2\times 2}$ reads

$$\sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{2.14}$$

The Hamiltonian $h$ from (2.7) corresponds to the isotropic XY chain, i.e. to the case where $\gamma = 0$.

The left and right reservoirs carry the inverse temperatures $\beta_L$ and $\beta_R$, respectively. *Pour fixer les idées*, we assume w.l.o.g. that they satisfy

$$0 < \beta_L \leq \beta_R < \infty. \tag{2.15}$$

We next specify the state in which the system is prepared initially. It consists of a KMS state at the corresponding temperature for each reservoir, and, w.l.o.g., of the chaotic state for the sample. For the definition of quasifree states, see Appendix A.

**Definition 2.3.** (Initial state) The initial state $\omega_0 \in \mathcal{Q}(\mathfrak{A})$ is the quasifree state specified by the density $S_0 \in \mathcal{L}(\mathfrak{h}^{\oplus 2})$ of the form

$$S_0 := s_{0,-} \oplus s_{0,+}, \tag{2.16}$$

where the operators $s_{0,\pm} \in \mathcal{L}(\mathfrak{h})$ are defined by

$$s_{0,\pm} := (1 + \mathrm{e}^{\pm k_0})^{-1}, \tag{2.17}$$

and $k_0 \in \mathcal{L}(\mathfrak{h} \simeq \mathfrak{h}_L \oplus \mathfrak{h}_{\mathcal{S}} \oplus \mathfrak{h}_R)$ is given by

$$k_0 := \beta_L h_L \oplus 0 \oplus \beta_R h_R. \tag{2.18}$$

Here, for $\alpha = L, \mathcal{S}, R$, we used the definitions $\mathfrak{h}_\alpha := \ell^2(\mathbb{Z}_\alpha)$ and $h_\alpha := i_\alpha^* h i_\alpha$, where $i_\alpha : \mathfrak{h}_\alpha \to \mathfrak{h}$ is the natural injection defined, for any $f \in \mathfrak{h}_\alpha$, by $i_\alpha(\{f(y)\}_{y\in\mathbb{Z}_\alpha})(x) := f(x)$ if $x \in \mathbb{Z}_\alpha$, and zero otherwise.

The following definition is due to Ruelle [15].

**Definition 2.4.** (NESS) A NESS associated with the $C^*$-dynamical system $(\mathfrak{A}, \tau)$ having the initial state $\omega_0 \in \mathcal{E}(\mathfrak{A})$ is a weak-$*$ limit point for $T \to \infty$ of the net

$$\left\{ \frac{1}{T}\int_0^T \mathrm{d}t\, \omega_0 \circ \tau^t \,\middle|\, T > 0 \right\}. \tag{2.19}$$

In the model specified by Definitions 2.1–2.3, we get the following NESS using the scattering approach of Ruelle [15].

**Theorem 2.1.** (XY NESS) *There exists a unique quasifree NESS $\omega \in \mathcal{Q}(\mathfrak{A})$ w.r.t. the initial state $\omega_0 \in \mathcal{Q}(\mathfrak{A})$ and the coupled dynamics $\tau^t \in \mathrm{Aut}(\mathfrak{A})$ whose density $S \in \mathcal{L}(\mathcal{H})$ reads*

$$S = s_- \oplus s_+, \tag{2.20}$$

*where the operators $\hat{s}_\pm \in \mathcal{L}(\hat{\mathfrak{h}})$ act in momentum space $\hat{\mathfrak{h}} := L^2(\mathbb{T})$ as multiplication by*

$$\hat{s}_\pm(\mathrm{e}^{\mathrm{i}k}) := \frac{1}{2}\,(1 \pm \varrho_\pm(\mathrm{e}^{\mathrm{i}k})), \tag{2.21}$$

*and the functions $\varrho_\pm : \mathbb{T} \to (-1,1)$ are defined by*

$$\varrho_\pm(\mathrm{e}^{\mathrm{i}k}) := \tanh\left[\frac{1}{2}(\beta \pm \mathrm{sign}(\sin k)\delta)(\lambda + \cos k)\right]. \tag{2.22}$$

*Here, we set $\beta := (\beta_R + \beta_L)/2$ and $\delta := (\beta_R - \beta_L)/2$, and the sign function $\mathrm{sign} : \mathbb{R} \to \{\pm 1\}$ is defined by $\mathrm{sign}(x) := 1$ if $x \geq 0$, and $\mathrm{sign}(x) := -1$ if $x < 0$.*

**Proof.** See Aschbacher and Pillet [9]. □

The main object of our study is the following.

**Definition 2.5.** (NESS EFP) Let $n \in \mathbb{N}$. The EFP observable $A_n \in \mathfrak{A}$ is defined by

$$A_n := \prod_{i=1}^{2n} B(F_i), \tag{2.23}$$

where, for all $i \in \mathbb{N}$, the form factors $F_i \in \mathfrak{h}^{\oplus 2}$ are given by

$$F_{2i-1} := u^i \oplus u^i\, G_1, \tag{2.24}$$

$$F_{2i} := u^i \oplus u^i\, G_2, \tag{2.25}$$

and the initial form factors $G_1, G_2 \in \mathfrak{h}^{\oplus 2}$ look like

$$G_1 := JG_2 := [0, \delta_0]. \tag{2.26}$$

Moreover, the expectation value $\mathrm{P} : \mathbb{N} \to [0,1]$ of the EFP observable $A_n \in \mathfrak{A}$ in the NESS $\omega \in \mathcal{E}(\mathfrak{A})$ is denoted by[1]

$$\mathrm{P}(n) := \omega(A_n). \tag{2.27}$$

[1]As for the name EFP, note that $A_n = \prod_{i=1}^n a_i a_i^*$, and that, for $B_n := \prod_{i=1}^n a_i$, we have

$$0 \leq \mathrm{P}(n) = \omega(B_n B_n^*) \leq \|B_n\|^2 \leq \prod_{i=1}^n \|\delta_i\|^2 = 1.$$

The next assertion states the main structural property of the EFP correlation function. For the basic facts of Toeplitz theory, see Appendix B.2.

**Proposition 2.1.** (EFP determinantal structure) *The NESS EFP* $\mathrm{P} : \mathbb{N} \to [0, 1]$ *is given by the determinant of the finite section of the Toeplitz operator* $T[\hat{s}_-] \in \mathcal{L}(\ell^2(\mathbb{N}))$,

$$\mathrm{P}(n) = \det(T_n[\hat{s}_-]). \tag{2.28}$$

**Proof.** Proceeding as in Aschbacher and Barbaroux [8], we have that, on one hand, the skew-symmetric EFP correlation matrix $\Omega_n \in \mathbb{R}^{2n\times 2n}$, defined, for $i$, $j = 1, \ldots, 2n$, by

$$\Omega_{n,ij} = \begin{cases} \omega(B(F_i)B(F_j)), & \text{if } i < j, \\ 0, & \text{if } i = j, \\ -\,\omega(B(F_j)B(F_i)), & \text{if } i > j, \end{cases} \tag{2.29}$$

where $F_i \in \mathfrak{h}^{\oplus 2}$ for $i \in \mathbb{N}$ are the form factors from Definition 2.5, relates to the EFP as

$$\mathrm{P}(n) = \mathrm{pf}(\Omega_n), \tag{2.30}$$

and, on the other hand, that it has the Toeplitz structure

$$\Omega_n = T_n[a_{\mathrm{P}}]. \tag{2.31}$$

Here, $a_{\mathrm{P}} \in L^\infty_{2\times 2}(\mathbb{T})$ is the block symbol of the Toeplitz operator $T[a_{\mathrm{P}}] \in \mathcal{L}(\ell^2_2(\mathbb{N}))$ which we computed in Aschbacher [6] to be of the form $a_{\mathrm{P}} = (\hat{s} - p)\sigma_1$, where $\hat{s} = \hat{s}_- \oplus \hat{s}_+$ is the density of the NESS $\omega \in \mathcal{Q}(\mathfrak{A})$ in momentum space and $p = (1 - \sigma_3)/2$. Theorem 2.1 then implies that, in the present case, the symbol has the form

$$a_{\mathrm{P}} = \begin{bmatrix} 0 & \hat{s}_- \\ \hat{s}_+ - 1 & 0 \end{bmatrix}. \tag{2.32}$$

Hence, there exists an $R \in O(2n)$ with $\det(R) = (-1)^{n(n-1)/2}$ s.t., using Lemma A.1, we can reduce the block Toeplitz Pfaffian to a scalar Toeplitz determinant,

$$\begin{aligned} \mathrm{P}(n) &= \mathrm{pf}(T_n[a_{\mathrm{P}}]) \\ &= (-1)^{\frac{n(n-1)}{2}}\, \mathrm{pf}\left(\begin{bmatrix} 0 & T_n[\hat{s}_-] \\ T_n[\hat{s}_+ - 1] & 0 \end{bmatrix}\right) \\ &= \det(T_n[\hat{s}_-]), \end{aligned} \tag{2.33}$$

where we used the fact that $T_n[\hat{s}_+ - 1] = -T_n[\hat{s}_-]^{\mathrm{t}}$.[m] This is the assertion. □

[m] $O(2n)$ stands for the orthogonal matrices in $\mathbb{R}^{2n\times 2n}$.

## 3. Subleading Order in the NESS EFP Asymptotics

Due to Proposition 2.1, the study of the large $n$ behavior of the EFP correlation function boils down to the analysis of a large truncated Toeplitz operator whose symbol is scalar and has the form given in Theorem 2.1,

$$\hat{s}_-(\mathrm{e}^{\mathrm{i}k}) = \frac{1}{2}\left(1 - \tanh\left[\frac{1}{2}(\beta - \mathrm{sign}(\sin k)\delta)(\lambda + \cos k)\right]\right), \tag{3.1}$$

see Fig. 1. In a true nonequilibrium situation, i.e. for $\delta > 0$, the R.H.S. of (3.1) is no longer continuous. Hence, as described in the introduction, we want to study the asymptotic behavior of the EFP NESS with the help of the so-called Fisher–Hartwig theory whose main content is summarized in Theorem B.2 of Appendix B.3. We first introduce the so-called pure jump symbols. For notation and definitions, see Appendix B.1.

**Definition 3.1.** (Pure jump) Let the argument function $\arg : \mathbb{C}\backslash\{0\} \to \mathbb{R}$ be defined by $z =: |z|\,\mathrm{e}^{\mathrm{i}\arg(z)}$ and $\arg(z) \in (-\pi, \pi]$ for all $z \in \mathbb{C}\backslash\{0\}$. For $\beta_0 \in \mathbb{C}$ and $t_0 \in \mathbb{T}$, the pure jump symbol $\varphi_{\beta_0,t_0} \in PC_0(\mathbb{T})$ is defined, for all $t \in \mathbb{T}$, by

$$\varphi_{\beta_0,t_0}(t) := \mathrm{e}^{\mathrm{i}\beta_0 \arg(-\frac{t}{t_0})}. \tag{3.2}$$

**Remark 3.1.** Note that $\varphi_{\beta_0,t_0} \in PC_0(\mathbb{T})$ has at most one jump discontinuity at the point $t_0$, namely

$$\varphi_{\beta_0,t_0}(t_0 \pm 0) = \mathrm{e}^{\mp\mathrm{i}\pi\beta_0}. \tag{3.3}$$

Moreover, the so-called jump phases are defined as follows.

**Definition 3.2.** (Jump phases) Let $a \in PC_0(\mathbb{T})$ with $\Lambda_a = \{t_j \in \mathbb{T} \,|\, j = 1, \ldots, m\}$, and let $a(t_j \pm 0) \neq 0$ for $j = 1, \ldots, m$. The numbers $\beta_j \in \mathbb{C}$ for $j = 1, \ldots, m$, called the pure jump phases, are defined by

$$\frac{a(t_j - 0)}{a(t_j + 0)} = \mathrm{e}^{2\pi\mathrm{i}\beta_j}. \tag{3.4}$$

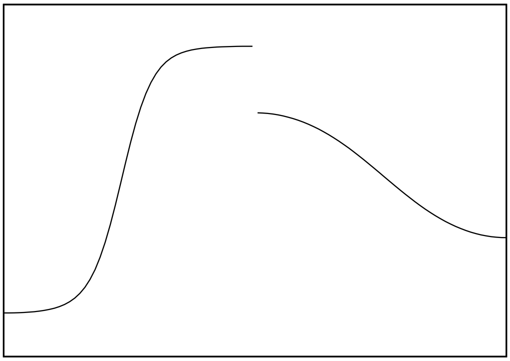

Fig. 1. The symbol $\hat{s}_-(\mathrm{e}^{\mathrm{i}k})$ with $k \in (-\pi, \pi]$ for $\beta = \frac{3}{2}$, $\delta = 1$, and $\lambda = \frac{1}{10}$.

Next, we define a regularized symbol which will be extracted from $\hat{s}_-$ below.

**Definition 3.3.** (Regularized symbol) Let $t_1 := 1$ and $t_2 := -1$. The regularized symbol $b_{\mathrm{P}} \in C(\mathbb{T})$ is defined by

$$b_{\mathrm{P}}(\mathrm{e}^{\mathrm{i}k}) := \left(\frac{\tau_L(t_1)}{\tau_R(t_1)}\frac{\tau_R(t_2)}{\tau_L(t_2)}\right)^{\frac{k}{2\pi}} \begin{cases} \sqrt{\frac{\tau_R(t_1)}{\tau_L(t_1)}}\,\tau_L(\mathrm{e}^{\mathrm{i}k}), & \text{if} \quad 0 \le k \le \pi, \\ \sqrt{\frac{\tau_L(t_1)}{\tau_R(t_1)}}\,\tau_R(\mathrm{e}^{\mathrm{i}k}), & \text{if} \quad -\pi < k < 0, \end{cases} \tag{3.5}$$

where, for $\alpha = L, R$, the function $\tau_\alpha : \mathbb{T} \to (0,1)$ has the form

$$\tau_\alpha(\mathrm{e}^{\mathrm{i}k}) := \frac{1}{2}\left(1 - \tanh\left[\frac{1}{2}\beta_\alpha(\lambda + \cos k)\right]\right), \tag{3.6}$$

see Fig. 2.

Using the pure jump phases and the regularized symbol, we can recast $\hat{s}_-$ into the following form.

**Lemma 3.1.** (Restricted Fisher–Hartwig form) *The NESS EFP symbol* $\hat{s}_- \in L^\infty(\mathbb{T})$ *has the following properties.*

(a) $\hat{s}_- \in PC_0(\mathbb{T})$,
(b) $\Lambda_{\hat{s}_-} = \{t_1, t_2\}$,
(c) *the jump phases of* $\hat{s}_-$ *at the points* $t_1$ *and* $t_2$ *are given by*

$$\beta_1 = -\frac{\mathrm{i}}{2\pi}\log\left(\frac{\tau_R(t_1)}{\tau_L(t_1)}\right), \tag{3.7}$$

$$\beta_2 = -\frac{\mathrm{i}}{2\pi}\log\left(\frac{\tau_L(t_2)}{\tau_R(t_2)}\right). \tag{3.8}$$

(d) *The symbol* $\hat{s}_- \in L^\infty(\mathbb{T})$ *can be written as*

$$\hat{s}_- = b_{\mathrm{P}}\varphi_{\beta_1,t_1}\varphi_{\beta_2,t_2}. \tag{3.9}$$

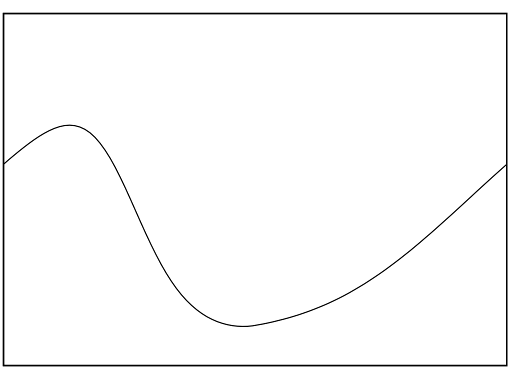

Fig. 2. The regularized symbol $b_{\mathrm{P}}(\mathrm{e}^{\mathrm{i}k})$ with $k \in (-\pi, \pi]$ for $\beta = \frac{3}{2}, \delta = 1$, and $\lambda = \frac{1}{10}$.

**Proof.** The assertions (a) and (b) immediately follow from the form of the symbol $\hat{s}_- \in L^\infty(\mathbb{T})$ given in (3.1). Moreover, using the choice

$$\beta_j = \frac{1}{2\pi}\,\arg\left(\frac{\hat{s}_-(t_j-0)}{\hat{s}_-(t_j+0)}\right) - \frac{\mathrm{i}}{2\pi}\,\log\left(\frac{\hat{s}_-(t_j-0)}{\hat{s}_-(t_j+0)}\right), \tag{3.10}$$

where the argument function is given in Definition 3.1, we get the pure jump phases (3.7) and (3.8) in assertion (c). As for assertion (d), writing, for $k \in (-\pi, \pi]$,

$$\varphi_{\beta_1,t_1}(\mathrm{e}^{\mathrm{i}k}) = \left(\frac{\tau_R(t_1)}{\tau_L(t_1)}\right)^{\frac{k+\operatorname{sign}(-k)\pi}{2\pi}}, \tag{3.11}$$

$$\varphi_{\beta_2,t_2}(\mathrm{e}^{\mathrm{i}k}) = \left(\frac{\tau_L(t_2)}{\tau_R(t_2)}\right)^{\frac{k}{2\pi}}, \tag{3.12}$$

with the sign function defined after (2.22), we get equality (3.9) in $L^\infty(\mathbb{T})$ involving the regularized symbol $b_{\mathrm{P}} \in C(\mathbb{T})$. □

In order to be able to apply the Fisher–Hartwig theory to the symbol $\hat{s}_-$, we have to make sure that the regularized symbol $b_{\mathrm{P}} \in C(\mathbb{T})$ is indeed sufficiently regular.

**Lemma 3.2.** (Fisher–Hartwig regularity) *The regularized symbol $b_{\mathrm{P}} \in C(\mathbb{T})$ has the following properties.*

(a) $b_{\mathrm{P}}(t) \neq 0$ *for all* $t \in \mathbb{T}$,
(b) $\operatorname{ind}(b_{\mathrm{P}}) = 0$,
(c) $b_{\mathrm{P}} \in B_1^1(\mathbb{T})$.

**Proof.** It follows from (3.5) that $b_{\mathrm{P}}(t) > 0$ for all $t \in \mathbb{T}$ which implies assertions (a) and (b). As for assertion (c), we use the fact given in Lemma C.1 (b) of Appendix B.3 that $b_{\mathrm{P}} \in C^1(\mathbb{T})$. This allows us to bound the integrand in (B.6) in Definition B.2 of the Besov space $B_1^1(\mathbb{T})$ as

$$\begin{aligned}\int_{-\pi}^{\pi}\frac{\mathrm{d}k}{k^2}\,\|\Delta_k^2 b_{\mathrm{P}}\|_{L^1(\mathbb{T})} &= \int_{-\pi}^{\pi}\frac{\mathrm{d}k}{k^2}\int_{-\pi}^{\pi}\mathrm{d}\theta\,|b_{\mathrm{P}}(\mathrm{e}^{\mathrm{i}(\theta+k)}) - 2b_P(\mathrm{e}^{\mathrm{i}\theta}) + b_{\mathrm{P}}(\mathrm{e}^{\mathrm{i}(\theta-k)})|\\ &\le \int_{-\pi}^{\pi}\frac{\mathrm{d}k}{|k|}\int_{-\pi}^{\pi}\mathrm{d}\theta\int_0^1\mathrm{d}t\,|b_{\mathrm{P}}'(\mathrm{e}^{\mathrm{i}(\theta+tk)}) - b_{\mathrm{P}}'(\mathrm{e}^{\mathrm{i}(\theta-tk)})|.\end{aligned} \tag{3.13}$$

Since, due to Lemma C.1 (a)–(c), $b_{\mathrm{P}}'$ is continuous and differentiable at all but finitely many points having a bounded derivative $\|b_{\mathrm{P}}''\|_{L^\infty(\mathbb{T})} < \infty$, we have $b_{\mathrm{P}}' \in AC(\mathbb{T})$, and, thus, it follows from the fundamental theorem of calculus that $b_{\mathrm{P}}' \in \operatorname{Lip}(\mathbb{T})$ with Lipschitz constant $\|b_{\mathrm{P}}''\|_{L^\infty(\mathbb{T})}$. Using the Lipschitz continuity on the R.H.S. of (3.13), we get

$$\int_{-\pi}^{\pi}\frac{\mathrm{d}k}{k^2}\,\|\Delta_k^2 b_{\mathrm{P}}\|_{L^1(\mathbb{T})} \le 4\pi^2\|b_{\mathrm{P}}''\|_{L^\infty(\mathbb{T})} < \infty. \tag{3.14}$$

Hence, we arrive at assertion (c). □

We are now ready to formulate the main result of this note.

**Theorem 3.1.** (NESS EFP asymptotics) *For $n \to \infty$, the NESS EFP behaves asymptotically as*

$$\mathrm{P}(n) \sim G(b_{\mathrm{P}})^n n^{Q_{\mathrm{P}}} F(\hat{s}_-), \tag{3.15}$$

*where the base of the exponential factor is given by*

$$G(b_{\mathrm{P}}) = \exp\left(\frac{1}{2}\sum_{\alpha=L,R}\int_{-\pi}^{\pi}\frac{\mathrm{d}k}{2\pi}\ \log(\tau_\alpha(\mathrm{e}^{\mathrm{i}k}))\right), \tag{3.16}$$

*satisfying $0 < G(b_{\mathrm{P}}) < 1$ for all inverse temperatures in the range $0 < \beta_L \leq \beta_R < \infty$. Furthermore, the exponent of the power law factor has the form*

$$Q_{\mathrm{P}} = \frac{1}{4\pi^2}\sum_{j=1,2}\left(\log\left(\frac{\tau_R(t_j)}{\tau_L(t_j)}\right)\right)^2. \tag{3.17}$$

*Thus, $Q_{\mathrm{P}} > 0$ if and only if $\beta_L \neq \beta_R$.*

**Proof.** Due to (3.9) of Lemma 3.1, the nonequilibrium symbol $\hat{s}_-$ has the form $\hat{s}_- = b_{\mathrm{P}}\varphi_{\beta_1,t_1}\varphi_{\beta_2,t_2}$, where $t_1 \neq t_2$ and, w.r.t. the form (B.13) of the restricted Fisher–Hartwig symbol, we have $\alpha_1 = \alpha_2 = 0$ and $\mathrm{Re}(\beta_1) = \mathrm{Re}(\beta_2) = 0$ from (3.7) and (3.8) in Lemma 3.1. Hence, assumptions (a) and (b) of Theorem B.2 from Appendix B.3 are satisfied. Moreover, due to Lemma 3.2, assumptions (c)–(d) of Theorem B.2 are also satisfied by the regularized symbol. Then, (3.15) follows from (B.14) in Theorem B.2, and it remains to derive the exponential, the power law, and the constant factors in (3.15) with the help of (B.15)–(B.17). As for $G(b_{\mathrm{P}})$, we get (3.16) from (B.15) and (3.5) in Definition 3.3. Moreover, substituting (3.7) and (3.8) into (B.16), we find (3.17). Finally, using (B.17), the last factor on the R.H.S. of (3.15) has the form

$$F(\hat{s}_-) = E(b_{\mathrm{P}})\,2^{2\beta_1\beta_2}\prod_{j=1,2}\left(\frac{b_{\mathrm{P},+}(t_j)}{b_{\mathrm{P},-}(t_j)}\right)^{\beta_j}\prod_{j=1,2}\mathrm{G}(1+\beta_j)\mathrm{G}(1-\beta_j), \tag{3.18}$$

where $E(b_{\mathrm{P}})$, $b_{\mathrm{P},\pm}(t_j)$, and $\mathrm{G}(1 \pm \beta_j)$ are given in (B.18), (B.19) and (B.21), respectively. □

**Remark 3.2.** In Aschbacher [6], we derived a bound on the decay rate of the exponential decay for the NESS EFP in the more general anisotropic XY chain. As noted there and discussed in the present introduction, Theorem 3.1 yields that this bound is exact for the special isotropic case at hand.[n]

[n] This can also be seen by directly using Szegő's first limit theorem, see for example Böttcher and Silbermann [11, p. 139].

## Appendix A. Fermionic Quasifree States

Let $\mathfrak{A}$ be the selfdual CAR algebra from Definition 2.1. We denote by $\mathcal{E}(\mathfrak{A})$ the set of states on the $C^*$ algebra $\mathfrak{A}$.[o]

**Definition A.1.** (Density) The density of a state $\omega \in \mathcal{E}(\mathfrak{A})$ is defined to be the operator $S \in \mathcal{L}(\mathfrak{h}^{\oplus 2})$ with $0 \leq S^* = S \leq 1$ and $JSJ = 1 - S$ satisfying, for all $F, G \in \mathfrak{h}^{\oplus 2}$,

$$\omega(B^*(F)B(G)) = (F, SG). \tag{A.1}$$

A special class of states are the important fermionic quasifree states.

**Definition A.2.** (Quasifree state) A state $\omega \in \mathcal{E}(\mathfrak{A})$ is called quasifree if it vanishes on the odd polynomials in the generators, and if it is a Pfaffian on the even polynomials in the generators, i.e. if, for all $F_1, \ldots, F_{2n} \in \mathfrak{h}^{\oplus 2}$ and for any $n \in \mathbb{N}$, we have

$$\omega(B(F_1) \cdots B(F_{2n})) = \mathrm{pf}(\Omega_n), \tag{A.2}$$

where the skew-symmetric matrix $\Omega_n \in \mathbb{C}_{ss}^{2n \times 2n}$ is defined, for $i, j = 1, \ldots, 2n$, by

$$\Omega_{n,ij} := \begin{cases} \omega(B(F_i)B(F_j)), & \text{if } i < j, \\ 0, & \text{if } i = j, \\ -\omega(B(F_j)B(F_i)), & \text{if } i > j. \end{cases} \tag{A.3}$$

Here, the Pfaffian $\mathrm{pf} : \mathbb{C}_{ss}^{2n \times 2n} \to \mathbb{C}$ is defined, on all skew-symmetric matrices $A \in \mathbb{C}_{ss}^{2n \times 2n} := \{A \in \mathbb{C}^{2n \times 2n} \mid A^{\mathrm{t}} = -A\}$,[p] by

$$\mathrm{pf}(A) := \sum_{\pi} \mathrm{sign}(\pi) \prod_{j=1}^{n} A_{\pi(2j-1),\pi(2j)}, \tag{A.4}$$

where the sum is running over all pairings of the set $\{1, 2, \ldots, 2n\}$, i.e. over all the $(2n)!/(2^n n!)$ permutations $\pi$ in the permutation group of $2n$ elements which satisfy $\pi(2j-1) < \pi(2j+1)$ and $\pi(2j-1) < \pi(2j)$, see Fig. 3. The set of quasifree states is denoted by $\mathcal{Q}(\mathfrak{A})$.

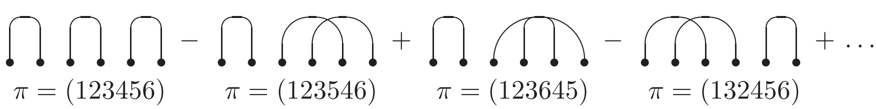


Fig. 3. Some of the pairings for $n = 3$. The total number of intersections $I$ relates to the signature as $\mathrm{sign}(\pi) = (-1)^I$.

[o] I.e. the normalized positive linear functionals on $\mathfrak{A}$.
[p] $A^{\mathrm{t}}$ is the transposition of the matrix $A \in \mathbb{C}^{n \times n}$.

The following lemma has been used in Sec. 2.

**Lemma A.1.** (Pfaffian) *The Pfaffian has the following properties.*

(a) *Let* $X, Y \in \mathbb{C}^{2n\times 2n}$ *with* $Y^{\mathrm{t}} = -Y$. *Then,*

$$\mathrm{pf}(XYX^{\mathrm{t}}) = \det(X)\,\mathrm{pf}(Y). \tag{A.5}$$

(b) *Let* $X \in \mathbb{C}^{n\times n}$. *Then,*

$$\mathrm{pf}\left(\begin{bmatrix} 0 & X \\ -X^{\mathrm{t}} & 0 \end{bmatrix}\right) = (-1)^{\frac{n(n-1)}{2}} \det(X). \tag{A.6}$$

**Proof.** See, for example, Stembridge [18]. □

## Appendix B. Toeplitz Theory

The material of this section is taken from Böttcher and Silbermann [11, 12].

### B.1. *Function classes*

Let $\mathbb{T} := \{t \in \mathbb{C} \,|\, |t| = 1\}$ stand for the unit circle. We denote by $C(\mathbb{T})$ the continuous functions, by $C^m(\mathbb{T})$ the $m$ times continuously differentiable functions, and by $L^p(\mathbb{T})$ with $1 \leq p \leq \infty$ the usual Lebesgue spaces. Moreover, $AC(\mathbb{T})$ and $\mathrm{Lip}(\mathbb{T})$ stand for the absolutely continuous and the Lipschitz continuous functions on $\mathbb{T}$. Finally, we need the following function class.

**Definition B.1.** (Piecewise continuous) The set of piecewise continuous functions is defined by

$$PC(\mathbb{T}) := \left\{ a \in L^\infty(\mathbb{T}) \,\middle|\, \text{The limits } \lim_{\varepsilon\to 0^+} a(\mathrm{e}^{\mathrm{i}(k\pm\varepsilon)}) \text{ exist for all } k \in (-\pi, \pi] \right\}. \tag{B.1}$$

For $a \in PC(\mathbb{T})$ and any $t \in \mathbb{T}$ of the form $t = \mathrm{e}^{\mathrm{i}k}$ with $k \in (-\pi, \pi]$, we use the notation

$$a(t \pm 0) := \lim_{\varepsilon\to 0^+} a(\mathrm{e}^{\mathrm{i}(k\pm\varepsilon)}). \tag{B.2}$$

Moreover, the set of jumps of $a \in PC(\mathbb{T})$ is defined by

$$\Lambda_a := \{t \in \mathbb{T} \,|\, a(t-0) \neq a(t+0)\}. \tag{B.3}$$

Finally, the set of piecewise continuous functions with finitely many jumps is defined by

$$PC_0(\mathbb{T}) := \{a \in PC(\mathbb{T}) \,|\, \mathrm{card}(\Lambda_a) < \infty\}. \tag{B.4}$$

In order to be able to make use of the Fisher–Hartwig theory from Appendix B.3, we also need to introduce the following function class.

**Definition B.2.** (Besov space) Let $1 \leq p < \infty$ and $k \in (-\pi, \pi]$. The operator $\Delta_k : L^p(\mathbb{T}) \to L^p(\mathbb{T})$ is defined, on all $f \in L^p(\mathbb{T})$, and for all $\theta \in (-\pi, \pi]$, by

$$(\Delta_k f)(\mathrm{e}^{\mathrm{i}\theta}) := f(\mathrm{e}^{\mathrm{i}(\theta+k)}) - f(\mathrm{e}^{\mathrm{i}\theta}). \tag{B.5}$$

Moreover, for any $n \in \mathbb{N}$, we recursively set $\Delta_k^n := \Delta_k \Delta_k^{n-1}$. For $\alpha > 0$ and $1 \leq p < \infty$, the Besov class is defined by

$$B_p^\alpha(\mathbb{T}) := \left\{ f \in L^p(\mathbb{T}) \,\middle|\, \int_{-\pi}^{\pi} \mathrm{d}k \; |k|^{-(1+\alpha p)} \, \|\Delta_k^n f\|_{L^p(\mathbb{T})}^p < \infty \right\}, \tag{B.6}$$

where $n \in \mathbb{N}$ is s.t. $n > \alpha$.[q]

Finally, we need the following definition.

**Definition B.3.** (Index) Let $a \in C(\mathbb{T})$ with $a(t) \neq 0$ for all $t \in \mathbb{T}$, and let $c : \mathbb{T} \to \mathbb{R}$ with $c \in C(\mathbb{T}\backslash\{1\})$ be s.t. $a = |a| \, \mathrm{e}^{\mathrm{i}c}$. The index (or winding number) of $a$ is defined by

$$\mathrm{ind}(a) := \frac{c(1-0) - c(1+0)}{2\pi}. \tag{B.7}$$

## B.2. *Toeplitz operators*

For $M \in \mathbb{N}$, we denote by $\ell_M^2(\mathbb{N})$ the space of all square-summable $\mathbb{C}^M$-valued sequences.[r] Moreover, we set

$$L_{M\times M}^\infty(\mathbb{T}) := \{ f : \mathbb{T} \to \mathbb{C}^{M\times M} \mid f_{ij} \in L^\infty(\mathbb{T}) \text{ for all } i, j = 1, \ldots, M \}. \tag{B.8}$$

We then have the following classical result.

**Theorem B.1.** (Toeplitz) *Let $\{a_x\}_{x\in\mathbb{Z}} \subset \mathbb{C}^{M\times M}$. The linear operator $A$ : $\mathrm{dom}\,(A) \subseteq \ell_M^2(\mathbb{N}) \to \ell_M^2(\mathbb{N})$ defined on all $f \in \mathrm{dom}\,(A)$ with maximal domain $\mathrm{dom}\,(A)$ by*

$$Af := \left\{ \sum_{j=1}^{\infty} a_{i-j} \, f_j \right\}_{i=1}^{\infty}, \tag{B.9}$$

*is a bounded operator on $\ell_M^2(\mathbb{N})$ if and only if there exists an $a \in L_{M\times M}^\infty(\mathbb{T})$ s.t. for all $x \in \mathbb{Z}$, it holds*

$$a_x = \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \; a(\mathrm{e}^{\mathrm{i}k}) \, \mathrm{e}^{-\mathrm{i}kx}. \tag{B.10}$$

[q]Note that the definition does not depend on the choice of such an $n$.
[r]W.r.t. the Euclidean norm on $\mathbb{C}^M$.

**Proof.** See Böttcher and Silbermann [11, p. 186]. □

We then make the following definition.

**Definition B.4.** (Symbol) Under the assumptions of Theorem B.1, we write the Toeplitz operator as $T[a] := A \in \mathcal{L}(\ell^2_M(\mathbb{N}))$. It has the matrix form

$$T[a] = \begin{bmatrix} a_0 & a_{-1} & a_{-2} & \cdots \\ a_1 & a_0 & a_{-1} & \cdots \\ a_2 & a_1 & a_0 & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix}. \tag{B.11}$$

The function $a \in L^\infty_{M\times M}(\mathbb{T})$ is called the symbol of $T[a]$. If $M = 1$, the symbol $a \in L^\infty(\mathbb{T}) = L^\infty_{1\times 1}(\mathbb{T})$ and the Toeplitz operator $T[a]$ are called scalar, whereas for $M > 1$ they are called block.

Finally, the Toeplitz operators are truncated as follows.

**Definition B.5.** (Finite section) Let $n \in \mathbb{N}$. The projection $P_n \in \mathcal{L}(\ell^2_M(\mathbb{N}))$ is defined, on all $f := \{x_1, \ldots, x_n, x_{n+1}, \ldots\} \in \ell^2_M(\mathbb{N})$, by

$$P_n f = \{x_1, \ldots, x_n, 0, 0, \ldots\}. \tag{B.12}$$

Moreover, the truncated Toeplitz matrices $T_n[a] \in \mathbb{C}^{Mn\times Mn}$ are defined by

$$T_n[a] := P_n T[a] P_n \restriction_{\mathrm{ran}\,(P_n)}.$$

### B.3. *Fisher–Hartwig symbols*

The following theorem summarizes the main results on the asymptotic behavior of Toeplitz determinants with Fisher–Hartwig symbols.

**Theorem B.2.** (Fisher–Hartwig) *Let $a \in L^\infty(\mathbb{T})$ be a restricted Fisher–Hartwig symbol, i.e. for all $t \in \mathbb{T}$, the symbol has the form*

$$a(t) = b(t) \prod_{j=1}^{m} |t - t_j|^{2\alpha_j} \varphi_{\beta_j, t_j}(t), \tag{B.13}$$

*and it satisfies the following assumptions*:

(a) $t_1, \ldots, t_m \in \mathbb{T}$ *are pairwise distinct points*,
(b) $\alpha_j, \beta_j \in \mathbb{C}$ *with* $|\mathrm{Re}(\alpha_j)| < \frac{1}{2}$ *and* $|\mathrm{Re}(\beta_j)| < \frac{1}{2}$ *for all* $j = 1, \ldots, m$,
(c) $b \in L^\infty(\mathbb{T}) \cap B^1_1(\mathbb{T})$,
(d) $b(t) \neq 0$ *for all* $t \in \mathbb{T}$,
(e) $\mathrm{ind}(b) = 0$.

*Then, for $n \to \infty$, the Toeplitz determinant has the asymptotic approximation*

$$\det(T_n[a]) \sim G(b)^n n^Q F(a), \tag{B.14}$$

*where the exponential factor and the power law factor are determined by*

$$G(b) := \exp[(\log b)_0], \tag{B.15}$$

$$Q := \sum_{j=1}^{m} (\alpha_j^2 - \beta_j^2). \tag{B.16}$$

*Here, $f_x$ for $x \in \mathbb{Z}$ denotes the $x$th Fourier coefficient of the function $f \in L^1(\mathbb{T})$. Moreover, the constant $F(a)$ is given by*

$$\begin{aligned} F(a) &:= E(b) \prod_{j=1}^{m} b_+(t_j)^{-(\alpha_j-\beta_j)} b_-(t_j)^{-(\alpha_j+\beta_j)} \prod_{j=1}^{m} \mathrm{G}_{\alpha_j,\beta_j} \\ &\quad \times \prod_{1\le i\ne j\le m} \left(1-\frac{t_i}{t_j}\right)^{-(\alpha_i-\beta_i)(\alpha_j+\beta_j)}, \end{aligned} \tag{B.17}$$

*where we define*[s]

$$E(b) := \exp\left(\sum_{l=1}^{\infty} l(\log b)_l (\log b)_{-l}\right), \tag{B.18}$$

$$b_\pm(t_j) := \exp\left(\sum_{l=1}^{\infty} (\log b)_{\pm l} t_j^{\pm l}\right), \tag{B.19}$$

$$\mathrm{G}_{\alpha_j,\beta_j} := \frac{\mathrm{G}(1+\alpha_j+\beta_j)\mathrm{G}(1+\alpha_j-\beta_j)}{\mathrm{G}(1+2\alpha_j)}. \tag{B.20}$$

*Finally, the function $\mathrm{G} : \mathbb{C} \to \mathbb{C}$ is the entire Barnes $\mathrm{G}$-function defined by*

$$\mathrm{G}(z+1) := (2\pi)^{z/2} \mathrm{e}^{-z(z+1)/2-\gamma_E z^2/2} \prod_{n=1}^{\infty} \left[\left(1+\frac{z}{n}\right)\mathrm{e}^{-z+z^2/(2n)}\right], \tag{B.21}$$

*where $\gamma_E$ is Euler's constant.*

**Proof.** See Böttcher and Silbermann [12, p. 582]. □

[s]Under the assumptions on $b$, there exists a logarithm $\log b \in W(\mathbb{T}) \cap B_2^{1/2}(\mathbb{T})$, where $W(\mathbb{T})$ denotes the Wiener algebra, see Böttcher and Silbermann [11, p. 123]. Therefore, $G(b)$, $E(b)$ and $b_\pm(t_j)$ for $j = 1, \ldots, m$ are well-defined, and the factors on the R.H.S. of (B.14) are independent of the choice of $\log b$.

## Appendix C. Regularized Symbol

Since we have to care about the behavior in the neighborhood of the discontinuities, we write the derivatives of the regularized symbol explicitly.

**Lemma C.1.** (Regularity) *Let* $\mathbb{T}_\pm := \{t \in \mathbb{T} \,|\, \mathrm{Im}(t) \neq 0, \mathrm{sign}(\mathrm{Im}(t)) = \pm 1\}$, *and set* $b_{\mathrm{P},\mathbb{T}_\pm} := b_\mathrm{P}\restriction_{\mathbb{T}_\pm}$. *Then, the regularized symbol* $b_\mathrm{P} \in C(\mathbb{T})$ *from Definition* 3.3 *has the following properties.*

(a) $b_{\mathrm{P},\mathbb{T}_\pm} \in C^\infty(\mathbb{T}_\pm)$,
(b) $b_\mathrm{P} \in C^1(\mathbb{T})$,
(c) *the left and right derivatives* $D_\pm b'_\mathrm{P}(t)$ *exist for all* $t \in \mathbb{T}$, *but, for* $j = 1, 2$, *we have*

$$D_- b'_\mathrm{P}(t_j) \neq D_+ b'_\mathrm{P}(t_j). \tag{C.1}$$

*Moreover, the second derivative is essentially bounded,*

$$\|b''_\mathrm{P}\|_{L^\infty(\mathbb{T})} < \infty. \tag{C.2}$$

**Proof.** Assertion (a) follows from the very form of (3.5). As for assertion (b), we find that the one-sided derivatives of $b_\mathrm{P}$ at the points $t_1$ and $t_2$ coincide, and, for $j = 1, 2$, are given by the expression

$$D_\pm b_\mathrm{P}(t_j) = \frac{1}{2\pi}\sqrt{\tau_R(t_j)\tau_L(t_j)}\,\log\left(\frac{\tau_L(t_1)\tau_R(t_2)}{\tau_R(t_1)\tau_L(t_2)}\right). \tag{C.3}$$

Here, for any $f : \mathbb{T} \to \mathbb{C}$, we used the notation

$$D_\pm f(t_1) := \lim_{\varepsilon\to 0^+} \frac{1}{\pm\varepsilon}(f(\mathrm{e}^{\pm\mathrm{i}\varepsilon}) - f(t_1)), \tag{C.4}$$

$$D_\pm f(t_2) := \lim_{\varepsilon\to 0^+} \frac{1}{\pm\varepsilon}(f(\mathrm{e}^{\mathrm{i}(\mp\pi\pm\varepsilon)}) - f(t_2)). \tag{C.5}$$

Combining (C.3) with the derivative of $b_{\mathrm{P},\mathbb{T}_\pm}$, we get

$$b'_\mathrm{P}(\mathrm{e}^{\mathrm{i}k}) = \left(\frac{\tau_L(t_1)\tau_R(t_2)}{\tau_R(t_1)\tau_L(t_2)}\right)^{\frac{k}{2\pi}} \cdot \begin{cases} \sqrt{\dfrac{\tau_R(t_1)}{\tau_L(t_1)}}\,\tau_L(\mathrm{e}^{\mathrm{i}k})\left(\dfrac{1}{2\pi}\log\left(\dfrac{\tau_L(t_1)\tau_R(t_2)}{\tau_R(t_1)\tau_L(t_2)}\right) + \beta_L\tilde{\tau}_L(\mathrm{e}^{\mathrm{i}k})\sin k\right), & \text{if } 0 \leq k \leq \pi, \\ \sqrt{\dfrac{\tau_L(t_1)}{\tau_R(t_1)}}\,\tau_R(\mathrm{e}^{\mathrm{i}k})\left(\dfrac{1}{2\pi}\log\left(\dfrac{\tau_L(t_1)\tau_R(t_2)}{\tau_R(t_1)\tau_L(t_2)}\right) + \beta_R\tilde{\tau}_R(\mathrm{e}^{\mathrm{i}k})\sin k\right), & \text{if } -\pi < k < 0, \end{cases} \tag{C.6}$$

where, for $\alpha = L, R$, we set $\tilde{\tau}_\alpha(\mathrm{e}^{\mathrm{i}k}) := \frac{1}{2}(1 + \tanh[\frac{1}{2}\beta_\alpha(\lambda + \cos k)])$. Hence, it follows from (C.6) that $b'_\mathrm{P} \in C(\mathbb{T})$. Finally, computing $b''_{\mathrm{P},\mathbb{T}_\pm}$ and the left and right derivatives of $b'_{\mathrm{P}}$ at the points $t_1$ and $t_2$,

$$D_+b'_{\mathrm{P}}(t_1) = \sqrt{\tau_R(t_1)\tau_L(t_1)}\left(\left[\frac{1}{2\pi}\log\left(\frac{\tau_L(t_1)\tau_R(t_2)}{\tau_R(t_1)\tau_L(t_2)}\right)\right]^2 + \beta_L\tilde{\tau}_L(t_1)\right), \tag{C.7}$$

$$D_-b'_{\mathrm{P}}(t_1) = \sqrt{\tau_R(t_1)\tau_L(t_1)}\left(\left[\frac{1}{2\pi}\log\left(\frac{\tau_L(t_1)\tau_R(t_2)}{\tau_R(t_1)\tau_L(t_2)}\right)\right]^2 + \beta_R\tilde{\tau}_R(t_1)\right), \tag{C.8}$$

$$D_+b'_{\mathrm{P}}(t_2) = \sqrt{\tau_R(t_2)\tau_L(t_2)}\left(\left[\frac{1}{2\pi}\log\left(\frac{\tau_L(t_1)\tau_R(t_2)}{\tau_R(t_1)\tau_L(t_2)}\right)\right]^2 - \beta_R\tilde{\tau}_R(t_2)\right), \tag{C.9}$$

$$D_-b'_{\mathrm{P}}(t_2) = \sqrt{\tau_R(t_2)\tau_L(t_2)}\left(\left[\frac{1}{2\pi}\log\left(\frac{\tau_L(t_1)\tau_R(t_2)}{\tau_R(t_1)\tau_L(t_2)}\right)\right]^2 - \beta_L\tilde{\tau}_L(t_2)\right), \tag{C.10}$$

we find, on one hand, that, for $j = 1, 2$,

$$D_-b'_{\mathrm{P}}(t_j) - D_+b'_{\mathrm{P}}(t_j) = \sqrt{\tau_R(t_j)\tau_L(t_j)}\,[\beta_R\tilde{\tau}_R(t_j) - \beta_L\tilde{\tau}_L(t_j)], \tag{C.11}$$

and, on the other hand, we get $b''_{\mathrm{P}}\restriction_{\mathbb{T}_\pm} \in C(\overline{\mathbb{T}}_\pm)$. Hence, we arrive at assertion (c). □

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