

Asymptotic behavior of Toeplitz determinants with a delta function singularity

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We find the asymptotic behaviors of Toeplitz determinants with symbols which are a sum of two contributions: one analytical and non-zero function in an annulus around the unit circle, and the other proportional to a Dirac delta function. The formulas are found by using the Wiener-Hopf procedure. The determinants of this type are found in computing the spin-correlation functions in low-lying excited states of some integrable models, where the delta function represents a peak at the momentum of the excitation. As a concrete example of applications of our results, using the derived asymptotic formulas we compute the spin-correlation functions in the lowest energy band of the frustrated quantum XY chain in zero field, and the ground state magnetization.

I. INTRODUCTION

We consider Toeplitz determinants

$$\tilde{D}_n(\tilde{f}) = \det(\tilde{f}_{j-k}^{(n)})_{j,k=1}^n, \quad \tilde{f}_j^{(n)} = \frac{1}{2\pi} \int_0^{2\pi} \tilde{f}(\theta, n) e^{-ij\theta} d\theta \quad (\text{I.1})$$

with a symbol

$$\tilde{f}(\theta, n) = f(e^{i\theta}) [1 + 2\pi z_n \delta(\theta - \theta_0)] \quad (\text{I.2})$$

Here δ is Dirac delta function, $\theta_0 \in [0, 2\pi)$, $(z_n)_{n \in \mathbb{N}}$ is an arbitrary sequence in \mathbb{C} and f is a continuous function on the unit circle.

It follows that for $\theta_0 \neq 0$ the elements $\tilde{f}_j^{(n)}$ are equal to

$$\tilde{f}_j^{(n)} = f_j + z_n f(e^{i\theta_0}) e^{-ij\theta_0}, \quad (\text{I.3})$$

where

$$f_j = \frac{1}{2\pi} \int_0^{2\pi} f(e^{i\theta}) e^{-ij\theta} d\theta. \quad (\text{I.4})$$

For $\theta_0 = 0$ there is an ambiguity in the delta function integral. In this case we use (I.3) to define the coefficients $\tilde{f}_j^{(n)}$ and the Toeplitz matrix $\tilde{D}_n(\tilde{f})$.

We restrict ourselves to symbols f that are non-zero and analytic in an annulus including the unit circle. A general such symbol can be written as

$$f(z) = a(z) z^\nu, \quad (\text{I.5})$$

where a is a function that is analytic and non-zero on the annulus and has zero winding number, while $\nu \in \mathbb{Z}$ is the winding number of the symbol f (see e.g. [1, 2]).

We are interested in asymptotic formulas for $\tilde{D}_n(\tilde{f})$ as $n \rightarrow \infty$. The asymptotic formulas for

$$D_n(f) = \det(f_{j-k})_{j,k=1}^n \quad (\text{I.6})$$

for analytic non-zero symbols f are by now considered classical, and exist under much more general conditions. For $\nu = 0$ they are given by the strong Szegő limit theorem (originally proven in [3], for a review of later developments see [4–6]). The asymptotic formulas for nonzero ν have been first obtained in [7, 8], and later under different conditions and using different methods in [9, 10]. The delta function in the symbol (I.2) might also be considered, in a suitable limit, as a singularity of the symbol, different from the widely studied Fisher-Hartwig singularities (for a review see [11]).

We decided to solve this problem motivated by the appearance of determinants of type (I.1) in spin-correlation functions of certain low energy states in quantum spin chains mappable to free fermionic systems. In such instances, the determinant $D_n(f)$ reflects the ground state correlations (in absence of frustration) and the delta function of the

symbol has a peak at the momentum of the fermionic excitation on the vacuum state. For chains with boundary frustration, the spin-correlation functions in the lowest admissible state are already determined by (I.1), where θ_0 emerges as the mode minimizing the energy and lying at the bottom of a band of states (in the thermodynamic limit) [12–16]. The leading asymptotic term for particular determinants of the type (I.1) in the case $\nu = 0$ was found in [13] in the context of the frustrated quantum Ising chain, without discussion of the subleading terms and without rigor: providing a reliable proof has been the initial inspiration for this work, together with the possibility of extending the conditions of applicability.

To introduce the notation, we are first going to review some results on the asymptotics of the determinant $D_n(f)$ where f is non-zero and analytic in an annulus around the unit circle. The asymptotic formulas of [7, 8] are appropriate for this case. The function $a(z) = \sum_{k=-\infty}^{\infty} a_k z^k$, defined in (I.5), is analytic in an annulus including the unit circle so

$$\limsup_{k \rightarrow \infty} |a_{-k}|^{1/k} = \rho_- < 1 < \rho_+ = \liminf_{k \rightarrow \infty} |a_k|^{-1/k}. \quad (\text{I.7})$$

An analytic logarithm of a on $\rho_- < |z| < \rho_+$ exists so we can introduce the Wiener-Hopf factorization (see e.g. [1, 17])

$$a_-(z) = \exp \sum_{k=1}^{\infty} (\log a)_{-k} z^{-k}, \quad a_+(z) = \exp \sum_{k=0}^{\infty} (\log a)_k z^k, \quad (\text{I.8})$$

where $\log a(z) = \sum_{k=-\infty}^{\infty} (\log a)_k z^k$ and thus $a = a_- a_+$. We also introduce the functions

$$b = a_- a_+^{-1}, \quad c = a_+ a_-^{-1}, \quad b c = 1. \quad (\text{I.9})$$

For expressing the subleading terms in the asymptotic formulas for $D_n(f)$ it is useful to define $\rho \in (0, 1)$ by

$$\rho_- < \rho < 1 < \rho^{-1} < \rho_+. \quad (\text{I.10})$$

The function a is then analytic on $\rho \leq |z| \leq \rho^{-1}$ and $a_j = O(\rho^j)$, $a_{-j} = O(\rho^j)$, for $j \geq 0$, for all ρ satisfying (I.10). Analogous relations hold for the functions b and c .

The asymptotic behavior of $D_n(f)$ in the case of zero winding number of the symbol ($\nu = 0$) is given by the strong Szegő limit theorem. The version of [7, 8] in the case of analytic symbol reads

$$D_n(a) = \exp \left[n(\log a)_0 + \sum_{k=1}^{\infty} k(\log a)_k (\log a)_{-k} + O(\rho^{2n}) \right] \quad \text{as } n \rightarrow \infty. \quad (\text{I.11})$$

We note that in the same reference an explicit formula for the term $O(\rho^{2n})$ in (I.11) is given, up to corrections $O(\rho^{4n})$.

For $\nu \neq 0$ the asymptotic behavior of $D_n(f)$ is determined by the asymptotic behavior of $D_n(a)$ and the determinant of the $|\nu| \times |\nu|$ Toeplitz matrix, defined by

$$\Delta_{\nu,n} = \det \left(d_{j-k}^{(n)} \right)_{j,k=1}^{|\nu|}, \quad \text{where } d_j^{(n)} = \begin{cases} b_{n+j} & \text{for } \nu < 0 \\ c_{-n-j} & \text{for } \nu > 0 \end{cases}. \quad (\text{I.12})$$

The asymptotic formula is

$$D_n(f) = (-1)^{n\nu} D_{n+|\nu|}(a) [\Delta_{\nu,n} + O(\rho^{n(|\nu|+3)})]. \quad (\text{I.13})$$

The formula (I.13) follows from the more precise result of [7, 8], given by Theorem 4 in [7] and Theorem 6 in [8].

We will extend these formulas to determinants of type (I.1). In order to do so, we first define the determinants $\tilde{\Delta}_{\nu,n}(l)$, for $l = 1, 2, \dots, |\nu|$, for $\nu \neq 0$, as the determinants of the matrix $(d_{j-k}^{(n)})_{j,k=1}^{|\nu|}$ with the column l replaced by the vector $(1, e^{-i\theta_0}, e^{-i2\theta_0}, \dots, e^{-i(|\nu|-1)\theta_0})^T$ for $\nu < 0$ and by $(1, e^{i\theta_0}, e^{i2\theta_0}, \dots, e^{i(\nu-1)\theta_0})^T$ for $\nu > 0$. This definition can be written as

$$\tilde{\Delta}_{\nu,n}(l) = \det \left(\tilde{d}_{j,k}^{(l)} \right)_{j,k=1}^{|\nu|}, \quad \text{where } \tilde{d}_{j,k}^{(l)} = \begin{cases} (1 - \delta_{k,l}) d_{j-k}^{(n)} + \delta_{k,l} e^{-i(j-1)\theta_0} & \text{for } \nu < 0 \\ (1 - \delta_{k,l}) d_{j-k}^{(n)} + \delta_{k,l} e^{i(j-1)\theta_0} & \text{for } \nu > 0 \end{cases}. \quad (\text{I.14})$$

The main results of this work are the following two theorems.

Theorem 1. *For $\nu = 0$ we have*

$$\tilde{D}_n(\tilde{f}) = D_n(a) \left\{ 1 + z_n \left[n + i \frac{d}{d\theta} \log b(e^{i\theta}) \Big|_{\theta=\theta_0} + O(\rho^n) \right] \right\} \quad \text{as } n \rightarrow \infty, \quad (\text{I.15})$$

where ρ is defined by (I.10).

Theorem 2. Let $\nu \neq 0$ and suppose $D_n(f) \neq 0$, $\Delta_{\nu,n} \neq 0$, for $n \geq n_0$, $n_0 \in \mathbb{N}$. If for sufficiently small ρ , satisfying (I.10), we have

$$\lim_{n \rightarrow \infty} \frac{\tilde{\Delta}_{\nu,n}(j)}{\Delta_{\nu,n}} \rho^{2n} = 0 \quad \text{for all } j \in \{1, 2, \dots, |\nu|\}, \quad (\text{I.16})$$

where $\tilde{\Delta}_{\nu,n}(j)$ are defined by (I.14), then for $n \geq n_0$

$$\tilde{D}_n(\tilde{f}) = D_n(f) \left\{ 1 + z_n \left[-b(e^{i\theta_0})e^{-i(n+1)\theta_0} \sum_{j=1}^{|\nu|} \frac{\tilde{\Delta}_{\nu,n}(j)}{\Delta_{\nu,n}} \left(e^{ij\theta_0} + O(\rho^n) \right) + n + O(1) \right] \right\} \quad \text{if } \nu < 0, \quad (\text{I.17})$$

$$\tilde{D}_n(\tilde{f}) = D_n(f) \left\{ 1 + z_n \left[-c(e^{i\theta_0})e^{i(n+1)\theta_0} \sum_{j=1}^{\nu} \frac{\tilde{\Delta}_{\nu,n}(j)}{\Delta_{\nu,n}} \left(e^{-ij\theta_0} + O(\rho^n) \right) + n + O(1) \right] \right\} \quad \text{if } \nu > 0. \quad (\text{I.18})$$

Compared to the usual behavior of Toeplitz determinants without delta-function singularities, in this case we see the emergence of algebraic contributions in the matrix rank n . The terms inside the sums in (I.17) and (I.18) are expected to be of the order of magnitude of the inverse of the coefficients $d_j^{(n)}$ for $|j| < |\nu|$. Therefore, since $d_j^{(n)} = O(\rho^n)$ as $n \rightarrow \infty$, they are expected typically to grow faster than ρ^{-n} , with exponentially suppressed subleading corrections.

We are going to derive these theorems by relating the determinant to a linear problem, which in turn can be expressed as a linear functional equation, whose solution can be obtained in the limit of large n . The leading contributions to this solution, obtained using the Wiener-Hopf procedure, provide the asymptotic formulas above for the determinant. The estimates on the order of magnitude of the corrections to the terms we have calculated explicitly rely on the intuitively clear property that a small perturbation to the functional equation yields a change to the solution of a similar order of magnitude. For the case of a zero winding number of the symbol we have also provided a rigorous proof of this statement, which makes Theorem 1 rigorous. For the case of a non-zero winding number we have not provided a rigorous proof, but the corrections are plausible for the same reasons and we have confirmed Theorem 2 numerically on a few relevant examples. The rigorous analysis of corrections is better established in the framework of the Riemann-Hilbert problem, an alternative technique that can be used, which will be the subject of another work.

We derive the theorems in section II. To give a concrete example of applications of these theorems (and to explicitly show the unusual behavior of these determinants) in section III we compute the spin-correlation functions in the lowest energy band of the frustrated quantum XY chain in zero magnetic field, and the ground state magnetization.

II. DERIVATION OF THE THEOREMS

A. Linear Problem

The first step in the derivation of the theorems is to use (I.3) and the basic property that determinant is alternating multilinear function of its columns, to expand $\tilde{D}_n(\tilde{f})$ as

$$\tilde{D}_n(\tilde{f}) = D_n(f) + z_n f(e^{i\theta_0}) \sum_{j=1}^n e^{i(j-1)\theta_0} D_{n,j}(f), \quad (\text{II.1})$$

where by $D_{n,j}(f)$ we denote the determinant obtained by replacing the column j in $D_n(f)$ by the column vector $(1, e^{-i\theta_0}, e^{-i2\theta_0}, \dots, e^{-i(n-1)\theta_0})^T$.

We assume that there is $n_0 \in \mathbb{N}$ such that $D_n(f) \neq 0$ for $n \geq n_0$. In the case $\nu = 0$ this assumption is justified by the Szegő theorem, while for nonzero ν we restrict ourselves to symbols for which this assumption holds. This assumption implies that there exists a unique solution $x_j^{(n)}$, $j = 0, 1, \dots, n-1$, of the linear problem

$$\sum_{k=0}^{n-1} f_{j-k} x_k^{(n)} = e^{-i\theta_0 j}, \quad \text{for } j = 0, 1, \dots, n-1, \quad (\text{II.2})$$

that is by Cramer's rule given by

$$x_j^{(n)} = \frac{D_{n,j+1}(f)}{D_n(f)}. \quad (\text{II.3})$$

This solution can be inserted in (II.1) to get

$$\tilde{D}_n(\tilde{f}) = D_n(f) \left[1 + z_n f(e^{i\theta_0}) \sum_{j=0}^{n-1} e^{i\theta_0 j} x_j^{(n)} \right]. \quad (\text{II.4})$$

Defining the analytic function

$$X^{(n)}(z) = \sum_{j=0}^{n-1} x_j^{(n)} z^j \quad (\text{II.5})$$

we have

$$\tilde{D}_n(\tilde{f}) = D_n(f) \left(1 + z_n f(e^{i\theta_0}) X^{(n)}(e^{i\theta_0}) \right). \quad (\text{II.6})$$

We are thus going to find an asymptotic formula for $X^{(n)}(z)$, and hence for $\tilde{D}_n(\tilde{f})$, by using the Wiener-Hopf procedure, similar to the one of [17, 18] used to compute the spin correlation functions of the Ising model. The prerequisites and details are given in the following sections.

Let us comment that the presented method of relating the determinant to a linear problem would not work with more than one delta function in the symbol (I.2). In arriving to expression (II.1) we have used the property that different column vectors resulting from the delta function in the symbol are one scalar multiple of the other. This has lead to many cancellations, since determinant is an alternating function. With more delta functions, column vectors arising from different delta functions could not anymore be related simply by scalar multiplication, which prevents cancellations.

B. Equivalent Problem

For a function $g(z) = \sum_{j=-\infty}^{\infty} g_j z^j$, defined and analytic in an annulus $\rho_- < |z| < \rho_+$ including the unit circle, we define its components

$$[g]_-(z) = \sum_{j=1}^{\infty} g_{-j} z^{-j}, \quad [g]_+(z) = \sum_{j=0}^{\infty} g_j z^j. \quad (\text{II.7})$$

The function $[g]_-$ is analytic on $|z| > \rho_-$, while the function $[g]_+$ is analytic on $|z| < \rho_+$. For definiteness, in the following we are going to restrict the domain of these functions to the annulus $\rho_- < |z| < \rho_+$, where both are analytic.

As shown in Appendix A, defining the coefficients

$$y_j^{(n)} = \begin{cases} e^{-ij\theta_0}, & j \in \{0, 1, \dots, n-1\} \\ 0, & j \in \mathbb{Z} \setminus \{0, 1, \dots, n-1\} \end{cases} \quad (\text{II.8})$$

and the analytic function

$$Y^{(n)}(z) = \sum_{j=0}^{n-1} y_j^{(n)} z^j \quad (\text{II.9})$$

solving the linear problem (II.2) is equivalent to finding functions $X^{(n)}, U^{(n)}, V^{(n)}$, defined and analytic on an annulus including the unit circle, satisfying

$$fX^{(n)} = Y^{(n)} + U^{(n)} z^n + V^{(n)} \quad (\text{II.10})$$

and having the properties

$$[X^{(n)}]_- = 0, \quad [X^{(n)} z^{-n}]_+ = 0, \quad [U^{(n)}]_- = 0, \quad [V^{(n)}]_+ = 0. \quad (\text{II.11})$$

With $D_n(f) \neq 0$ the solution exists and is unique, with $X^{(n)}$ corresponding to (II.5). By solving this equivalent problem we find the asymptotic formula for $X^{(n)}(e^{i\theta_0})$ in (II.6).

C. Evaluating the components

Following the standard Wiener-Hopf approach, we seek the solution of (II.10) by exploiting the different analytical properties of the different components of the functions appearing in it. The components (II.7) can be evaluated as the following integrals. Let z belong to the annulus $\rho_- < |z| < \rho_+$, and let $\rho_1 \in (\rho_-, |z|)$, $\rho_2 \in (|z|, \rho_+)$. Then

$$[g]_-(z) = \frac{1}{2\pi i} \oint_{|w|=\rho_1} \frac{g(w)}{z-w} dw, \quad [g]_+(z) = \frac{1}{2\pi i} \oint_{|w|=\rho_2} \frac{g(w)}{w-z} dw. \quad (\text{II.12})$$

These formulas can be shown by summing, in accordance with definition (II.7), the Laurent series coefficients

$$g_k = \frac{1}{2\pi i} \oint_{|w|=\rho_1} g(w) \frac{dw}{w^{k+1}} = \frac{1}{2\pi i} \oint_{|w|=\rho_2} g(w) \frac{dw}{w^{k+1}} \quad (\text{II.13})$$

and interchanging the sum and the integral, which is valid since the Laurent series is uniformly convergent on every closed subannulus in the interior of its annulus.

In the derivation of the theorems we are going to encounter functions G , analytic on the annulus $\rho_- < |z| < \rho_+$, that are of the form

$$G(z) = \frac{g(z) - g(e^{i\theta_0})}{z - e^{i\theta_0}} \quad \text{for } z \neq e^{i\theta_0}, \quad G(e^{i\theta_0}) = \left. \frac{dg(z)}{dz} \right|_{z=e^{i\theta_0}}, \quad (\text{II.14})$$

where g is analytic on the same annulus. For instance, the function (II.9) satisfies

$$Y^{(n)}(z) = e^{-i(n-1)\theta_0} \frac{z^n - e^{in\theta_0}}{z - e^{i\theta_0}}, \quad Y^{(n)}(e^{i\theta_0}) = n = e^{-i(n-1)\theta_0} \left. \frac{dz^n}{dz} \right|_{z=e^{i\theta_0}}. \quad (\text{II.15})$$

For $z \neq e^{i\theta_0}$, it will be convenient to consider the function G as a sum of two functions with a singularity on the unit circle, or, as we are about to show, the sum of two functions analytical inside/outside the unit circle. We thus need to introduce another structure. Let \mathcal{G} be defined by the rule

$$\mathcal{G}(z) = \frac{g(z)}{z - e^{i\theta_0}} \quad \text{for } \rho_- < |z| < \rho_+, \quad z \neq e^{i\theta_0}, \quad (\text{II.16})$$

with g being a function analytic on the annulus $\rho_- < |z| < \rho_+$. The function \mathcal{G} is thus analytic on the annuli $\rho_- < |z| < 1$ and $1 < |z| < \rho_+$. Its Laurent series coefficients are different on two different annuli, let us denote them by

$$\mathcal{G}(z) = \sum_{j=-\infty}^{\infty} \mathcal{G}_j^{(<)} z^j \quad \text{for } \rho_- < |z| < 1, \quad \mathcal{G}(z) = \sum_{j=-\infty}^{\infty} \mathcal{G}_j^{(>)} z^j \quad \text{for } 1 < |z| < \rho_+. \quad (\text{II.17})$$

There are thus two ways of defining $+$ and $-$ components of the functions \mathcal{G} . We define

$$[\mathcal{G}]_-^{(<)}(z) = \sum_{j=1}^{\infty} \mathcal{G}_{-j}^{(<)} z^{-j}, \quad [\mathcal{G}]_+^{(<)}(z) = \sum_{j=0}^{\infty} \mathcal{G}_j^{(<)} z^j, \quad (\text{II.18})$$

$$[\mathcal{G}]_-^{(>)}(z) = \sum_{j=1}^{\infty} \mathcal{G}_{-j}^{(>)} z^{-j}, \quad [\mathcal{G}]_+^{(>)}(z) = \sum_{j=0}^{\infty} \mathcal{G}_j^{(>)} z^j. \quad (\text{II.19})$$

In this work we are going to make use of the functions $[\mathcal{G}]_-^{(<)}$ and $[\mathcal{G}]_+^{(>)}$, both of which are analytic on $\rho_- < |z| < \rho_+$. We are going to use the obvious notation

$$\left[\frac{g}{z - e^{i\theta_0}} \right]_-^{(<)} = [\mathcal{G}]_-^{(<)}, \quad \left[\frac{g}{z - e^{i\theta_0}} \right]_+^{(>)} = [\mathcal{G}]_+^{(>)}. \quad (\text{II.20})$$

Analogously to (II.12) we have the integral representation

$$\begin{aligned} \left[\frac{g}{z - e^{i\theta_0}} \right]_-^{(<)}(z) &= \frac{1}{2\pi i} \oint_{|w|=\rho_1} \frac{g(w)}{(w - e^{i\theta_0})(z - w)} dw, \quad \text{where } \rho_1 \in (\rho_-, \min\{1, |z|\}), \\ \left[\frac{g}{z - e^{i\theta_0}} \right]_+^{(>)}(z) &= \frac{1}{2\pi i} \oint_{|w|=\rho_2} \frac{g(w)}{(w - e^{i\theta_0})(w - z)} dw, \quad \text{where } \rho_2 \in (\max\{1, |z|\}, \rho_+). \end{aligned} \quad (\text{II.21})$$

Expanding $1/(w - e^{i\theta_0})$ under integrals into series and interchanging the series and the integral, we get the following representation:

$$\begin{aligned} \left[\frac{g}{z - e^{i\theta_0}} \right]_-^{(<)}(z) &= \sum_{j=0}^{\infty} e^{-i(j+1)\theta_0} [gz^j]_-(z), \\ \left[\frac{g}{z - e^{i\theta_0}} \right]_+^{(>)}(z) &= \sum_{j=0}^{\infty} e^{ij\theta_0} [gz^{-j-1}]_+(z). \end{aligned} \quad (\text{II.22})$$

With the introduced definitions, for the function G defined by (II.14) we have

$$\begin{aligned} [G]_- &= \left[\frac{g - g(e^{i\theta_0})}{z - e^{i\theta_0}} \right]_-^{(<)} = \left[\frac{g}{z - e^{i\theta_0}} \right]_-^{(<)}, \\ [G]_+ &= \left[\frac{g - g(e^{i\theta_0})}{z - e^{i\theta_0}} \right]_+^{(>)} = \left[\frac{g}{z - e^{i\theta_0}} \right]_+^{(>)}, \end{aligned} \quad (\text{II.23})$$

where the first equality follows immediately from the integral representations and the second is obtained using

$$\left[\frac{g(e^{i\theta_0})}{z - e^{i\theta_0}} \right]_-^{(<)} = 0, \quad \left[\frac{g(e^{i\theta_0})}{z - e^{i\theta_0}} \right]_+^{(>)} = 0, \quad (\text{II.24})$$

which follows from (II.22). From (II.23) it follows

$$G = \left[\frac{g}{z - e^{i\theta_0}} \right]_-^{(<)} + \left[\frac{g}{z - e^{i\theta_0}} \right]_+^{(>)}. \quad (\text{II.25})$$

We clearly have also the following linear property. Let h be a function analytic on the same annulus as g . Then

$$[hG]_- = \left[\frac{hg}{z - e^{i\theta_0}} \right]_-^{(<)} - \left[\frac{hg(e^{i\theta_0})}{z - e^{i\theta_0}} \right]_-^{(<)}, \quad [hG]_+ = \left[\frac{hg}{z - e^{i\theta_0}} \right]_+^{(>)} - \left[\frac{hg(e^{i\theta_0})}{z - e^{i\theta_0}} \right]_+^{(>)}. \quad (\text{II.26})$$

The definitions we have introduced are going to be useful because of the following two elementary lemmas that we state and prove.

Lemma 1. *Let g be a function analytic on an annulus $\rho_- < |z| < \rho_+$, that includes the unit circle. Then for $z \neq e^{i\theta_0}$ belonging to the annulus*

$$\left[\frac{g}{z - e^{i\theta_0}} \right]_-^{(<)}(z) = \frac{[g]_-(z) - [g]_-(e^{i\theta_0})}{z - e^{i\theta_0}}, \quad \left[\frac{g}{z - e^{i\theta_0}} \right]_+^{(>)}(z) = \frac{[g]_+(z) - [g]_+(e^{i\theta_0})}{z - e^{i\theta_0}}. \quad (\text{II.27})$$

Proof. Let us prove the first equality. From the representation (II.22) it follows

$$\left[\frac{[g]_+}{z - e^{i\theta_0}} \right]_-^{(<)} = 0, \quad (\text{II.28})$$

which implies

$$\left[\frac{g}{z - e^{i\theta_0}} \right]_-^{(<)} = \left[\frac{[g]_-}{z - e^{i\theta_0}} \right]_-^{(<)}. \quad (\text{II.29})$$

We now define a function $G^{(-)}$ as

$$G^{(-)}(z) = \frac{[g]_-(z) - [g]_-(e^{i\theta_0})}{z - e^{i\theta_0}} \quad \text{for } z \neq e^{i\theta_0}, \rho_- < |z| < \rho_+, \quad G^{(-)}(e^{i\theta_0}) = \left. \frac{d}{dz} [g]_-(z) \right|_{z=e^{i\theta_0}}, \quad (\text{II.30})$$

and, using the decomposition (II.25) for this function, we have

$$G^{(-)} = \left[\frac{[g]_-}{z - e^{i\theta_0}} \right]_-^{(<)} + \left[\frac{[g]_-}{z - e^{i\theta_0}} \right]_+^{(>)} = \left[\frac{[g]_-}{z - e^{i\theta_0}} \right]_-^{(<)}, \quad (\text{II.31})$$

where the last equality follows from (II.22). Combining (II.29) and (II.31) proves the first equality of the lemma. The second equality is proven in an analogous way. \square

Lemma 2. Let $(g_n)_{n \in \mathbb{N}}$ be a sequence of functions analytic on an annulus $\rho_- < |z| < \rho_+$, that includes the unit circle, and let $\rho_- < \rho_1 < 1 < \rho_2 < \rho_+$. Moreover, let $(s_n)_{n \in \mathbb{N}}$ be a sequence of positive numbers.

(a) If $g_n = O(s_n)$ uniformly in z at the circle $|z| = \rho'_1$, for some $\rho'_1 \in (\rho_-, \rho_1)$, then

$$[g_n]_-(z) = O(s_n), \quad \left[\frac{g_n}{z - e^{i\theta_0}} \right]_-^{(<)}(z) = O(s_n) \quad (\text{II.32})$$

uniformly in z on $\rho_1 \leq |z| \leq \rho_2$.

(b) If $g_n = O(s_n)$ uniformly in z at the circle $|z| = \rho'_2$, for some $\rho'_2 \in (\rho_2, \rho_+)$, then

$$[g_n]_+(z) = O(s_n), \quad \left[\frac{g_n}{z - e^{i\theta_0}} \right]_+^{(>)}(z) = O(s_n) \quad (\text{II.33})$$

uniformly in z on $\rho_1 \leq |z| \leq \rho_2$.

Proof. Let us prove the first part of (a). By assumption there is $K > 0$ such that

$$|g_n(z)| \leq K s_n \quad \text{for all } z \text{ on the circle } |z| = \rho'_1. \quad (\text{II.34})$$

For $\rho_1 \leq |z| \leq \rho_2$ we have, from (II.12), the integral representation

$$[g]_-(z) = \frac{1}{2\pi i} \oint_{|w|=\rho'_1} \frac{g(w)}{z-w} dw. \quad (\text{II.35})$$

Then from the assumption (II.34) and using $|z-w| \geq \rho_1 - \rho'_1$ it follows

$$|[g]_-(z)| \leq \frac{K \rho'_1}{\rho_1 - \rho'_1} s_n, \quad (\text{II.36})$$

which means that $[g]_-(z) = O(s_n)$ uniformly in z on $\rho_1 \leq |z| \leq \rho_2$. The other parts of the lemma are proven in an analogous way by using the integral representations (II.12) and (II.21). \square

D. Solution for the zero winding number case

Having introduced the tools for the separation in components of the various functions, we can present the solutions. In the case $\nu = 0$, on the basis of a Wiener-Hopf procedure, presented in Appendix B, we construct the following functions, which are the specialization of (B.27), (B.22), and (B.15) and are defined and analytic on the annulus (I.7), given for $z \neq e^{i\theta_0}$ by

$$X_1^{(n)}(z) = e^{-i(n-1)\theta_0} a_+^{-1}(e^{i\theta_0}) a_+^{-1}(z) \frac{z^n c(z) - e^{in\theta_0} c(e^{i\theta_0})}{z - e^{i\theta_0}}, \quad (\text{II.37})$$

$$U_1^{(n)}(z) = -e^{-i(n-1)\theta_0} a_+(z) \frac{a_+^{-1}(z) - a_+^{-1}(e^{i\theta_0})}{z - e^{i\theta_0}}, \quad (\text{II.38})$$

$$V_1^{(n)}(z) = e^{i\theta_0} a_-(z) \frac{a_-^{-1}(z) - a_-^{-1}(e^{i\theta_0})}{z - e^{i\theta_0}}, \quad (\text{II.39})$$

and for $z = e^{i\theta_0}$ by continuity. It's easy to see that these functions satisfy the equation (II.10)

$$aX_1^{(n)} = Y^{(n)} + U_1^{(n)} z^n + V_1^{(n)}, \quad (\text{II.40})$$

where, in this case, according to (I.5), $f = a$, and the function a_{\pm} in (II.37) have been defined in (I.8) and we remind that $c = a_+ a_-^{-1}$.

Let ρ be defined by (I.10). A straightforward application of Lemma 1 and Lemma 2 yields the properties

$$[X_1^{(n)}]_- = O(\rho^n), \quad [X_1^{(n)} z^{-n}]_+ = O(\rho^n), \quad [U_1^{(n)}]_- = 0, \quad [V_1^{(n)}]_+ = 0, \quad (\text{II.41})$$

where $O(\rho^n)$ holds on $\rho \leq |z| \leq \rho^{-1}$, uniformly in z . For example, let us show the first property. We have

$$[X_1^{(n)}]_- = e^{-\imath(n-1)\theta_0} a_+^{-1}(e^{\imath\theta_0}) \left[\frac{z^n a_-^{-1}}{z - e^{\imath\theta_0}} \right]_-^{(<)} - e^{\imath\theta_0} a_-^{-1}(e^{\imath\theta_0}) \left[\frac{a_+^{-1}}{z - e^{\imath\theta_0}} \right]_-^{(<)}. \quad (\text{II.42})$$

Applying Lemma 2 on the first term, with $\rho'_1 \in (\rho_-, \rho)$, $\rho_1 = \rho$, $\rho_2 = \rho^{-1}$, $s_n = \rho^n$, we see that it is equal to $O(\rho^n)$ on $\rho \leq |z| \leq \rho^{-1}$, uniformly in z . The second term is zero, by Lemma 1. The other properties in (II.41) are shown in an analogous way.

The properties (II.41) should be compared with (II.11). They imply that the function $X_1^{(n)}$ with the components $j < 0$ and $j \geq n$ removed, i.e. the function $X_2^{(n)} = X_1^{(n)} - [X_1^{(n)}]_- - z^n [X_1^{(n)} z^{-n}]_+$, is a solution of the problem

$$aX_2^{(n)} = Y_2^{(n)} + U_2^{(n)} z^n + V_2^{(n)} \quad (\text{II.43})$$

$$[X_2^{(n)}]_- = 0, \quad [X_2^{(n)} z^{-n}]_+ = 0, \quad [U_2^{(n)}]_- = 0, \quad [V_2^{(n)}]_+ = 0, \quad (\text{II.44})$$

where $[Y_2^{(n)}]_- = 0$, $[Y_2^{(n)} z^{-n}]_+ = 0$, and

$$Y_2^{(n)}(z) - Y^{(n)}(z) = O(\rho^n) \quad \text{uniformly in } z \text{ on the unit circle } |z| = 1. \quad (\text{II.45})$$

Thus, we have constructed a linear problem whose corresponding functional equation is a $O(\rho^n)$ perturbation of the original one on the unit circle. It is intuitively clear that the solution $X^{(n)}$ will result into a $O(\rho^n)$ perturbation of $X_2^{(n)}$ on the unit circle. This passage is made rigorous by applying Lemma 3, stated and proven in Appendix C, on $X^{(n)}$ and $X_2^{(n)}$. It follows

$$X_2^{(n)}(z) - X^{(n)}(z) = O(\rho^n) \quad \text{uniformly in } z \text{ on the unit circle } |z| = 1 \quad (\text{II.46})$$

and therefore, since $X_2^{(n)}(z) - X_1^{(n)}(z) = O(\rho^n)$ uniformly in z on the unit circle, we have

$$X^{(n)}(z) = X_1^{(n)}(z) + O(\rho^n) \quad \text{uniformly in } z \text{ on the unit circle } |z| = 1. \quad (\text{II.47})$$

This, together with (II.37), gives

$$X^{(n)}(e^{\imath\theta_0}) = a_+^{-1}(e^{\imath\theta_0}) a_-^{-1}(e^{\imath\theta_0}) n + e^{\imath\theta_0} a_+^{-2}(e^{\imath\theta_0}) \left. \frac{dc(z)}{dz} \right|_{z=e^{\imath\theta_0}} + O(\rho^n). \quad (\text{II.48})$$

It follows

$$a(e^{\imath\theta_0}) X^{(n)}(e^{\imath\theta_0}) = n - \imath \left. \frac{d}{d\theta} \log c(e^{\imath\theta}) \right|_{\theta=\theta_0} + O(\rho^n). \quad (\text{II.49})$$

Theorem 1 follows from (II.6) and (II.49). Let us comment here that the leading term in this solution was already determined in [12, 13], but without rigor, with a cavalier use of the component analysis and an improper analytical continuation. Most of all, the approach employed there does not allow to treat the non-zero winding number case.

E. Solution for the non-zero winding number case

Let us assume that $\nu > 0$. The result for $\nu < 0$ follows from this one by transposing the original Toeplitz matrix in (I.1) and doing the integral transformation $\theta \rightarrow -\theta$. On the basis of the Wiener-Hopf procedure presented in Appendix B, as a specialization of (B.27), (B.22) and (B.15) we construct the functions $X_1^{(n)}$, $U_1^{(n)}$, $V_1^{(n)}$, analytic on

the annulus (I.7). For $z \neq e^{i\theta_0}$, $\rho_- < |z| < \rho_+$, they are defined by the rule

$$X_1^{(n)}(z)z^\nu = e^{-i(n+\nu-1)\theta_0} a_+^{-1}(z) a_+^{-1}(e^{i\theta_0}) \frac{c(z)z^{n+\nu} - c(e^{i\theta_0})e^{i(n+\nu)\theta_0}}{z - e^{i\theta_0}} \\ + e^{-i(n-1)\theta_0} a_-^{-1}(z) z^{n+\nu} \sum_{k=0}^{\nu-1} (a_+^{-1})_k \frac{z^{k-\nu} - e^{i(k-\nu)\theta_0}}{z - e^{i\theta_0}} + a_+^{-1}(z) \sum_{k=1}^{\nu} \alpha_k^{(n)} [c z^{n+\nu-k}]_+(z), \quad (\text{II.50})$$

$$U_1^{(n)} z^{-\nu} = -e^{-i(n-1)\theta_0} a_+(z) \frac{[a_+^{-1} z^{-\nu}]_+(z) - [a_+^{-1} z^{-\nu}]_+(e^{i\theta_0})}{z - e^{i\theta_0}} + a_+(z) \sum_{k=1}^{\nu} \alpha_k^{(n)} z^{-k}, \quad (\text{II.51})$$

$$V_1^{(n)}(z) = e^{i\theta_0} a_-(z) \frac{a_-^{-1}(z) - a_-^{-1}(e^{i\theta_0})}{z - e^{i\theta_0}} - a_-(z) \sum_{k=1}^{\nu} \alpha_k^{(n)} [c z^{n+\nu-k}]_-(z), \quad (\text{II.52})$$

and for $z = e^{i\theta_0}$ by continuity. Here $\alpha_1^{(n)}, \alpha_2^{(n)}, \dots, \alpha_\nu^{(n)} \in \mathbb{C}$ are for the moment unspecified, and it is simple to check that for any choice of them the functions above satisfy (II.10) as

$$az^\nu X_1^{(n)} = Y^{(n)} + U_1^{(n)} z^n + V_1^{(n)}. \quad (\text{II.53})$$

Let ρ be defined by (I.10). As in the previous section, a straightforward application of Lemma 1 and Lemma 2 yields

$$[X_1^{(n)} z^\nu]_-(z) = O(\rho^n), \quad [U_1^{(n)}]_- = 0, \quad [V_1^{(n)}]_+ = 0, \quad (\text{II.54})$$

where $O(\rho^n)$ holds on $\rho \leq |z| \leq \rho^{-1}$, uniformly in z . The coefficients $\alpha_1^{(n)}, \alpha_2^{(n)}, \dots, \alpha_\nu^{(n)}$ are chosen to satisfy

$$(X_1^{(n)} z^\nu)_j = O(\rho^n) \quad \text{for } j = 0, 1, \dots, \nu - 1, \quad (\text{II.55})$$

thus extending (II.54) to also $[X_1^{(n)}]_- = O(\rho^n)$.

Thus, one computes the components $(X_1^{(n)} z^\nu)_j$ using (II.13), by integrating at the circle $|w| = \rho$, and imposes (II.55). As shown in Appendix B, this procedure results in

$$\alpha_k^{(n)} = -a_-^{-1}(e^{i\theta_0}) e^{-i(\nu-1)\theta_0} \frac{\tilde{\Delta}_{\nu,n}(k)}{\Delta_{\nu,n}}, \quad (\text{II.56})$$

where $\Delta_{\nu,n}$ is defined by (I.12) and $\tilde{\Delta}_{\nu,n}(k)$ by (I.14).

We have shown so far

$$[X_1^{(n)}]_- = O(\rho^n), \quad [U_1^{(n)}]_- = 0, \quad [V_1^{(n)}]_+ = 0, \quad (\text{II.57})$$

which should be compared to (II.11). It remains to discuss $[X_1^{(n)} z^{-n}]_+$. Application of Lemmas 1 and 2 yields

$$[X_1^{(n)} z^{-n}]_+ = O(\rho^n) + \sum_{k=1}^{\nu} \alpha_k^{(n)} \left[a_+^{-1} z^{-(n+\nu)} [c z^{n+\nu-k}]_+ \right]_+. \quad (\text{II.58})$$

We have further

$$\alpha_k^{(n)} \left[a_+^{-1} z^{-(n+\nu)} [c z^{n+\nu-k}]_+ \right]_+ = -\alpha_k^{(n)} \left[a_+^{-1} z^{-(n+\nu)} [c z^{n+\nu-k}]_- \right]_+ = -\alpha_k^{(n)} O(\rho_1^n) \quad (\text{II.59})$$

where in the last equality we have applied Lemma 2 two successive times for for some $\rho_1 \in (\rho_-, \rho)$, and $O(\rho_1^{2n})$ holds on $\rho \leq |z| \leq \rho^{-1}$, uniformly in z . Now, assuming that the condition (I.16) of Theorem 2 holds, using (II.56) we get

$$\alpha_k^{(n)} O(\rho_1^{2n}) = O((\rho_1/\rho)^2) \quad (\text{II.60})$$

Defining

$$\sigma = \max\{(\rho_1/\rho)^2, \rho\} \quad (\text{II.61})$$

we have thus

$$[X_1^{(n)}]_-(z) = O(\sigma^n), \quad [X_1^{(n)}z^{-n}]_+ = O(\sigma^n), \quad [U_1^{(n)}]_- = 0, \quad [V_1^{(n)}]_+ = 0, \quad (\text{II.62})$$

where $O(\sigma^n)$ holds on $\rho \leq |z| \leq \rho^{-1}$, uniformly in z . These properties should be compared with (II.11). Because of the same reasoning as for the zero winding number case we expect

$$X^{(n)}(z) = X_1(z) + O(\sigma^n) \quad (\text{II.63})$$

on the unit circle $|z| = 1$. In this case we cannot provide a rigorous proof for this estimate, but we find it very natural and we have checked numerically that the final result, i.e. Theorem 2, holds in several relevant cases.

It follows

$$\begin{aligned} X^{(n)}(e^{i\theta_0})e^{\nu\theta_0} &= e^{-i(n+\nu-1)\theta_0}a_+^{-2}(e^{i\theta_0})\frac{d}{dz}\left(c(z)z^{n+\nu}\right)\Big|_{z=e^{i\theta_0}} \\ &+ e^{i(\nu+1)\theta_0}a_-^{-1}(e^{i\theta_0})\sum_{k=0}^{\nu-1}(a_+^{-1})_k\frac{d}{dz}z^{k-\nu}\Big|_{z=e^{i\theta_0}} + a_+^{-1}(e^{i\theta_0})\sum_{k=1}^{\nu}\alpha_k^{(n)}[cz^{n+\nu-k}]_+(e^{i\theta_0}) + O(\sigma^n) \end{aligned} \quad (\text{II.64})$$

from which we get

$$\begin{aligned} X^{(n)}(e^{i\theta_0})e^{\nu\theta_0} &= a_+^{-1}(e^{i\theta_0})a_-^{-1}(e^{i\theta_0})(n+\nu) + e^{i\theta_0}a_+^{-2}(e^{i\theta_0})\frac{dc(z)}{dz}\Big|_{z=e^{i\theta_0}} \\ &+ a_-^{-1}(e^{i\theta_0})\sum_{k=0}^{\nu-1}(k-\nu)(a_+^{-1})_ke^{ik\theta_0} + a_+^{-1}(e^{i\theta_0})\sum_{k=1}^{\nu}\alpha_k^{(n)}[cz^{n+\nu-k}]_+(e^{i\theta_0}) + O(\sigma^n). \end{aligned} \quad (\text{II.65})$$

Lemma 2 gives a simplification

$$[cz^{n+\nu-k}]_+(e^{i\theta_0}) = c(e^{i\theta_0})e^{i(n+\nu-k)\theta_0} + O(\rho^n) \quad (\text{II.66})$$

from which it follows

$$X^{(n)}(e^{i\theta_0})e^{\nu\theta_0} = a_-^{-1}(e^{i\theta_0})\sum_{k=1}^{\nu}\alpha_k^{(n)}(e^{i(n+\nu-k)\theta_0} + O(\rho^n)) + a_+^{-1}(e^{i\theta_0})a_-^{-1}(e^{i\theta_0})n + O(1). \quad (\text{II.67})$$

Theorem 2 follows directly from (II.6) and (II.67), where the result for the case $\nu < 0$ descends from the one for $\nu > 0$ by transposing the original Toeplitz matrix in (I.1) and making the integral transformation $\theta \rightarrow -\theta$.

III. APPLICATION OF THE RESULTS: FRUSTRATED QUANTUM XY CHAIN IN ZERO FIELD

As an example of a concrete application of our results we compute the lowest energy band spin-correlation functions and the ground state magnetization for the frustrated quantum spin chain defined by the Hamiltonian

$$H = \sum_{j=1}^N \left(\sigma_j^x \sigma_{j+1}^x - \lambda \sigma_j^y \sigma_{j+1}^y \right), \quad (\text{III.1})$$

where $\lambda \in (0, 1)$ is the anisotropy parameter, $N = 2M + 1$ is the number of lattice sites, which is imposed to be odd, σ^α for $\alpha = x, y, z$, are Pauli matrices, and periodic boundary conditions are imposed ($\sigma_j^\alpha = \sigma_{j+N}^\alpha$). This kind of models, known as XY chains, have been introduced in [19] and its ground state spin-correlation functions have been computed in [19–21]. However, in (III.1) we take the dominant interaction (along the x component of the spins) to favor antiferromagnetic order. This choice, coupled with the periodic boundary conditions on a ring with an odd number of sites N , introduces *boundary frustration* different properties, which have been studied in [12–16]. The frustrated model is interesting also because it demonstrates that different boundary conditions and different parities in N can result in different ground state order even in the thermodynamic limit ($N \rightarrow \infty$).

We briefly review some properties of the model, found in [14, 15], to introduce the notation. Denoting by $\Pi^\alpha = \prod_{j=1}^N \sigma_j^\alpha$, for $\alpha = x, y, z$, the parity operators, we have that all three commute with the Hamiltonian (III.1) $[\Pi^\alpha, H] = 0$, but, with odd N , satisfy a non-commuting algebra $[\Pi^\alpha, \Pi^\beta] = i\varepsilon^{\alpha,\beta,\gamma}2(-1)^{\frac{N-1}{2}}\Pi^\gamma$, which is essentially $SU(2)$. More

interestingly for us, the parities anticommute $\{\Pi^\alpha, \Pi^\beta\} = \delta_{\alpha,\beta}$. Because of these symmetries, every eigenstate of the spin chain (III.1) is at least two-fold degenerate. In fact, if $|\Omega\rangle$ is an eigenstate of (III.1) with, for instance, positive z -parity $\Pi^z |\Omega\rangle = |\Omega\rangle$, then $\Pi^x |\Omega\rangle$ has the same energy eigenvalue with respect to H and opposite z -parity.

In each sector of given z -parity, the XY chain can be mapped exactly, although non-locally, to a system of free fermions [22]. This mapping allows to represent every state in a Fock space: one defines a vacuum $|0^\pm\rangle$ which is annihilated by fermionic operators a_q , with $q \in \Gamma^\pm$ belonging to a different set (of integers or half-integers) depending on the parity ($\Gamma^\pm = \{\frac{\pi}{N}(2j + \frac{1+\Pi^z}{2}) : j = 0, 1, \dots, N-1\}$), $a_q |0^\pm\rangle = 0$ for all $q \in \Gamma^\pm$, and applies the Bogoliubov creation operators a_q^\dagger to create all other states. Only states with a number of excitations compatible with the parity are admissible in the Hilbert space of (III.1): assigning zero excitations to the vacua $|0^\pm\rangle$, each a_q^\dagger adds one. Even excitation states belong to the positive z -parity sector, while odd excitation ones have negative z -parity.

It is convenient to work just in a single z -parity (we will take $\Pi^z = -1$) and generate all (the degenerate) states with opposite parity through the application of Π^x . Due to the frustrated boundary conditions, the system is gapless with the energy gap between the states closing as $1/N^2$. This means that the lowest energy state is part of a band, spanned by the (single excitation) states $|q\rangle = a_q^\dagger |0^-\rangle$, which have negative z -parity $\Pi^z = -1$, and the states $\Pi^x |q\rangle = i(-1)^{(N-1)/2} \Pi^y |q\rangle$, which have the opposite z -parity $\Pi^z = 1$. The energy of the states $|q\rangle$ and $\Pi^x |q\rangle$ is equal and the index q is the momentum of the excitation, that can be related to lattice translations [15]. The ground state, in particular, has momentum $q = 0$, and is two-fold degenerate [14]. A generic ground state is, therefore, a superposition

$$|g\rangle = \cos \theta |g^-\rangle + \sin \theta e^{i\psi} |g^+\rangle, \quad (\text{III.2})$$

where $|g^-\rangle = |q = 0\rangle$, $|g^+\rangle = \Pi^x |g^-\rangle$, $\theta \in [0, 2\pi)$ and $\psi \in [0, 2\pi)$.

We are interested in the spin correlation functions $\langle q | \sigma_1^x \sigma_{1+n}^x | q \rangle$ and $\langle q | \sigma_1^y \sigma_{1+n}^y | q \rangle$, and in the ground state magnetizations $\langle g | \sigma_1^x | g \rangle$ and $\langle g | \sigma_1^y | g \rangle$. Note that, as a consequence of the symmetries and of the exact degeneracies, it is possible to have a spontaneous finite magnetization even for finite N .

1. Spin-correlation functions

Using the Majorana fermions representation of the spin operators and performing the Wick contractions as in [12], the spin correlation functions can be expressed in terms of Toeplitz determinants

$$\langle q | \sigma_1^\alpha \sigma_{1+n}^\alpha | q \rangle = (-1)^n \left[\left(\tilde{D}_n(\tilde{f}) + \text{c.c.} \right) - D_n(f) \right], \quad (\text{III.3})$$

where c.c. stands for the complex conjugate and

$$\tilde{f}_j^{(n)} = f_j - \frac{1}{N} f(e^{iq}) e^{-iqj}, \quad (\text{III.4})$$

$$f_j = \frac{1}{N} \sum_{\theta \in \Gamma^-} f(e^{i\theta}) e^{-ij\theta} \stackrel{N \rightarrow \infty}{\simeq} \frac{1}{2\pi} \int_0^{2\pi} f(e^{i\theta}) e^{-ij\theta} d\theta, \quad (\text{III.5})$$

$$f(z) = a(z) z^\nu, \quad a(z) = \sqrt{\frac{1 - \lambda z^{-2}}{1 - \lambda z^2}}. \quad (\text{III.6})$$

$$(\text{III.7})$$

The winding number is $\nu = 0$ for $\alpha = x$ and $\nu = 2$ for $\alpha = y$. Comparing with (I.3) we see that $z_n = -1/N$, thus a constant with respect to n , although, from physical considerations, we must have $n < N/2$.

We see that a is analytic on $\lambda^{1/2} < |z| < \lambda^{-1/2}$ and by inspection we find

$$a_+(z) = a_-^{-1}(z^{-1}) = (1 - \lambda z^2)^{-1/2}, \quad c(z) = b^{-1}(z) = a_+(z) a_-^{-1}(z) = [(1 - \lambda z^2)(1 - \lambda z^{-2})]^{-1/2}. \quad (\text{III.8})$$

The determinant $D_n(f)$ has already been computed in [20] because it determines the ground state spin-correlation functions in absence of frustration. For $\nu = 0$ it is given by

$$D_n(f) \quad (\text{III.9})$$

$$= (1 - \lambda^2)^{1/2} \left[1 + 4 \left(\frac{\lambda}{1 - \lambda^2} \right)^2 \frac{\lambda^n}{\pi n^2} (1 + O(n^{-1})) \right], \quad \text{for } n = 2m \text{ as } m \rightarrow \infty, \quad (\text{III.10})$$

$$= (1 - \lambda^2)^{1/2} \left[1 + 2 \frac{1 + \lambda^2}{\lambda} \left(\frac{\lambda}{1 - \lambda^2} \right)^2 \frac{\lambda^n}{\pi n^2} (1 + O(n^{-1})) \right], \quad \text{for } n = 2m + 1 \text{ as } m \rightarrow \infty. \quad (\text{III.11})$$

Applying Theorem 1, with the term

$$\left. \frac{d}{d\theta} \log b(e^{i\theta}) \right|_{\theta=q} = \frac{2\lambda \sin q}{1 + \lambda^2 - 2\lambda \cos 2q} \in \mathbb{R} \quad (\text{III.12})$$

not contributing in (III.3), we find

$$\langle q | \sigma_1^x \sigma_{1+n}^x | q \rangle \quad (\text{III.13})$$

$$= (1 - \lambda^2)^{1/2} \left[1 + 4 \left(\frac{\lambda}{1 - \lambda^2} \right)^2 \frac{\lambda^n}{\pi n^2} (1 + O(n^{-1})) \right] \left[1 - \frac{2n}{N} (1 + O(\lambda^{\frac{n}{2}(1+\varepsilon)})) \right], \quad \text{for } n = 2m \text{ as } m \rightarrow \infty, \quad (\text{III.14})$$

$$= -(1 - \lambda^2)^{1/2} \left[1 + 2 \frac{1 + \lambda^2}{\lambda} \left(\frac{\lambda}{1 - \lambda^2} \right)^2 \frac{\lambda^n}{\pi n^2} (1 + O(n^{-1})) \right] \left[1 - \frac{2n}{N} (1 + O(\lambda^{\frac{n}{2}(1+\varepsilon)})) \right], \quad \text{for } n = 2m + 1 \text{ as } m \rightarrow \infty, \quad (\text{III.15})$$

where $\varepsilon > 0$ is arbitrarily small.

To compute $\langle q | \sigma_1^y \sigma_{1+n}^y | q \rangle$ using Theorem 2 we need to find

$$c_{-n} = \frac{1}{2\pi i} \oint_{|w|=1} \frac{w^{n-1}}{[(1 - \lambda z^2)(1 - \lambda z^{-2})]^{1/2}} dw. \quad (\text{III.16})$$

Integrals of this type have been computed in [17, 18, 20, 21], for the purpose of computing the ground state spin-correlation functions, using the properties of the hypergeometric functions. This one is given by

$$c_{-n} = \frac{2^{1/2}}{(1 - \lambda^2)^{1/2}} \frac{\lambda^{\frac{n}{2}}}{\sqrt{\pi n}} (1 + O(n^{-1})) \quad \text{for } n = 2m \text{ as } m \rightarrow \infty. \quad (\text{III.17})$$

$$c_{-n} = 0 \quad \text{for } n = 2m + 1. \quad (\text{III.18})$$

Applying Theorem 2, where the condition (I.16) of the theorem is satisfied for ρ close to $\sqrt{\lambda}$, and using the result (I.13) for $D_n(f)$, we find

$$\langle q | \sigma_1^y \sigma_{1+n}^y | q \rangle \quad (\text{III.19})$$

$$= \frac{2}{1 - \lambda} \frac{\lambda^n}{\pi n} (1 + O(n^{-1})) + 2^{5/2} \frac{\cos nq}{(1 + \lambda^2 - 2\lambda \cos 2q)^{1/2}} \frac{\lambda^{\frac{n}{2}}}{N \sqrt{\pi n}} (1 + O(n^{-1})) \quad \text{for } n = 2m \text{ as } m \rightarrow \infty. \quad (\text{III.20})$$

$$= \frac{2}{1 - \lambda} \frac{\lambda^n}{\pi n} (1 + O(n^{-1})) + 2^{3/2} \frac{\lambda^{-\frac{1}{2}} \cos[(n+1)q] + \lambda^{\frac{1}{2}} \cos[(n-1)q]}{(1 + \lambda^2 - 2\lambda \cos 2q)^{1/2}} \frac{\lambda^{\frac{n}{2}}}{N \sqrt{\pi n}} (1 + O(n^{-1})) \quad \text{for } n = 2m + 1 \text{ as } m \rightarrow \infty. \quad (\text{III.21})$$

In the ground state ($q = 0$) terms proportional to $1/N$ in (III.13) and (III.19) are due to the delta-function singularity in the symbol and make the difference between the frustrated model and the model without frustration (that is, periodic boundary conditions with $N = 2M$ or free boundary conditions). In this case, the difference is relevant only at distances n comparable to the system size N . Without these terms, the x correlation function would converge exponentially fast to a saturation value as the distance between sites is increased, while the y correlation decays to zero, reflecting a spontaneous magnetization developing only in the x direction. The dependence (III.13) implies, instead, that the correlations between the most distant spins, separated by $n = (N - 1)/2$, decay as $1/N$ as we increase the (odd) system size N . This kind of behavior in frustrated quantum chains was first found in [23, 24] and later further discussed, and checked numerically, in [12–14, 16].

2. The ground state magnetization

As discussed in [14, 15], the magnetization in the ground state is mesoscopic (that is, finite in finite systems) and ferromagnetic, i.e. $\langle g | \sigma_1^x | g \rangle = \langle g | \sigma_j^x | g \rangle$ for $j = 2, 3, \dots, N$, in a generic ground state $|g\rangle$ defined by (III.2). It is given by

$$\langle g | \sigma_1^x | g \rangle = \cos \psi \sin 2\theta \langle g^- | \sigma_1^x \Pi^x | g^- \rangle \quad (\text{III.22})$$

$$\langle g | \sigma_1^y | g \rangle = (-1)^{\frac{N-1}{2}} \sin \psi \sin 2\theta \langle g^- | \sigma_1^y \Pi^y | g^- \rangle \quad (\text{III.23})$$

The absolute values of the quantities $\langle g | \sigma_1^\alpha \Pi^\alpha | g \rangle$, for $\alpha = x, y$, are the maximal values of the magnetization on the ground state manifold, and it has been shown in [14] that these quantities can be expressed as Toeplitz determinants, as

$$\langle g^- | \sigma_1^\alpha \Pi^\alpha | g^- \rangle \stackrel{N \rightarrow \infty}{\simeq} (-1)^n \tilde{D}_n(\tilde{f}), \quad (\text{III.24})$$

where

$$n = \frac{N-1}{2}, \quad \tilde{f}_j^{(n)} = f_j - \frac{2}{N}, \quad (\text{III.25})$$

$$f_j = \frac{1}{2\pi} \int_0^{2\pi} f(e^{i\theta}) e^{-ij\theta} d\theta, \quad (\text{III.26})$$

$$f(z) = a(z)z^\nu, \quad a(z) = \sqrt{\frac{1-\lambda z^{-1}}{1-\lambda z}}. \quad (\text{III.27})$$

Here the winding number is $\nu = 0$ for $\alpha = x$ and $\nu = 1$ for $\alpha = y$. Theorems 1 and 2 can be applied with $z_n = 1/N = 1/(2n+1)$.

We proceed in a similar way to the previous section. The function $a(z)$ is analytic on $\lambda < |z| < \lambda^{-1}$, and by inspection we find

$$a_+(z) = a_-^{-1}(z^{-1}) = (1-\lambda z)^{-1/2}, \quad c(z) = b^{-1}(z) = a_+(z)a_-^{-1}(z) = [(1-\lambda z)(1-\lambda z^{-1})]^{-1/2}. \quad (\text{III.29})$$

The coefficients c_{-n} are given by

$$c_{-n} = \frac{1}{2\pi i} \oint_{|w|=1} \frac{w^{n-1}}{[(1-\lambda z)(1-\lambda z^{-1})]^{1/2}} dw = \frac{\lambda^n}{\sqrt{\pi n}} \left(1 + O(n^{-1})\right). \quad (\text{III.30})$$

Applying Theorems 1 and 2 we find

$$\langle g^- | \sigma_1^x \Pi^x | g^- \rangle = (-1)^{\frac{N-1}{2}} \frac{1}{N} (1-\lambda^2)^{\frac{1}{4}} \left(1 + O(\lambda^{\frac{N}{2}(1+\varepsilon)})\right), \quad (\text{III.31})$$

$$\langle g^- | \sigma_1^y \Pi^y | g^- \rangle = \frac{2}{N} \frac{(1+\lambda)^{\frac{1}{4}}}{(1-\lambda)^{\frac{3}{4}}} \left(1 + O(\lambda^{\frac{N}{2}(1+\varepsilon)})\right), \quad (\text{III.32})$$

where $N = 2M + 1$, as $M \rightarrow \infty$. Here $\varepsilon > 0$ is arbitrarily small.

We remark that without frustration (that is, without the delta-function in the symbol) the Toeplitz determinant in (III.31) would approach a constant exponentially fast, while the one in (III.32) would similarly decay to zero, while with the delta-function they both show an algebraic decay in the matrix rank. We conclude that both magnetizations go to zero as $N = 2M + 1, M \rightarrow \infty$, which is in a striking difference from the behavior of the model in the limit $N = 2M, M \rightarrow \infty$, and from the behavior of the model with free boundary conditions.

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Appendix A: Existence and uniqueness of the solution

For all $n \geq n_0$ we have $D_n(f) \neq 0$ so there exists a unique solution $x_j^{(n)}$, for $j = 0, 1, \dots, n-1$, of the linear problem

$$\sum_{k=0}^{n-1} f_{j-k} x_k^{(n)} = y_j^{(n)}, \quad \text{for } j = 0, 1, \dots, n-1, \quad (\text{A.1})$$

for arbitrary complex numbers $y_j^{(n)}$, $j = 0, 1, \dots, n-1$. We define the coefficients

$$u_j^{(n)} = \begin{cases} \sum_{k=0}^{n-1} f_{j-k+n} x_k^{(n)}, & \text{for } j = 0, 1, 2, \dots \\ 0, & \text{for } j = -1, -2, \dots \end{cases}, \quad v_j^{(n)} = \begin{cases} 0, & \text{for } j = 0, 1, 2, \dots \\ \sum_{k=0}^{n-1} f_{j-k} x_k^{(n)}, & \text{for } j = -1, -2, \dots \end{cases} \quad (\text{A.2})$$

and the functions

$$U^{(n)} = \sum_{j=0}^{\infty} u_j^{(n)} z^j, \quad V^{(n)} = \sum_{j=1}^{\infty} v_{-j}^{(n)} z^{-j}. \quad (\text{A.3})$$

The functions $U^{(n)}$ and $V^{(n)}$ are well defined, and therefore analytic, on the same annulus as $f(z)$, the one defined by (I.7). To see this pick some z from the annulus. We have

$$\begin{aligned} \sum_{j=1}^{\infty} |v_{-j}^{(n)}| |z|^{-j} &\leq \sum_{j=1}^{\infty} \sum_{k=0}^{n-1} |f_{-j-k}| |x_k^{(n)}| |z|^{-j} = \sum_{k=0}^{n-1} |x_k^{(n)}| |z|^k \sum_{j=1}^{\infty} |f_{-j-k}| |z|^{-j-k} \\ &\leq \left(\sum_{j=-\infty}^{\infty} |f_j| |z|^j \right) \left(\sum_{k=0}^{n-1} |x_k^{(n)}| |z|^k \right) < \infty, \end{aligned} \quad (\text{A.4})$$

where the last inequality holds because Laurent series is absolutely convergent in the interior of its annulus. In an analogous way it is shown that $U^{(n)}$ is well defined.

It follows from definition (A.2) that the equation

$$\sum_{k=0}^{n-1} f_{j-k} x_k^{(n)} = y_j^{(n)} + u_{j-n}^{(n)} + v_j^{(n)}, \quad (\text{A.5})$$

with $y_j^{(n)}$ defined to be zero for $j < 0$ and $j \geq n$, holds for all $j \in \mathbb{Z}$. Multiplying the equation by z^j , with z belonging to the annulus (I.7), and summing from $j = -\infty$ to $j = \infty$ it follows

$$f(z)X^{(n)}(z) = Y^{(n)}(z) + U^{(n)}(z)z^n + V^{(n)}(z), \quad (\text{A.6})$$

where

$$X^{(n)}(z) = \sum_{j=0}^{n-1} x_j^{(n)} z^j, \quad Y^{(n)}(z) = \sum_{j=0}^{n-1} y_j^{(n)} z^j. \quad (\text{A.7})$$

Thus we have shown that, for arbitrary polynomials $Y^{(n)}$ of degree not greater than $n-1$, i.e. analytic functions with the properties

$$[Y^{(n)}]_- = 0, \quad [Y^{(n)} z^{-n}]_+ = 0, \quad (\text{A.8})$$

that the functions $X^{(n)}, U^{(n)}, V^{(n)}$ are the solution of the functional equation

$$fX^{(n)} = Y^{(n)} + U^{(n)}z^n + V^{(n)} \quad (\text{A.9})$$

on the annulus and by construction they have the properties

$$[X^{(n)}]_- = 0, \quad [X^{(n)} z^{-n}]_+ = 0, \quad [U^{(n)}]_- = 0, \quad [V^{(n)}]_+ = 0. \quad (\text{A.10})$$

The uniqueness of the solution of (A.1) implies the uniqueness of the solution of (A.9) under constraint (A.10).

Appendix B: Wiener-Hopf procedure

1. Wiener-Hopf equations

We assume $\nu \geq 0$. The determinant (I.1) for $\nu < 0$ can be obtained simply by transposing the Toeplitz matrix for the opposite sign of ν and making the integral transformation $\theta \rightarrow -\theta$. From (A.9) it follows, separating the components,

$$a_+ z^\nu X^{(n)} - [a_-^{-1} Y^{(n)}]_+ - [a_-^{-1} U^{(n)} z^n]_+ = a_-^{-1} V^{(n)} + [a_-^{-1} Y^{(n)}]_- + [a_-^{-1} U^{(n)} z^n]_-, \quad (\text{B.1})$$

where a_{\pm} have been defined in (I.8). We now use the standard Wiener-Hopf argument [17]. Namely, the properties (A.10) imply that through it's Laurent series the left-hand side defines a function analytic on $|z| < \rho_+$, while the right-hand side defines a function analytic on $|z| > \rho_-$, that goes to zero for $|z| \rightarrow \infty$. The two sides together define a function analytic on the whole plane and zero at infinity, thus, by Liouville's theorem, zero on the whole plane. It follows

$$X^{(n)}z^{\nu} = a_+^{-1}([a_-^{-1}Y^{(n)}]_+ + [a_-^{-1}U^{(n)}z^n]_+), \quad (\text{B.2})$$

$$V^{(n)} = -a_-([a_-^{-1}Y^{(n)}]_- + [a_-^{-1}U^{(n)}z^n]_-). \quad (\text{B.3})$$

Similarly, denoting

$$\alpha_k^{(n)} = (a_+^{-1}U^{(n)}z^{-\nu})_{-k}, \quad (\text{B.4})$$

and multiplying (A.9) by $a_+^{-1}z^{-(n+\nu)}$, we can make the separation

$$\begin{aligned} & \left(a_+^{-1}U^{(n)}z^{-\nu} - \sum_{k=1}^{\nu} \alpha_k^{(n)}z^{-k} \right) + [a_+^{-1}Y^{(n)}z^{-(n+\nu)}]_+ + [a_+^{-1}V^{(n)}z^{-(n+\nu)}]_+ \\ &= a_-X^{(n)}z^{-n} - [a_+^{-1}Y^{(n)}z^{-(n+\nu)}]_- - [a_+^{-1}V^{(n)}z^{-(n+\nu)}]_- - \sum_{k=1}^{\nu} \alpha_k^{(n)}z^{-k}. \end{aligned} \quad (\text{B.5})$$

It follows

$$U^{(n)}z^{-\nu} = -a_+([a_+^{-1}Y^{(n)}z^{-(n+\nu)}]_+ + [a_+^{-1}V^{(n)}z^{-(n+\nu)}]_+) + a_+ \sum_{k=1}^{\nu} \alpha_k^{(n)}z^{-k}, \quad (\text{B.6})$$

$$X^{(n)}z^{-n} = a_-^{-1}([a_+^{-1}Y^{(n)}z^{-(n+\nu)}]_- + [a_+^{-1}V^{(n)}z^{-(n+\nu)}]_-) + a_-^{-1} \sum_{k=1}^{\nu} \alpha_k^{(n)}z^{-k}. \quad (\text{B.7})$$

This result is also valid for $\nu = 0$ adopting the convention $\sum_{k=1}^0 = 0$.

The solution of the set of equations (B.2), (B.3), (B.6) and (B.7), together with the requirement

$$(X^{(n)}z^{\nu})_j = 0 \quad \text{for } j = 0, 1, \dots, \nu - 1, \quad (\text{B.8})$$

that fixes the coefficients $\alpha_1^{(n)}, \alpha_2^{(n)}, \dots, \alpha_{\nu}^{(n)}$, is the solution of (A.9) with the desired properties (A.10).

2. The solution

In this section we solve asymptotically the functional equation (A.9) with $Y^{(n)}$ defined by (II.8) and (II.9). For the set of equations (B.2), (B.3), (B.6) and (B.7) a solution in the closed form might not exist so we follow the standard approach [17, 18] and we look for the solution by making an assumption on the function $U^{(n)}$ and then checking whether the final solution we obtain is consistent with this assumption.

We assume that

$$U^{(n)}z^{-\nu} - a_+ \sum_{k=1}^{\nu} \alpha_k^{(n)}z^{-k} = O(1) \quad \text{uniformly in } z, \text{ on } \rho \leq |z| \leq \rho^{-1}, \text{ for all } \rho \text{ defined by (I.10)}. \quad (\text{B.9})$$

The second term in (B.3) is equal to

$$[a_-^{-1}U^{(n)}z^n]_- = \left[a_-^{-1}z^{n+\nu} \left(U^{(n)}z^{-\nu} - a_+ \sum_{k=1}^{\nu} \alpha_k^{(n)}z^{-k} \right) \right]_- + \left[a_+a_-^{-1} \sum_{k=1}^{\nu} \alpha_k^{(n)}z^{n+\nu-k} \right]_-. \quad (\text{B.10})$$

Applying Lemma 2 on the first term in (B.10) gives

$$[a_-^{-1}U^{(n)}z^n]_- = \left[a_+a_-^{-1} \sum_{k=1}^{\nu} \alpha_k^{(n)}z^{n+\nu-k} \right]_- + O(\rho^n), \quad (\text{B.11})$$

where $O(\rho^n)$ holds on $\rho \leq |z| \leq \rho^{-1}$, uniformly in z , for all ρ satisfying (I.10). From now on it is always the case and we don't write every time that O holds uniformly in z on $\rho \leq |z| \leq \rho^{-1}$, for all ρ satisfying (I.10). We can thus write (B.3) as

$$V^{(n)}(z) = -a_-(z)[a_-^{-1}Y^{(n)}]_-(z) - a_-(z) \sum_{k=1}^{\nu} \alpha_k^{(n)} [a_+ a_-^{-1} z^{n+\nu-k}]_-(z) + O(\rho^n). \quad (\text{B.12})$$

We use (II.15) to rewrite the first term on the RHS of (B.12) as

$$[a_-^{-1}Y^{(n)}]_- = e^{-i(n-1)\theta_0} \left[\frac{a_-^{-1}z^n}{z - e^{i\theta_0}} \right]_-^{(<)} - e^{i\theta_0} \left[\frac{a_-^{-1}}{z - e^{i\theta_0}} \right]_-^{(<)}. \quad (\text{B.13})$$

The first term here is $O(\rho^n)$ by Lemma 2. Applying Lemma 1 to the second term gives

$$[a_-^{-1}Y^{(n)}]_-(z) = -e^{i\theta_0} \frac{a_-^{-1}(z) - a_-^{-1}(e^{i\theta_0})}{z - e^{i\theta_0}} + O(\rho^n) \quad \text{for } z \neq e^{i\theta_0}, \rho \leq |z| \leq \rho^{-1}. \quad (\text{B.14})$$

The value at $z = e^{i\theta_0}$ is obtained by continuity and from now on we omit writing $z \neq e^{i\theta_0}$, $\rho \leq |z| \leq \rho^{-1}$ every time. It follows

$$V^{(n)}(z) = e^{i\theta_0} a_-(z) \frac{a_-^{-1}(z) - a_-^{-1}(e^{i\theta_0})}{z - e^{i\theta_0}} - a_-(z) \sum_{k=1}^{\nu} \alpha_k^{(n)} [a_-^{-1} a_+ z^{n+\nu-k}]_-(z) + O(\rho^n). \quad (\text{B.15})$$

This expression can be used in (B.6) to find $U^{(n)}$. Before we do so, we use (II.15) again to get for the first term on the RHS of (B.6):

$$[a_+^{-1}Y^{(n)} z^{-(n+\nu)}]_+ = e^{-i(n-1)\theta_0} \left[\frac{a_+^{-1} z^{-\nu}}{z - e^{i\theta_0}} \right]_+^{(>)} - e^{i\theta_0} \left[\frac{a_+^{-1} z^{-(n+\nu)}}{z - e^{i\theta_0}} \right]_+^{(>)}. \quad (\text{B.16})$$

The second term is $O(\rho^n)$ by Lemma 2. Applying Lemma 1 to the first term we get

$$[a_+^{-1}Y^{(n)} z^{-(n+\nu)}]_+(z) = e^{-i(n-1)\theta_0} \frac{[a_+^{-1} z^{-\nu}]_+(z) - [a_+^{-1} z^{-\nu}]_+(e^{i\theta_0})}{z - e^{i\theta_0}} + O(\rho^n). \quad (\text{B.17})$$

We can now substitute (B.15) in (B.6) and apply Lemma 2 to the second term on the RHS of (B.6) to get

$$[a_+^{-1}V^{(n)} z^{-(n+\nu)}]_+(z) = - \sum_{k=1}^{\nu} \alpha_k^{(n)} [a_- a_+^{-1} z^{-(n+\nu)} [a_-^{-1} a_+ z^{n+\nu-k}]_-]_+(z) + O(\rho^n). \quad (\text{B.18})$$

Collecting everything it follows from (B.6)

$$\begin{aligned} U^{(n)} z^{-\nu} = & - e^{-i(n-1)\theta_0} a_+(z) \frac{[a_+^{-1} z^{-\nu}]_+(z) - [a_+^{-1} z^{-\nu}]_+(e^{i\theta_0})}{z - e^{i\theta_0}} + \\ & + a_+(z) \sum_{k=1}^{\nu} \alpha_k^{(n)} \left(z^{-k} + [a_- a_+^{-1} z^{-(n+\nu)} [a_-^{-1} a_+ z^{n+\nu-k}]_-]_+(z) \right) + O(\rho^n). \end{aligned} \quad (\text{B.19})$$

The coefficients $\alpha_1^{(n)}, \alpha_2^{(n)}, \dots, \alpha_{\nu}^{(n)}$ remain to be determined. However, if we assume that, for sufficiently small ρ , they satisfy

$$\alpha_k^{(n)} O(\rho^{2n}) = O(1), \quad \text{for } k = 1, 2, \dots, \nu, \quad (\text{B.20})$$

then, taking a ρ_1 such that $\rho_- < \rho_1 < \rho < 1 < \rho^{-1} < \rho_1^{-1} < \rho_+$, the last term in (B.19) is, by Lemma 2,

$$a_+(z) \sum_{k=1}^{\nu} \alpha_k^{(n)} [a_- a_+^{-1} z^{-(n+\nu)} [a_-^{-1} a_+ z^{n+\nu-k}]_-]_+(z) = a_+(z) \sum_{k=1}^{\nu} \alpha_k^{(n)} O(\rho_1^{2n}) = O((\rho_1/\rho)^2), \quad \text{on } \rho \leq |z| \leq \rho^{-1}. \quad (\text{B.21})$$

It follows

$$U^{(n)} z^{-\nu} = -e^{-\iota(n-1)\theta_0} a_+(z) \frac{[a_+^{-1} z^{-\nu}]_+(z) - [a_+^{-1} z^{-\nu}]_+(e^{\iota\theta_0})}{z - e^{\iota\theta_0}} + a_+(z) \sum_{k=1}^{\nu} \alpha_k^{(n)} z^{-k} + O(\sigma^n), \quad (\text{B.22})$$

where $\sigma = \max\{(\rho_1/\rho)^2, \rho\}$. Then (B.22) is consistent with the starting assumption (B.9), while assumption (B.20) will be checked below for its consistency.

Finally, $X^{(n)}$ is computed using (B.2). The first term in (B.2) is found from (II.15) and (B.14), using

$$[a_-^{-1} Y^{(n)}]_+ = a_-^{-1} Y^{(n)} - [a_-^{-1} Y^{(n)}]_- . \quad (\text{B.23})$$

We get

$$[a_-^{-1} Y^{(n)}]_+(z) = e^{-\iota(n-1)\theta_0} \frac{a_-^{-1}(z) z^n - a_-^{-1}(e^{\iota\theta_0}) e^{\iota n \theta_0}}{z - e^{\iota\theta_0}} + O(\rho^n). \quad (\text{B.24})$$

The second term in (B.2) is found from (B.11) and (B.22),

$$\begin{aligned} [a_-^{-1} U^{(n)} z^n]_+ &= a_-^{-1} U^{(n)} z^n - [a_-^{-1} U^{(n)} z^n]_- \\ &= -e^{-\iota(n-1)\theta_0} a_-^{-1}(z) a_+(z) z^{n+\nu} \frac{a_+^{-1}(z) z^{-\nu} - a_+^{-1}(e^{\iota\theta_0}) e^{-\iota\nu\theta_0}}{z - e^{\iota\theta_0}} \\ &\quad + e^{-\iota(n-1)\theta_0} a_-^{-1}(z) a_+(z) z^{n+\nu} \sum_{k=0}^{\nu-1} (a_+^{-1})_k \frac{z^{k-\nu} - e^{\iota(k-\nu)\theta_0}}{z - e^{\iota\theta_0}} \\ &\quad + \left[a_+ a_-^{-1} \sum_{k=1}^{\nu} \alpha_k^{(n)} z^{n+\nu-k} \right]_+ (z) + O(\sigma^n), \end{aligned} \quad (\text{B.25})$$

where we used

$$[a_+^{-1} z^{-\nu}]_+ = a_+^{-1} z^{-\nu} - \sum_{k=0}^{\nu-1} (a_+^{-1})_k z^{k-\nu}. \quad (\text{B.26})$$

Now, summing (B.24) and (B.25) in (B.2) gives

$$\begin{aligned} X^{(n)}(z) z^\nu &= e^{-\iota(n+\nu-1)\theta_0} a_+^{-1}(z) a_+^{-1}(e^{\iota\theta_0}) \frac{a_+(z) a_-^{-1}(z) z^{n+\nu} - a_+(e^{\iota\theta_0}) a_-^{-1}(e^{\iota\theta_0}) e^{\iota(n+\nu)\theta_0}}{z - e^{\iota\theta_0}} \\ &\quad + e^{-\iota(n-1)\theta_0} a_-^{-1}(z) z^{n+\nu} \sum_{k=0}^{\nu-1} (a_+^{-1})_k \frac{z^{k-\nu} - e^{\iota(k-\nu)\theta_0}}{z - e^{\iota\theta_0}} + a_+^{-1}(z) \sum_{k=1}^{\nu} \alpha_k^{(n)} [a_-^{-1} a_+ z^{n+\nu-k}]_+(z) + O(\sigma^n). \end{aligned} \quad (\text{B.27})$$

It remains to determine the coefficients $\alpha_1^{(n)}, \alpha_2^{(n)}, \dots, \alpha_\nu^{(n)}$ from requirement (B.8) and to see whether (B.20) is satisfied. We compute the coefficients $(X^{(n)} z^{-\nu})_j$ by (II.13), integrating at $|w| = \rho$. All the terms in (B.27) containing the factor z^n result in $O(\rho^n)$ corrections, while

$$\frac{1}{2\pi i} \oint_{|w|=\rho} \frac{a_+^{-1}(w)}{w - e^{\iota\theta_0}} \frac{dw}{w^{j+1}} = -e^{-\iota\theta_0} \sum_{k=0}^j (a_+^{-1})_k e^{-\iota(j-k)\theta_0}. \quad (\text{B.28})$$

It follows

$$(X^{(n)} z^\nu)_j = \sum_{k=1}^{\nu} \alpha_k^{(n)} \left(a_+^{-1} [c z^{n+\nu-k}]_+ \right)_j + a_-^{-1}(e^{\iota\theta_0}) \sum_{k=0}^j (a_+^{-1})_k e^{-\iota(j-k)\theta_0} + O(\sigma^n), \quad (\text{B.29})$$

where $c = a_+ a_-^{-1}$.

Thus if the coefficients $\alpha_1^{(n)}, \alpha_2^{(n)}, \dots, \alpha_\nu^{(n)}$ satisfy

$$0 = \sum_{k=1}^{\nu} \alpha_k^{(n)} \left(a_+^{-1} [c z^{n+\nu-k}]_+ \right)_j + a_-^{-1}(e^{\iota\theta_0}) \sum_{k=0}^j (a_+^{-1})_k e^{-\iota(j-k)\theta_0}, \quad \text{for } j = 0, 1, \dots, \nu-1, \quad (\text{B.30})$$

then

$$(X^{(n)}z^\nu)_j = O(\sigma^n), \quad \text{for } j = 0, 1, \dots, \nu - 1. \quad (\text{B.31})$$

Using

$$\left(a_+^{-1}[cz^{n+\nu-k}]_+\right)_j = \sum_{m=0}^j (a_+^{-1})_m c_{j-m-n-\nu+k} \quad (\text{B.32})$$

it's easy to see that (B.30) is equivalent to

$$\sum_{k=1}^{\nu} \alpha_k^{(n)} c_{j-n-\nu+k} = -a_-^{-1}(e^{i\theta_0})e^{-ij\theta_0}, \quad \text{for } j = 0, 1, \dots, \nu - 1. \quad (\text{B.33})$$

The set of equations (B.33) is solved by Cramer's rule. The solution is

$$\alpha_j^{(n)} = -a_-^{-1}(e^{i\theta_0})e^{-i(\nu-1)\theta_0} \frac{\tilde{\Delta}_{\nu,n}(j)}{\Delta_{\nu,n}} \quad (\text{B.34})$$

where $\Delta_{\nu,n}$ and $\tilde{\Delta}_{\nu,n}(j)$ are defined by (I.12) and (I.14) respectively. We see that the condition (B.9) of Theorem 2 ensures that the assumption (B.20) is satisfied.

The solution of equations (B.2), (B.3) and (B.6) we have found is consistent with assumptions (B.9) and (B.20), that we have made to find it, up to $O(\sigma^n)$ terms. On the basis of this solution we construct the functions $X_1^{(n)}$, $U_1^{(n)}$ and $V_1^{(n)}$ discussed in sections IID and IIE.

Appendix C: Remarks on rigor

To prove theorems 1 and 2 we have used the intuitive property that a small perturbation to the functional equation (A.9) results only in a small perturbation to the solutions. Here we show it rigorously for the case of a zero winding number of the symbol, and thus make Theorem 1 rigorous.

The result we need is given by Lemma 3, that we are going to state and prove. The proof of the lemma uses a similar procedure to the one used in the proof of Szegő theorem in chapter X of [17], based on the Wiener-Hopf equations. Let us note that the complication with non-zero winding number is the presence of the third term in (B.6) and we omit this case.

Before introducing the lemma let us introduce two norms for functions analytic on an annulus around the unit circle. The first one is the supremum norm on the unit circle. Let g be analytic on the annulus $\rho_- < |z| < \rho_+$ that includes the unit circle. We define

$$\|g\| = \sup_{z \in \mathbb{C}: |z|=1} |g(z)|. \quad (\text{C.1})$$

The second norm is defined as the sum of the absolute values of Laurent series coefficients of g , which is well defined since the Laurent series is absolutely convergent in the interior of its annulus. If $g(z) = \sum_{j=-\infty}^{\infty} g_j z^j$, we denote

$$\|g\|_1 = \sum_{j=-\infty}^{\infty} |g_j|. \quad (\text{C.2})$$

We have clearly

$$\|g\| \leq \|g\|_1. \quad (\text{C.3})$$

Let us discuss the properties of the norms related to the components (II.7). From their integral representation (II.12) we have

$$\|[g]_-\| \leq \frac{\rho_1}{1 - \rho_1} \sup_{z: |z|=\rho_1} \{|g(z)|\}, \quad \|[g]_+\| \leq \frac{\rho_2}{\rho_2 - 1} \sup_{z: |z|=\rho_2} |g(z)|, \quad (\text{C.4})$$

for any choice $\rho_1 \in (\rho_-, 1)$, $\rho_2 \in (1, \rho_+)$. On the other hand, the second norm clearly satisfies

$$\|[g]_-\|_1 \leq \|g\|_1, \quad \|[g]_+\|_1 \leq \|g\|_1. \quad (\text{C.5})$$

If g and h are two functions analytic on an annulus around the unit circle we have

$$\|gh\| \leq \|g\| \|h\|, \quad \|gh\|_1 \leq \|g\|_1 \|h\|_1, \quad (\text{C.6})$$

where the first inequality is trivial and the second is proven easily using the absolute convergence of the Laurent series inside the annulus. Finally, for a sequence of functions $(g^{(n)})_{n \in \mathbb{N}}$ analytic on an annulus around the unit circle and a sequence of positive numbers $(s_n)_{n \in \mathbb{N}}$ we have clearly that

$$g^{(n)}(z) = O(s_n) \quad \text{uniformly in } z \text{ on the unit circle } |z| = 1 \quad \text{if and only if} \quad \|g^{(n)}\| = O(s_n). \quad (\text{C.7})$$

Lemma 3. *Let a be non-zero analytic function on an annulus around the unit circle, defined by (I.7), and with a zero winding number. Let $Y_j^{(n)}$, for $j = 1, 2$ and $n \in \mathbb{N}$, be polynomials of degree not greater than $n - 1$, i.e. analytic functions with*

$$[Y_j^{(n)}]_- = 0, \quad [Y_j^{(n)} z^{-n}]_+ = 0, \quad (\text{C.8})$$

and let $X_j^{(n)}, U_j^{(n)}, V_j^{(n)}$, for $j = 1, 2$, be analytic solutions of the functional equation

$$aX_j^{(n)} = Y_j^{(n)} + U_j^{(n)} z^n + V_j^{(n)} \quad (\text{C.9})$$

on the annulus, such that they satisfy the properties

$$[X_j^{(n)}]_- = 0, \quad [X_j^{(n)} z^{-n}]_+ = 0, \quad [U_j^{(n)}]_- = 0, \quad [V_j^{(n)}]_+ = 0. \quad (\text{C.10})$$

If

$$Y_1^{(n)}(z) - Y_2^{(n)}(z) = O(s_n) \quad \text{uniformly in } z \text{ on the unit circle } |z| = 1 \quad (\text{C.11})$$

then

$$X_1^{(n)}(z) - X_2^{(n)}(z) = O(ns_n) \quad \text{uniformly in } z \text{ on the unit circle } |z| = 1. \quad (\text{C.12})$$

Proof. Defining

$$Y^{(n)} = Y_1^{(n)} - Y_2^{(n)}, \quad X^{(n)} = X_1^{(n)} - X_2^{(n)}, \quad U^{(n)} = U_1^{(n)} - U_2^{(n)}, \quad V^{(n)} = V_1^{(n)} - V_2^{(n)}, \quad (\text{C.13})$$

proving the lemma becomes equivalent to showing that if $\|Y^{(n)}\| = O(s_n)$ then the solution $X^{(n)}$ of the problem (A.9) (for $\nu = 0$) and (A.10) satisfies $\|X^{(n)}\| = O(ns_n)$.

The lines of the proof are the following. First we use the Wiener-Hopf equations (B.3) and (B.6) to show that $\|U^{(n)}\| = O(ns_n)$ and $\|V^{(n)}\| = O(ns_n)$. Then we recognize that directly from (A.9) and the properties of the norm it follows

$$\|X^{(n)}\| \leq \|a^{-1}\| \left(\|Y^{(n)}\| + \|U^{(n)}\| + \|V^{(n)}\| \right), \quad (\text{C.14})$$

and conclude that since the right hand side of the inequality is $O(ns_n)$, so is the left side.

We now work out the details. Note first that the Laurent series coefficients $y_j^{(n)}$ of the function $Y^{(n)}(z) = \sum_{j=0}^{n-1} y_j^{(n)} z^j$ satisfy $|y_j^{(n)}| \leq \|Y^{(n)}\|$, which can be seen easily from the integral representation of the coefficients. It follows

$$\|Y^{(n)}\|_1 \leq n \|Y^{(n)}\|. \quad (\text{C.15})$$

From the Wiener-Hopf equation (B.3) we get

$$\|V^{(n)}\| = \|a_-\| \left\| [a_+^{-1} Y^{(n)}]_- \right\| + \|a_-\| \left\| [a_+^{-1} U^{(n)} z^n]_- \right\|. \quad (\text{C.16})$$

To bound the first term we notice

$$\left\| [a_-^{-1} Y^{(n)}]_- \right\| \leq \left\| [a_-^{-1} Y^{(n)}]_- \right\|_1 \leq \left\| a_-^{-1} Y^{(n)} \right\|_1 \leq \|a_-^{-1}\|_1 \left\| Y^{(n)} \right\|_1 \leq \|a_-^{-1}\|_1 n \left\| Y^{(n)} \right\|, \quad (\text{C.17})$$

where all the inequalities except the last follow simply from the discussed properties of the norms, and the last one follows from (C.15). To bound the second term in (C.16) we use (C.4) with $\rho_1 = \rho$ for some ρ defined by (I.10). We have

$$\left\| [a_-^{-1} U^{(n)} z^n]_- \right\| \leq \frac{\rho^{n+1}}{1-\rho} \sup_{z:|z|=\rho} \{|a_-^{-1}(z)U^{(n)}(z)|\}. \quad (\text{C.18})$$

Since the Laurent series coefficients of $U^{(n)}$ define a function analytic inside the whole circle $|z| < \rho^{-1}$ we can apply the maximum modulus principle to conclude

$$\sup_{z:|z|=\rho} \{|U^{(n)}(z)|\} \leq \sup_{z:|z|=1} \{|U^{(n)}(z)|\} = \left\| U^{(n)} \right\|. \quad (\text{C.19})$$

It follows

$$\left\| [a_-^{-1} U^{(n)} z^n]_- \right\| \leq \frac{\rho^{n+1}}{1-\rho} \sup_{z:|z|=\rho} \{|a_-^{-1}(z)|\} \left\| U^{(n)} \right\|. \quad (\text{C.20})$$

We conclude that there are positive constants λ_1 and λ_2 (independent of n) such that

$$\left\| V^{(n)} \right\| \leq \lambda_1 n \left\| Y^{(n)} \right\| + \lambda_2 \rho^n \left\| U^{(n)} \right\|. \quad (\text{C.21})$$

Using the same methods we conclude from the Wiener-Hopf equation (B.6) that there are positive constants λ_3 and λ_4 such that

$$\left\| U^{(n)} \right\| \leq \lambda_3 n \left\| Y^{(n)} \right\| + \lambda_4 \rho^n \left\| V^{(n)} \right\|. \quad (\text{C.22})$$

We have obtained a system of two inequalities. Inserting the second into the first, and rearranging the terms, we get

$$(1 - \lambda_2 \lambda_4 \rho^{2n}) \left\| V^{(n)} \right\| \leq (\lambda_1 + \lambda_2 \lambda_3 \rho^n) n \left\| Y^{(n)} \right\|. \quad (\text{C.23})$$

For sufficiently large n the factor on the right is positive and greater than, say, $1/2$, so we conclude

$$\left\| V^{(n)} \right\| = O(ns_n). \quad (\text{C.24})$$

Using (C.22) again we get also

$$\left\| U^{(n)} \right\| = O(ns_n). \quad (\text{C.25})$$

Finally, from (C.14) we get then $\left\| X^{(n)} \right\| = O(ns_n)$, which completes the proof. \square

In applying Lemma 3 for functions $Y_2^{(n)}$ and $Y^{(n)}$ in section IID we have $s_n = \rho^n$, for any ρ defined by (I.10). Note that since ρ can always be made smaller, the factor n in $O(ns_n)$ in (C.12) is irrelevant.

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