

Entanglement entropy of two disjoint intervals separated by one spin in a chain of free fermion

Article

Published Version

Creative Commons: Attribution 4.0 (CC-BY)

Open Access

Brightmore, L., Gehér, G. P., Its, A. R., Korepin, V., Mezzadri, F., Mo, M. Y. and Virtanen, J. (2020) Entanglement entropy of two disjoint intervals separated by one spin in a chain of free fermion. *Journal of Physics A: Mathematical and Theoretical*, 53. 345303. ISSN 1751-8113 doi: <https://doi.org/10.1088/1751-8121/ab9cf2> Available at <https://centaur.reading.ac.uk/91293/>

It is advisable to refer to the publisher's version if you intend to cite from the work. See [Guidance on citing](#).

To link to this article DOI: <http://dx.doi.org/10.1088/1751-8121/ab9cf2>

Publisher: IOP

All outputs in CentAUR are protected by Intellectual Property Rights law, including copyright law. Copyright and IPR is retained by the creators or other copyright holders. Terms and conditions for use of this material are defined in the [End User Agreement](#).

www.reading.ac.uk/centaur

CentAUR

Central Archive at the University of Reading

Reading's research outputs online

PAPER • OPEN ACCESS

Entanglement entropy* of two disjoint intervals separated by one spin in a chain of free fermion

To cite this article: L Brightmore *et al* 2020 *J. Phys. A: Math. Theor.* **53** 345303

View the [article online](#) for updates and enhancements.



IOP | ebooks™

Bringing together innovative digital publishing with leading authors from the global scientific community.

Start exploring the collection—download the first chapter of every title for free.

Entanglement entropy of two disjoint intervals separated by one spin in a chain of free fermion*

L Brightmore¹, G P Geher^{2,5} , A R Its³, V E Korepin⁴,
F Mezzadri¹ , M Y Mo¹ and J A Virtanen²

¹ School of Mathematics, University of Bristol, Fry Building, Woodland Road, Bristol BS8 1UG, United Kingdom

² Department of Mathematics and Statistics, University of Reading, Whiteknights, P.O. Box 220, Reading RG6 6AX, United Kingdom

³ Department of Mathematical Sciences, Indiana University-Purdue University Indianapolis, 402 N. Blackford St., Indianapolis, IN 46202-3267, United States of America

⁴ C.N. Yang Institute for Theoretical Physics, State University of New York at Stony Brook, Stony Brook, NY 11794-3840, United States of America

E-mail: G.P.Geher@reading.ac.uk, gehergyuri@gmail.com, aits@iupui.edu, korepin@gmail.com, F.Mezzadri@bristol.ac.uk and j.a.virtanen@reading.ac.uk

Received 18 December 2019, revised 22 May 2020

Accepted for publication 15 June 2020

Published 3 August 2020



CrossMark

Abstract

We calculate the entanglement entropy of a non-contiguous subsystem of a chain of free fermions. The starting point is a formula suggested by Jin and Korepin, [arXiv:1104.1004](https://arxiv.org/abs/1104.1004), for the reduced density of states of two disjoint intervals with lattice sites $P = \{1, 2, \dots, m\} \cup \{2m + 1, 2m + 2, \dots, 3m\}$, which applies to this model. As a first step in the asymptotic analysis of this system, we consider its simplification to two disjoint intervals separated just by one site, and we rigorously calculate the mutual information between these two blocks and the rest of the chain. In order to compute the

*Gehér was supported by the Leverhulme Trust Early Career Fellowship (ECF-2018-125), and by the Hungarian National Research, Development and Innovation Office (Grant No. K115383). Its was supported by the NSF grant DMS-1700261. Virtanen was supported in part by EPSRC grants EP/M024784/1 and EP/T008636/1. Gehér and Virtanen also thank the American Institute of Mathematics and the SquaRE program for their support.

⁵Author to whom any correspondence should be addressed.



Original content from this work may be used under the terms of the [Creative Commons Attribution 4.0 licence](https://creativecommons.org/licenses/by/4.0/). Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.

entropy we need to study the asymptotic behaviour of an inverse Toeplitz matrix with Fisher–Hartwig symbol using the the Riemann–Hilbert method.

Keywords: quantum spin chain, quantum entanglement entropy, mutual information, Riemann–Hilbert problems

(Some figures may appear in colour only in the online journal)

1. Introduction

Quantum systems that are spatially separated can share information that cannot be accounted for by the relativistic laws of classical physics. This fundamental property of quantum mechanics, which plays a crucial role in quantum information, is known as *entanglement* and its measurement is still largely an open problem. There is not a unique way of quantifying entanglement; however, in bipartite systems one of the most popular and successful measure of entanglement is the von Neumann entropy [9].

Suppose that the system is in a pure state $|\psi\rangle$. The density matrix is simply the projection operator $\rho_{PQ} = |\psi\rangle\langle\psi|$, where P and Q refer to the two parts and the Hilbert space $\mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_Q$. The von Neumann entropy is defined as

$$S(\rho_P) = S(\rho_Q) = -\text{Tr}(\rho_P \log \rho_P) = -\text{Tr}(\rho_Q \log \rho_Q), \quad (1.1)$$

where

$$\rho_P = \text{Tr}_Q \rho_{PQ}, \quad \rho_Q = \text{Tr}_P \rho_{PQ} \quad (1.2)$$

and Tr_P and Tr_Q denote the partial traces over the degrees of freedom of P and Q , respectively.

In this paper we study the entropy of a two-block subsystem is a chain of free fermions. More precisely, we consider the chain

$$H_F = -\sum_{j=1}^N b_j^\dagger b_{j+1} + b_j b_{j+1}^\dagger, \quad (1.3)$$

where the Fermi operators b_j are defined by the anticommutation relations

$$\{b_j, b_k\} = 0 \quad \text{and} \quad \{b_j, b_k^\dagger\} = \delta_{jk}. \quad (1.4)$$

The starting point for this analysis is an integral representation for the von Neumann entropy of the subsystem P of fermions on lattice sites

$$P = \{1, 2, \dots, m\} \cup \{2m+1, 2m+2, \dots, 3m\}. \quad (1.5)$$

This was derived by Jin and the fourth co-author in [26], and followed on from the success of this approach to calculating the entropy of a contiguous block of spins in the XX model [25]. Our goal is to compute the entanglement entropy between the subsystem (1.5) and the rest of the chain in the limit as $m \rightarrow \infty$.

Over the past two decades the entanglement of bipartite systems have been extensively studied in one-dimensional quantum critical systems, in particular quantum spin chains. Consider a spin chain with N spins; at zero temperature the Hamiltonian is in the ground state and in the thermodynamic limit $N \rightarrow \infty$ it undergoes a phase transition for some critical value of a parameter, e.g. the magnetic field. This quantum phase transition is characterized by an infinite spin-spin correlation length. Several papers have addressed the problem of computing the

entanglement of the first L consecutive spins and the rest of the chain in various contexts [1, 21, 23, 25, 27, 28, 30, 33, 34, 38]. It is well known that the entanglement entropy grows as

$$S(\rho_P) \propto \log L, \quad L \rightarrow \infty. \tag{1.6}$$

Recently, there has been considerable interest in computing $S(\rho_P)$ in quantum spin chains when P is made of disjoint regions of space. Up to now this problem has received attention within the framework conformal field theory (CFT) [2, 11–13, 17, 18]. One-dimensional quantum critical systems can be described in terms of a massless CFT. More general holographic descriptions are given in [32, 35]. When P is one interval, then the coefficient of the logarithm in (1.6) is proportional to the central charge c , which is a characteristic of the theory [10]. If the theory is bosonic, i.e. if c is an integer, then in the two-interval case the von Neumann entropy depends on the compactification radius of the bosonic field [18]. In the papers [11, 12] the moments of the density matrix were obtained for two-intervals as ratios of Jacobi theta-functions. Unfortunately, they could not compute the analytic continuation of their formulae in terms of the exponent of the moments, which would have led them to an expression for the von Neumann entropy, except in the asymptotic limit of small intervals [12].

A well established approach to solve quantum spin chains that goes back to Lieb *et al* [31] is to map the spin operators into Fermi operators using the Jordan–Wigner transformation. For example, the XX chain

$$H_{\text{XX}} = - \sum_{j=1}^N \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y \tag{1.7}$$

is mapped into (1.3). This approach works well when computing the von Neuman and Reny entropies of a single contiguous interval, as the entropy of the first L spins coincides with that of the first L fermions in (1.3). However, in the case of disjoint intervals in a spin chain there is the extra complication due to the fact that in the fermionic space the operators between blocks contribute to the entropy, because the Jordan–Wigner transformation is not local. This problem was tackled using CFT by Fagotti and Calabrese [17]. In order to avoid this technicality, our starting point is the fermionic chain (1.3). In the model (1.3), the Fermi operators in between blocks do not appear in the computation of the reduced density of states; therefore, the approach adopted in [26] applies. This simplification allows a rigorous computation of the asymptotic behaviour of the entanglement entropy as $m \rightarrow \infty$ while at the same time preserving the physical phenomenon that we want to study. This idea is not new and was adopted by Ares *et al* [3], who performed a numerical study and conjectured a formula of the entropy of several disjoint blocks in a chain of Fermi operators. In fact, our main result—formula (2.12)—seems to be consistent with Ares–Esteve–Falceto conjecture. We hope to address this issue in all detail in the forthcoming publication.

One of the main features of this representation of the von Neumann entropy derived in [26] for the two-blocks (1.5) is that the computation of the entanglement reduces to an integral involving the determinant of a block-matrix, whose two block-diagonal entries are Toeplitz determinants, see formulae (41), (48)–(51) in [26], or (2.1)–(2.4) below. This calculation would be the ultimate goal, but at the moment it is out of our reach—remark 1 in section 3. In this paper, instead, we consider a simplified example of a subsystem consisting of two intervals separated by just one lattice site. The asymptotic analysis of this model is already much more difficult than that of a single block Hamiltonian. Indeed, we not only have to evaluate the asymptotics of the Toeplitz determinant itself, but we also need to extract detailed information on the asymptotic behaviour of the inverse Toeplitz matrix.

It should also be noticed that, besides its intrinsic interest as a physical problem, the study of the asymptotics of Toeplitz determinants has a long history going back to Szegő [36, 37] as such matrices are ubiquitous in mathematics and physics. Indeed, starting from the seminal works of Szegő, Kaufman and Onsager, the Toeplitz determinants have been playing a very important role in many areas of analysis and mathematical physics. Moreover, a growing interest has been recently developed to the study of certain generalizations of Toeplitz determinants. The most known among those are the determinants of Toeplitz plus Hankel matrices—see [8, 16, 19], the bordered Toeplitz determinants [4], and the integrable Fredholm determinants [15, 20]. These determinants appear in the study of Ising model in the zig-zag layered half-plane [14], in the spectral analysis of the Hankel matrices, in the study of the next-to-diagonal correlation functions in the Ising model ([4]), and in the theory of exactly solvable quantum models. In this paper, motivated by the physical model in the context of quantum information, we are concerned with yet another generalization of Toeplitz determinants, which are certain finite rank deformations of the standard Toeplitz matrices. In order to study such deformations, we need to analyse the asymptotic behaviour not only of the Toeplitz determinants *per se* but of the inverse Toeplitz matrices as well. The evaluation of the asymptotic behaviour of this new class of determinants which is done in this paper is, we believe, an important analytical result in its own right.

To summarize, in this article we compute the mutual information between a two blocks of Fermi operators separated by one lattice site and the rest of the chain in the Hamiltonian (1.3) explicitly. Our approach is based on the Riemann–Hilbert method, which has the additional advantage of being mathematically rigorous.

2. The main result

Let C denote the unit circle on the complex plane and

$$g : C \rightarrow \mathbb{C}, \quad g(z) = \begin{cases} 1 & \Re z > 0, \\ -1 & \Re z < 0. \end{cases}$$

The Fourier coefficients of g are

$$g_l := \frac{1}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{3\pi}{2}} e^{-il\theta} g(e^{i\theta}) d\theta = \oint_C z^{-l} g(z) \frac{dz}{2\pi iz} = \frac{2}{l\pi} \sin \frac{l\pi}{2} = \begin{cases} 0 & l \text{ is even,} \\ (-1)^{\frac{l-1}{2}} \frac{2}{l\pi} & l \text{ is odd.} \end{cases}$$

In general, the $m \times m$ Toeplitz matrix and determinant with symbol $\phi \in L^\infty(C)$ will be denoted by $T_m[\phi]$ and $D_m[\phi]$, respectively. As it is well-known, the spectral norm (or operator norm) of $T_m[\phi]$ satisfies $\|T_m[\phi]\| \leq \|\phi\|_\infty$. In particular, as $T_m[g]$ is a self-adjoint matrix, we obtain the relation $\sigma(T_m[g]) \subseteq [-1, 1]$ for its spectrum.

Let $k, m, n \in \mathbb{N}$. We introduce the following matrix and determinant

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \in \mathbb{C}^{(m+n) \times (m+n)}, \quad D(\lambda) = \det(\lambda I - A) \quad (\lambda \in \mathbb{C}) \quad (2.1)$$

where

$$\begin{aligned} A_{11} &= -T_m[g] \in \mathbb{C}^{m \times m}, & A_{22} &= -T_n[g] \in \mathbb{C}^{n \times n}, \\ A_{12} &= A_{21}^T = (\mathcal{A}_{ij})_{i=1, \dots, m; j=1, \dots, n} \in \mathbb{C}^{m \times n}, \end{aligned} \quad (2.2)$$

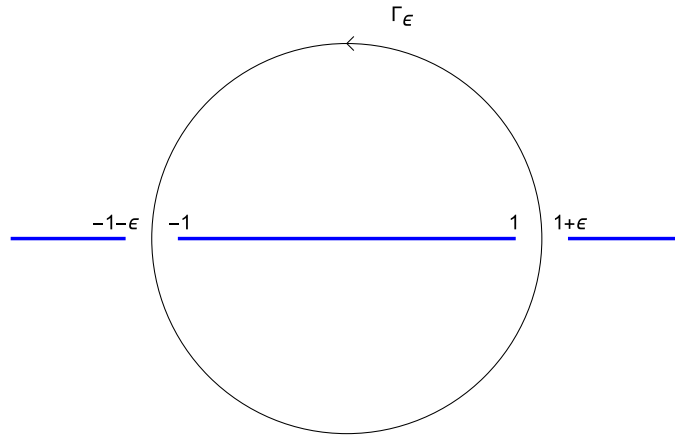


Figure 1. The cuts and the contour in (2.4).

and

$$A_{ij} = - \begin{vmatrix} g_{i-j-m-k} & g_{i-m-1} & g_{i-m-2} & \cdots & g_{i-m-k} \\ g_{1-j-k} & g_0 & g_{-1} & \cdots & g_{1-k} \\ g_{2-j-k} & g_1 & g_0 & \cdots & g_{2-k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ g_{-j} & g_{k-1} & g_{k-2} & \cdots & g_0 \end{vmatrix}, \quad (2.3)$$

which is the determinant of a $(k + 1) \times (k + 1)$ matrix, $k \in \mathbb{N}$.

Define the quantity

$$S(\rho_P) = \lim_{\varepsilon \searrow 0} \frac{1}{2\pi i} \oint_{\Gamma_\varepsilon} e(1 + \varepsilon, \lambda) \frac{d}{d\lambda} \ln D(\lambda) d\lambda, \quad (2.4)$$

where

$$e(x, v) := - \frac{x + v}{2} \ln \frac{x + v}{2} - \frac{x - v}{2} \ln \frac{x - v}{2}.$$

The contour Γ_ε goes around the $[-1, 1]$ interval once in the positive direction avoiding the cuts $(-\infty, -1 - \varepsilon] \cup [1 + \varepsilon, \infty)$ of $e(1 + \varepsilon, \cdot)$, see figure 1. For instance Γ_ε can be the circle $(1 + \frac{1}{2}\varepsilon)C$. For a general k, m, n we interpret the quantity in (2.4) as a measure of entanglement (kind of an entropy) between the subsystem

$$P = \{1, 2, \dots, m\} \cup \{m + k + 1, m + k + 2, \dots, m + k + n\}. \quad (2.5)$$

and the rest of the chain of free fermions (1.3) in the limit $N \rightarrow \infty$. Here is our motivation for this interpretation.

Let \mathcal{H} be an Hilbert space spanned by the fermions in the chain (1.3). Decompose \mathcal{H} in the direct product $\mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_Q$, where \mathcal{H}_P is the space generated by the fermions b_j at the lattice sites P indicated in (2.5). Write $P = P_1 \cup P_2$, where $P_1 = \{1, \dots, m\}$ and $P_2 = \{m + k + 1, \dots, m + k + n\}$ and denote by ℓ_{P_1} and ℓ_{P_2} the sizes of P_1 and P_2 , respectively. A standard

calculation leads to the formula

$$\rho_P = \frac{1}{2^{\ell_{P_1} + \ell_{P_2}}} \sum_{a=0,1} \left\langle \left(\prod_{j \in P} b_j^a \right) \right\rangle \left(\prod_{j \in P} b_j^a \right)^\dagger \quad (2.6)$$

for the reduced density matrix. The angle brackets in this equation denote the expectation value with respect to the ground state. Applying Wick's theorem gives

$$\rho_P = \prod_{j \in P} \left(\langle b_j^\dagger b_j \rangle b_j^\dagger b_j + \langle b_j b_j^\dagger \rangle b_j b_j^\dagger \right). \quad (2.7)$$

The above subsystem consists of two blocks/intervals of m and n fermions separated by a gap of length k . Using (2.7), it was shown in [26] that in the special case when $k = m = n$, and in the thermodynamical limit $N \rightarrow \infty$, the quantity $S(\rho_P)$ is indeed the von Neumann entropy of (2.5). We refer the reader to [26] for more details.

Our ultimate interest is to analyse $S(\rho_P)$ as $k, m, n \rightarrow \infty$, however, at this point the general problem seems to be far too complicated to attack directly (see remark 1 in section 3 below). Therefore we decided to start with the easier case when the gap between the two intervals is fixed to be $k = 1$, that is, when (2.5) becomes

$$P = \{1, 2, \dots, m\} \cup \{m + 2, m + 3, \dots, m + n + 1\}. \quad (2.8)$$

In this case the entries of A_{12} in (2.3) become

$$\mathcal{A}_{ij} = - \begin{vmatrix} g_{i-j-m-1} & g_{i-m-1} \\ g_{-j} & g_0 \end{vmatrix}$$

and, taking into account that $g_0 = 0$,

$$\mathcal{A}_{ij} = g_{i-m-1} \cdot g_{-j}. \quad (2.9)$$

As we shall see, this simplest case already leads to a mathematically very challenging problem.

The asymptotic behaviour of the von Neumann entropy $S(\rho_P^{(n)})$ of the interval $\{1, 2, \dots, n\}$ was calculated in [25]. In particular, it was shown there that

$$S(\rho_P^{(n)}) = \lim_{\varepsilon \searrow 0} \frac{1}{2\pi i} \oint_{\Gamma_\varepsilon} e(1 + \varepsilon, \lambda) \frac{d}{d\lambda} \ln D_n[\phi] d\lambda, \quad (2.10)$$

where $\phi(z) = g(z) + \lambda(z \in C)$. Therefore the problem of calculating the limiting behaviour of the entropy of (2.8) reduces to the calculation of the *mutual information* between the two intervals:

$$S(\rho_P^{(m)}) + S(\rho_P^{(n)}) - S(\rho_P) = \lim_{\varepsilon \searrow 0} \frac{1}{2\pi i} \oint_{\Gamma_\varepsilon} e(1 + \varepsilon, \lambda) \frac{d}{d\lambda} (\ln D_m[\phi] + \ln D_n[\phi] - \ln D(\lambda)) d\lambda$$

To analyse the asymptotic behaviour of this quantity as $m, n \rightarrow \infty$ is still mathematically very complicated. However, as we expect this quantity to converge to a finite number, it makes sense to consider the following limit instead, where the ε and m, n limits are interchanged:

$$\lim_{\varepsilon \searrow 0} \lim_{m, n \rightarrow \infty} \frac{1}{2\pi i} \oint_{\Gamma_\varepsilon} e(1 + \varepsilon, \lambda) \frac{d}{d\lambda} (\ln D_m[\phi] + \ln D_n[\phi] - \ln D(\lambda)) d\lambda. \quad (2.11)$$

We point out that a similar interchanged limit was considered in [22, 25] for the case of one interval. The value of the limit (2.11) is what we shall calculate and interpret as the mutual

information between the two intervals. It will turn out that indeed this is a finite number, which is stated in our main theorem.

Theorem 2.1. *Let $\widehat{D}(\lambda) = \frac{D(\lambda)}{D_m[\phi] \cdot D_n[\phi]}$ ($\lambda \in \mathbb{C} \setminus [-1, 1]$). The limiting mutual information between the two intervals of the subsystem P from (2.8) is*

$$\lim_{\varepsilon \searrow 0} \lim_{m, n \rightarrow \infty} \frac{-1}{2\pi i} \oint_{\Gamma_\varepsilon} e(1 + \varepsilon, \lambda) \frac{d}{d\lambda} \ln \widehat{D}(\lambda) d\lambda = 2 \ln 2 - 1 \approx 0.386294. \tag{2.12}$$

The main tool in the proof of the above theorem will be an asymptotic analysis of an inner product involving the inverse Toeplitz matrix $T_m[\phi]^{-1}$. We phrase the related statement in the next section as lemma 3.2. We also notice that the asymptotics of the Toeplitz determinants $D_m[\phi]$ and $D_n[\phi]$ are described by the Fisher–Hartwig conjecture which, for the class of the symbols where the symbol ϕ belongs to, was proven by E Basor in [7].

3. Some preliminary calculations

We introduce the notations

$$\vec{g}_1 = (g_{-m}, g_{-m+1}, \dots, g_{-1})^T \in \mathbb{C}^m, \quad \vec{g}_2 = (g_{-1}, g_{-2}, \dots, g_{-n})^T \in \mathbb{C}^n, \\ \vec{\mathfrak{G}}_1 = T_m[\phi]^{-1} \vec{g}_1 \in \mathbb{C}^m, \quad \vec{\mathfrak{G}}_2 = T_n[\phi]^{-1} \vec{g}_2 \in \mathbb{C}^n.$$

Notice that for all $\lambda \in \mathbb{C} \setminus [-1, 1]$ we have (see also (2.9))

$$\lambda I - A = \begin{pmatrix} T_m[\phi] & -\vec{g}_1 \vec{g}_2^T \\ -\vec{g}_2 \vec{g}_1^T & T_n[\phi] \end{pmatrix} = \begin{pmatrix} T_m[\phi] & 0 \\ 0 & T_n[\phi] \end{pmatrix} \cdot \left[I - \begin{pmatrix} 0 & \vec{\mathfrak{G}}_1 \vec{\mathfrak{G}}_2^T \\ \vec{\mathfrak{G}}_2 \vec{\mathfrak{G}}_1^T & 0 \end{pmatrix} \right].$$

Therefore we obtain

$$D(\lambda) = D_m[\phi] \cdot D_n[\phi] \cdot \det \left(I - \vec{\mathfrak{G}}_1 \vec{\mathfrak{G}}_2^T \vec{\mathfrak{G}}_2 \vec{\mathfrak{G}}_1^T \right) = D_m[\phi] \cdot D_n[\phi] \cdot \left(1 - \langle \vec{\mathfrak{G}}_1, \vec{g}_1 \rangle \langle \vec{\mathfrak{G}}_2, \vec{g}_2 \rangle \right)$$

where we used standard facts about rank-one matrices and the following identity for block-matrices:

$$I - \begin{pmatrix} 0 & B \\ C & 0 \end{pmatrix} = \begin{pmatrix} I - BC & -B \\ 0 & I \end{pmatrix} \cdot \begin{pmatrix} I & 0 \\ -C & I \end{pmatrix}.$$

In particular, we infer

$$\widehat{D}(\lambda) = 1 - \langle \vec{\mathfrak{G}}_1, \vec{g}_1 \rangle \langle \vec{\mathfrak{G}}_2, \vec{g}_2 \rangle.$$

Thus in order to compute the mutual information, we need to deal with the inner products $\langle \vec{\mathfrak{G}}_j, \vec{g}_j \rangle$. It turns out that it is sufficient to handle the case $j = 1$.

Proposition 3.1. *Let us use the notations $\vec{g}_1^{(m)} = \vec{g}_1$, $\vec{\mathfrak{G}}_1^{(m)} = \vec{\mathfrak{G}}_1$, $\vec{g}_2^{(n)} = \vec{g}_2$, $\vec{\mathfrak{G}}_2^{(n)} = \vec{\mathfrak{G}}_2$, which indicates the m - or n -dependence of the vectors. Then, we have*

$$\langle \vec{\mathfrak{G}}_2^{(n)}, \vec{g}_2^{(n)} \rangle = \langle \vec{\mathfrak{G}}_1^{(m)}, \vec{g}_1^{(m)} \rangle.$$

Proof. Consider the $n \times n$ matrix $J = (\delta_{i+j-n+1})_{i,j=0}^{n-1}$ where δ denotes the Kronecker delta symbol. Since we have $JT_n[g]J = T_n[g]$, we obtain $JT_n[\phi]^{-1}J = T_n[\phi]^{-1}$, and thus

$$\langle \vec{\mathfrak{G}}_2^{(n)}, \vec{\mathfrak{g}}_2^{(n)} \rangle = \langle JT_n[\phi]^{-1} J \vec{\mathfrak{g}}_2^{(n)}, \vec{\mathfrak{g}}_2^{(n)} \rangle = \langle T_n[\phi]^{-1} \vec{\mathfrak{g}}_1^{(n)}, \vec{\mathfrak{g}}_1^{(n)} \rangle.$$

□

Remark 1. Notice that for a general gap of length k , the matrix $\lambda I - A$ whose determinant is needed to be evaluated, can be written as

$$\begin{aligned} \lambda I - A = & \begin{pmatrix} (\phi_{i-j})_{i,j=1,\dots,m} & \gamma(g_{i-j-m-1})_{i=1,\dots,m} \\ \gamma(g_{j-i-m-1})_{i=1,\dots,n} & (\phi_{i-j})_{i,j=1,\dots,n} \end{pmatrix} \\ & - \sum_{d,l=1}^k \gamma_{dl} \begin{pmatrix} 0 & -\vec{\mathfrak{g}}_d \vec{\mathfrak{g}}_{k+l}^T \\ -\vec{\mathfrak{g}}_{k+l} \vec{\mathfrak{g}}_d^T & 0 \end{pmatrix} \end{aligned} \tag{3.1}$$

where

$$\vec{\mathfrak{g}}_d = (g_{1-m-d}, g_{2-m-d}, \dots, g_{-d})^T, \quad \vec{\mathfrak{g}}_{k+d} = (g_{d-1-k}, g_{d-2-k}, \dots, g_{d-n-k})^T, \quad d = 1, 2, \dots, k,$$

and the scalar coefficients γ and γ_{dl} are certain $k \times k$, independent of n, m , determinants. This shows what are the new technical challenges when one passes from $k = 1$ to the values $k > 1$. The ‘principal’ determinant is not a block diagonal Toeplitz determinant anymore; indeed, the non-trivial off-diagonal Toeplitz blocks, generated by new symbols, appear. Moreover, the finite rank perturbation is of rank $2k$ and, therefore, ceases to be ‘finite rank’ as we consider the most general setting of the problem when all three sizes, m, n , and k become arbitrarily large.

From now on, until the end of section 8, our goal is to prove the following lemma, which then we shall apply in section 9 to prove theorem 2.1.

Lemma 3.2. Define $\beta := \frac{1}{2\pi i} \ln \frac{\lambda+1}{\lambda-1}$. As $m \rightarrow \infty$ we have

$$\langle \vec{\mathfrak{G}}_1, \vec{\mathfrak{g}}_1 \rangle = \langle T_m[\phi]^{-1} \vec{\mathfrak{g}}_1, \vec{\mathfrak{g}}_1 \rangle = i \tan\left(\frac{\pi}{2}\beta\right) + O(m^{-\frac{1}{4}}), \tag{3.2}$$

where the error term is uniform in λ on compact subsets of $|\lambda| > 1$.

In order to analyse $\langle \vec{\mathfrak{G}}_1, \vec{\mathfrak{g}}_1 \rangle$, we shall express it in terms of a Riemann–Hilbert problem (RHP) that arises in the theory of integrable operators, see [6, section 5.6] (see also [15], or [24]). Define the kernel

$$K(z, s) = \frac{1 - \phi(s)}{2\pi i} \frac{z^m s^{-m} - 1}{z - s} = \frac{\vec{f}(z)^T \vec{h}(s)}{z - s} \quad (z, s \in C),$$

where

$$\vec{f}(z) = \begin{pmatrix} f_1(z) \\ f_2(z) \end{pmatrix} = \begin{pmatrix} z^m \\ 1 \end{pmatrix}, \quad \vec{h}(s) = \begin{pmatrix} h_1(s) \\ h_2(s) \end{pmatrix} = \frac{1 - \phi(s)}{2\pi i} \begin{pmatrix} s^{-m} \\ -1 \end{pmatrix},$$

which also satisfy $\langle \vec{f}(z), \vec{h}(z) \rangle = 0 \quad (z \in C)$, where $\langle \vec{a}, \vec{b} \rangle = \sum_j a_j b_j$. This kernel defines a very special type of bounded singular integral operators on $L^2(C)$, namely a so-called (completely) *integrable operator* in the following way:

$$K[u](z) = \int_C K(z, s)u(s) ds \quad (u \in L^2(C), z \in C),$$

where the integral is meant in the principal value sense, and we put the function in between $[\cdot]$.

By well-known properties of this operator, for all $\lambda \in \mathbb{C} \setminus [-1, 1]$ we have $0 \neq D_m[\phi] = \det(1 - K)$ and

$$T_m[\phi]^{-1} = \left(((1 - K)^{-1}[z^j], z^k) \right)_{j,k=0}^{m-1}, \tag{3.3}$$

where (\cdot, \cdot) denotes the complex inner product on $L^2(C)$. In particular, the connection between the two determinants can be shown by repeating the argument of [6, page 123]. In order to obtain (3.3) we observe that (by (5.157)–(5.158) in [6, page 123]) $1 - K$ has the block-matrix

form $\begin{pmatrix} 1 & 0 & 0 \\ * & T_m[\phi] & * \\ 0 & 0 & 1 \end{pmatrix}$, hence the (2.2) block of $(1 - K)^{-1}$ is $T_m[\phi]^{-1}$. Furthermore, by [6, theorem 5.21] (see also [15], or [24]),

$$\vec{F}(z) = \begin{pmatrix} F_1(z) \\ F_2(z) \end{pmatrix} := (1 - K)^{-1}[\vec{f}](z) = Y_{K-}(z)\vec{f}(z) = \begin{pmatrix} Y_{K-,11}(z)z^m + Y_{K-,12}(z) \\ Y_{K-,21}(z)z^m + Y_{K-,22}(z) \end{pmatrix}, \tag{3.4}$$

where Y_K is the unique solution of the following RHP.

Y_K —Riemann–Hilbert problem

$$Y_K : \mathbb{C} \setminus C \rightarrow \mathbb{C}^{2 \times 2} \text{ is analytic,} \tag{3.5}$$

$$Y_{K+}(z) = Y_{K-}(z) \cdot \begin{pmatrix} \phi(z) & -(\phi(z) - 1)z^m \\ (\phi(z) - 1)z^{-m} & 2 - \phi(z) \end{pmatrix} \quad (\text{a.e. } z \in C), \tag{3.6}$$

$$Y_K(z) = I + O(z^{-1}) \quad \text{as } z \rightarrow \infty. \tag{3.7}$$

The unit circle is oriented in the usual positive direction, and the jump condition (3.6) is meant in the L^2 sense, see [6, definition 5.16].

In the next section we will connect the Y_K —RHP with another RHP, but for the rest of this section our aim is to express the inner product $\langle \vec{\mathfrak{G}}_1, \vec{\mathfrak{g}}_1 \rangle$ in terms of Y_K .

Proposition 3.3. *We have*

$$\langle \vec{\mathfrak{G}}_1, \vec{\mathfrak{g}}_1 \rangle = -\frac{2}{\pi} \sum_{\ell=1}^m \frac{\sin \frac{\ell\pi}{2}}{\ell} M_{\ell,11}, \tag{3.8}$$

where

$$Y_K(z) = I + \sum_{\ell=1}^{\infty} M_{\ell} z^{-\ell} \quad \text{as } z \rightarrow \infty.$$

Proof. First, by (3.3) we have

$$\begin{aligned} \langle \vec{\mathfrak{G}}_1, \vec{\mathfrak{g}}_1 \rangle &= \vec{\mathfrak{g}}_1^T T_m[\phi]^{-1} \vec{\mathfrak{g}}_1 = \sum_{j,k=0}^{m-1} g_{j-m} g_{k-m} ((1 - K)^{-1}[z^j], z^k) \\ &= \left((1 - K)^{-1} \left[\sum_{j=0}^{m-1} g_{j-m} z^j \right], \sum_{k=0}^{m-1} g_{k-m} z^k \right). \end{aligned}$$

Next, since $g(z) = (\phi(z) - 1) + (1 - \lambda)$, we calculate

$$\begin{aligned} \sum_{j=0}^{m-1} g_{j-m} z^j &= \sum_{j=0}^{m-1} \oint_C g(s) s^{m-j} z^j \frac{ds}{2\pi i s} = \sum_{j=0}^{m-1} \oint_C (\phi(s) - 1) s^{m-j} z^j \frac{ds}{2\pi i s} \\ &= \oint_C \frac{\phi(s) - 1}{2\pi i} s^m \sum_{j=0}^{m-1} \left(\frac{z}{s}\right)^j \frac{ds}{s} = - \oint_C K(z, s) s^m ds = -K[z^m](z). \end{aligned}$$

Therefore, by (3.4) and (3.7)

$$\begin{aligned} \langle \vec{\mathfrak{G}}_1, \vec{\mathfrak{g}}_1 \rangle &= - \left((1 - K)^{-1} K[z^m], \sum_{k=0}^{m-1} g_{k-m} z^k \right) = - \left((1 - K)^{-1} [z^m] - z^m, \sum_{k=0}^{m-1} g_{k-m} z^k \right) \\ &= - \left(F_1, \sum_{k=0}^{m-1} g_{k-m} z^k \right) = - \sum_{k=0}^{m-1} g_{k-m} \oint_C F_1(z) z^{-k} \frac{dz}{2\pi i z} \\ &= - \sum_{k=0}^{m-1} g_{k-m} \oint_C Y_{K-,11}(z) z^{m-k} + Y_{K-,12}(z) z^{-k} \frac{dz}{2\pi i z} \\ &= - \sum_{k=0}^{m-1} g_{k-m} \oint_C Y_{K-,11}(z) z^{m-k} \frac{dz}{2\pi i z} = - \sum_{k=0}^{m-1} g_{k-m} M_{m-k,11}, \end{aligned}$$

from which we conclude (3.8). □

4. Expressing the inner product in terms of the R—Riemann—Hilbert problem

Note that for all $\lambda \in \mathbb{C} \setminus [-1, 1]$ the function ϕ possesses Fisher–Hartwig singularities at $z_1 = i = e^{i\frac{\pi}{2}}$ and $z_2 = -i = e^{i\frac{3\pi}{2}}$; thus, we can apply the results in [16]. To be more precise, using the notation of (1.2) in [16], we can write ϕ in the following form:

$$\phi(z) = e^{V_0} g_1(z) g_2(z) z_1^{-\beta_1} z_2^{-\beta_2}$$

with $\alpha_1 = \alpha_2 = 0, \theta_1 = \frac{\pi}{2}, \theta_2 = \frac{3\pi}{2}$,

$$\beta = \beta(\lambda) := \beta_1 = -\beta_2 = \frac{1}{2\pi i} \cdot \ln \frac{\lambda + 1}{\lambda - 1} = \frac{1}{2\pi i} [\ln(\lambda + 1) - \ln(\lambda - 1)], \tag{4.1}$$

$$V(z) = V_0 = \frac{1}{2} [\ln(\lambda - 1) + \ln(\lambda + 1)], \tag{4.2}$$

$$g_1(z) g_2(z) = \begin{cases} 1 & \Re z > 0 \\ e^{-2i\pi\beta} & \Re z < 0 \end{cases} = \begin{cases} 1 & \Re z > 0 \\ \frac{\lambda - 1}{\lambda + 1} & \Re z < 0 \end{cases} \tag{4.3}$$

$$z_1^{-\beta_1} z_2^{-\beta_2} = e^{\frac{1}{2}[\ln(\lambda+1) - \ln(\lambda-1)]}. \tag{4.4}$$

Note that throughout this paper, $\ln z$ denotes the principal branch of the logarithm, that is, $-\pi < \arg z < \pi$. Since $\frac{\lambda+1}{\lambda-1}$ is a fractional linear map, we can easily examine the real- and imaginary

parts of β . We have

$$\Re\beta = \frac{1}{2\pi} \arg \frac{\lambda + 1}{\lambda - 1}, \quad \Im\beta = \frac{-1}{2\pi} \ln \left| \frac{\lambda + 1}{\lambda - 1} \right| = \frac{1}{2\pi} \ln \left| \frac{\lambda - 1}{\lambda + 1} \right|, \quad (4.5)$$

therefore we see that $\Im\beta$ stays bounded on compact subsets of $\mathbb{C} \setminus [-1, 1]$. In addition, $|\Re\beta| < \frac{1}{2}$ for all $\lambda \in \mathbb{C} \setminus [-1, 1]$. However, notice that a simple calculation gives that

$$|\Re\beta| < \frac{1}{4} \iff |\lambda| > 1,$$

which is the reason why we shall take $\Gamma_\varepsilon = (1 + \frac{1}{2}\varepsilon)C$ in (2.12) in our calculations. Let us also note that β does not vanish on \mathbb{C} .

Next, we shall connect the Y_K —RHP with the Y —RHP, see e.g. [16] or [5] for details.

Y —Riemann–Hilbert problem for orthogonal polynomials on the circle

$$Y : \mathbb{C} \setminus C \rightarrow \mathbb{C}^{2 \times 2} \text{ is analytic,} \quad (4.6)$$

$$Y_+(z) = Y_-(z) \cdot \begin{pmatrix} 1 & \phi(z)z^{-m} \\ 0 & 1 \end{pmatrix} \quad (z \in C \setminus \{i, -i\}), \quad (4.7)$$

$$Y(z) = (I + O(z^{-1})) \begin{pmatrix} z^m & 0 \\ 0 & z^{-m} \end{pmatrix} \quad \text{as } z \rightarrow \infty, \quad (4.8)$$

$$Y(z) = \begin{pmatrix} O(1) & O(\ln |z \mp i|) \\ O(1) & O(\ln |z \mp i|) \end{pmatrix} \quad \text{as } z \rightarrow \pm i. \quad (4.9)$$

The jump condition (4.7) is meant in the sense that Y is continuous up to C from both sides, except at the points $\pm i$.

It is well-known that this RHP has a unique solution which can be given in terms of orthogonal polynomials. An easy calculation shows the following connection between the unique solutions Y_K and Y :

$$Y_K(z) = \begin{cases} \sigma_3 Y(z) \sigma_3 \begin{pmatrix} z^m & -1 \\ 1 & 0 \end{pmatrix}^{-1}, & |z| < 1 \\ \sigma_3 Y(z) \sigma_3 \begin{pmatrix} z^m & 0 \\ 1 & z^{-m} \end{pmatrix}^{-1}, & |z| > 1 \end{cases} \quad (4.10)$$

where $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ is the Pauli matrix. We point out that a similar connection was observed in [5]. Note that even though the jump conditions (3.6) and (4.7) are meant in different ways, one verifies easily that indeed the above Y_K solves the Y_K —RHP in the L^2 sense. The advantage of involving Y in our analysis is that we can use the powerful results of [16], in particular, we can express our inner product in terms of the R —RHP which can be estimated effectively. Let us recall the R —RHP next, whose associated contour Γ_R is shown in figure 2. Notice that the circles ∂U_1 and ∂U_2 around $\pm i$ are oriented in the negative direction.

R —Riemann–Hilbert problem

$$R : \mathbb{C} \setminus \Gamma_R \rightarrow \mathbb{C}^{2 \times 2} \text{ is analytic,} \quad (4.11)$$

$$R_+(z) = R_-(z) \cdot N(z) \begin{pmatrix} 1 & 0 \\ \phi(z)^{-1}z^{-m} & 1 \end{pmatrix} N(z)^{-1} \quad (z \in \Sigma_j^{\text{out}}), \quad (4.12)$$

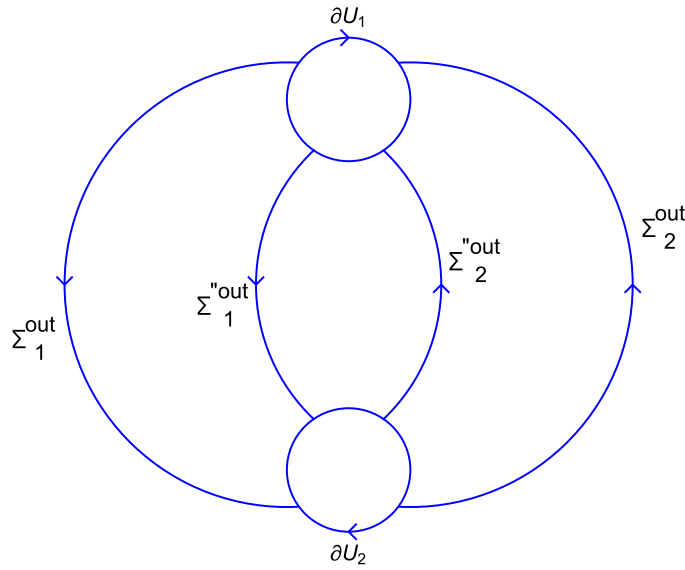


Figure 2. The contour Γ_R for the R —RHP.

$$R_+(z) = R_-(z) \cdot N(z) \begin{pmatrix} 1 & 0 \\ \phi(z)^{-1}z^m & 1 \end{pmatrix} N(z)^{-1} \quad (z \in \Sigma_j^{\text{out}}), \tag{4.13}$$

$$R_+(z) = R_-(z) \cdot P_j(z)N(z)^{-1} \quad (z \in \partial U_j \setminus \{\text{intersection points}\}), \tag{4.14}$$

$$R(z) = I + O(z^{-1}) \quad \text{as } z \rightarrow \infty. \tag{4.15}$$

The jump conditions (4.12)–(4.14) are meant in the sense that R is continuous up to Γ_R from each side. The functions N and P_j denote the global and local parametries, respectively, see [16, subsections 4.1–4.2]. Namely,

$$N(z) = \begin{cases} \mathcal{D}(z)^{\sigma_3} & |z| > 1 \\ \mathcal{D}(z)^{\sigma_3} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} & |z| < 1 \end{cases} \tag{4.16}$$

where $\mathcal{D}(z) = \exp\left(\frac{1}{2\pi i} \int_C \frac{\ln \phi(s)}{s-z} ds\right)$ stands for the Szegő function. The local parametries will be discussed in detail in section 7.

From (4.10) we calculate

$$Y_{K,11}(z) = Y_{11}(z)z^{-m} + Y_{12}(z) \quad (|z| \geq 2).$$

If we trace back the transformations $Y \rightarrow T \rightarrow S \rightarrow R$ performed in [16], we obtain

$$Y(z) = R(z)N(z)z^{m\sigma_3} = R(z)\mathcal{D}(z)^{\sigma_3}z^{m\sigma_3} \quad (|z| \geq 2).$$

In particular,

$$Y_{11}(z)z^{-m} = R_{11}(z)\mathcal{D}(z), \quad Y_{12}(z) = R_{12}(z)\mathcal{D}(z)^{-1}z^{-m} \quad (|z| \geq 2).$$

Notice that $Y_{12}(z) = O(z^{-m-1})$ as $z \rightarrow \infty$, hence by (3.8) it does not contribute to our inner product. Therefore we have

$$M_{\ell,11} = d_\ell + \oint_{|z|=2} (R_{11}(z) - 1) \mathcal{D}(z) z^\ell \frac{dz}{2\pi iz} \quad (\ell = 1, \dots, m),$$

where $\mathcal{D}(z) = 1 + \sum_{j=1}^\infty d_j z^{-j}$ ($|z| > 1$). Thus, from (3.8) we obtain

$$\langle \vec{\mathfrak{G}}_1, \vec{\mathfrak{g}}_1 \rangle = -\frac{2}{\pi} \sum_{\ell=1}^m \frac{\sin \frac{\ell\pi}{2}}{\ell} d_\ell - \frac{2}{\pi} \oint_{|z|=2} (R_{11}(z) - 1) \mathcal{D}(z) f_m(z) \frac{dz}{2\pi iz}, \quad (4.17)$$

where

$$f_m(z) = \sum_{\ell=1}^m \frac{\sin \frac{\ell\pi}{2}}{\ell} z^\ell. \quad (4.18)$$

Now, set $M = \lfloor \frac{m-1}{2} \rfloor$ and notice that for all $z \in \mathbb{C}$, $\Re z \neq 0$, we have

$$\begin{aligned} f_m(z) &= \sum_{k=0}^M \frac{(-1)^k}{2k+1} z^{2k+1} = \frac{1}{i} \sum_{k=0}^M \frac{(iz)^{2k+1}}{2k+1} = \frac{1}{i} \sum_{k=0}^M \int_0^{iz} s^{2k} ds = \frac{1}{i} \int_0^{iz} \frac{1 - s^{2M+2}}{1 - s^2} ds \\ &= \int_0^z \frac{1 + (-1)^M y^{2M+2}}{1 + y^2} dy = \arctan z + (-1)^M \int_0^z \frac{y^{2M+2}}{1 + y^2} dy \\ &= \frac{1}{2i} \ln \frac{z-i}{z+i} + \frac{\pi}{2} \operatorname{sgn} \Re z + (-1)^M \int_0^z \frac{y^{2M+2}}{1 + y^2} dy \\ &= \frac{1}{2i} \ln \frac{z-i}{z+i} + \widetilde{f}_m(z) = \frac{1}{2i} \ln \frac{z-i}{z+i} + \frac{\pi}{2} \operatorname{sgn} \Re z + \widetilde{f}_{m,1}(z), \end{aligned} \quad (4.19)$$

where the integration is meant along a line segment and $\widetilde{f}_m, \widetilde{f}_{m,1}$ are implicitly defined in the above equation-chain. Note that $\frac{1}{2i} \ln \frac{z-i}{z+i}$ and \widetilde{f}_m are analytic in $\mathbb{C} \setminus [-i, i]$, and that the integral expression $\widetilde{f}_{m,1}$ is analytic in $\mathbb{C} \setminus ([i, i\infty) \cup [-i, -i\infty))$. Since $(R_{11}(z) - 1) \mathcal{D}(z) = O(1/z)$ and $\frac{1}{2i} \ln \frac{z-i}{z+i} = O(1/z)$ as $z \rightarrow \infty$, we easily obtain that

$$\langle \vec{\mathfrak{G}}_1, \vec{\mathfrak{g}}_1 \rangle = -\frac{2}{\pi} \sum_{\ell=1}^m \frac{\sin \frac{\ell\pi}{2}}{\ell} d_\ell - \frac{2}{\pi} \oint_{|z|=2} (R_{11}(z) - 1) \mathcal{D}(z) \widetilde{f}_m(z) \frac{dz}{2\pi iz}, \quad (4.20)$$

To summarise, we have two kinds of contributions to the inner product, one which comes from the Szegő function and another coming from $R - I$. Next, we compute the contribution coming from $\mathcal{D}(z)$.

5. The contribution from the Szegő function

Here we calculate the asymptotic behaviour of $-\frac{2}{\pi} \sum_{\ell=1}^m \frac{\sin \frac{\ell\pi}{2}}{\ell} d_\ell = -\sum_{\ell=1}^m g_\ell d_\ell$ as $m \rightarrow \infty$. For that, we need a formula for the Szegő function. By (4.8) (or (4.10)) in [16], a short calculation gives

$$\mathcal{D}(z) = \exp \left(\beta \cdot \ln \frac{z-i}{z+i} \right) = \left(\frac{z-i}{z+i} \right)^\beta \quad (|z| > 1), \quad (5.1)$$

where the right-hand side is analytic outside $[-i, i]$, and

$$\mathcal{D}(z) = \left(\frac{z-i}{z+i}\right)^\beta \phi(z) \quad (|z| < 1). \tag{5.2}$$

A simple calculation gives

$$D(e^{i\theta}) = \left(\frac{e^{i\theta} - e^{i\frac{\pi}{2}}}{e^{i\theta} + e^{i\frac{\pi}{2}}}\right)^\beta = \left(i \frac{\sin\left(\frac{\theta}{2} - \frac{\pi}{4}\right)}{\cos\left(\frac{\theta}{2} - \frac{\pi}{4}\right)}\right)^\beta = \left(i \tan\left(\frac{\theta}{2} - \frac{\pi}{4}\right)\right)^\beta \quad (\theta \in \mathbb{R}).$$

Therefore, since $\mathcal{D}(1/z) = 1 + \sum_{j=1}^\infty d_j z^j$ belongs to the Hardy class H^2 , we obtain the following expression for the limit of the sum:

$$\begin{aligned} -\sum_{l=1}^\infty g_l d_l &= -\frac{1}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{3\pi}{2}} \mathcal{D}(e^{-i\theta}) \overline{g(e^{i\theta})} d\theta = -\frac{1}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{3\pi}{2}} \mathcal{D}(e^{i\theta}) g(e^{i\theta}) d\theta \\ &= -\frac{1}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{3\pi}{2}} \mathcal{D}(e^{i\theta}) d\theta + \frac{1}{\pi} \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} \mathcal{D}(e^{i\theta}) d\theta = -1 + \frac{1}{\pi} \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} \mathcal{D}(e^{i\theta}) d\theta \\ &= -1 + \frac{1}{\pi} \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} \left(i \tan\left(\frac{\theta}{2} - \frac{\pi}{4}\right)\right)^\beta d\theta = -1 + \frac{2 \cdot i^\beta}{\pi} \int_0^{\frac{\pi}{2}} (\tan \vartheta)^\beta d\vartheta \\ &= -1 + \frac{2 \cdot i^\beta}{\pi} \int_0^\infty \frac{u^\beta}{1+u^2} du = i \tan\left(\frac{\pi}{2}\beta\right), \end{aligned}$$

where we substituted $u = \tan \vartheta$ and used standard residue calculus.

We estimate the speed of convergence below.

Proposition 5.1. *We have*

$$-\frac{2}{\pi} \sum_{\ell=1}^m \frac{\sin \frac{\ell\pi}{2}}{\ell} d_\ell = i \tan\left(\frac{\pi}{2}\beta\right) + O(m^{-\frac{1}{2}}) \tag{5.3}$$

as $m \rightarrow \infty$, where the error is uniform in λ on compact subsets of $\mathbb{C} \setminus [-1, 1]$.

Proof. Note that

$$\begin{aligned} |\mathcal{D}(e^{i\theta})| &= \left| \left(e^{i\pi/2} \tan\left(\frac{\theta}{2} - \frac{\pi}{4}\right) \right)^\beta \right| = e^{-\frac{\pi}{2}\Im\beta} \left(\left| \frac{\theta - \frac{3\pi}{2}}{\theta - \frac{\pi}{2}} \right| \left| \tan\left(\frac{\theta}{2} - \frac{\pi}{4}\right) \right| \right)^{\Re\beta} \\ &\quad \times \left| \theta - \frac{\pi}{2} \right|^{\Re\beta} \left| \theta - \frac{3\pi}{2} \right|^{-\Re\beta} \\ &\leq e^{-\frac{\pi}{2}\Im\beta} 3^{1/2} \left| \theta - \frac{\pi}{2} \right|^{\Re\beta} \left| \theta - \frac{3\pi}{2} \right|^{-\Re\beta} \quad \left(\frac{\pi}{2} < \theta < \frac{3\pi}{2} \right). \end{aligned}$$

and similarly

$$|\mathcal{D}(e^{i\theta})| = \left| \left(e^{-i\pi/2} \tan\left(\frac{\theta}{2} - \frac{\pi}{4}\right) \right)^\beta \right| \leq e^{\frac{\pi}{2}\Im\beta} 3^{1/2} \left| \theta - \frac{\pi}{2} \right|^{\Re\beta} \left| \theta + \frac{\pi}{2} \right|^{-\Re\beta} \quad \left(-\frac{\pi}{2} < \theta < \frac{\pi}{2} \right).$$

Hence the squared L^2 -norm of the Szegő function can be estimated as follows:

$$\begin{aligned} \frac{1}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{3\pi}{2}} |\mathcal{D}(e^{i\theta})|^2 d\theta &\leq \frac{e^{\pi|\Im\beta|} 3}{2\pi} \left(\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \left| \theta - \frac{\pi}{2} \right|^{2\Re\beta} \left| \theta + \frac{\pi}{2} \right|^{-2\Re\beta} d\theta \right. \\ &\quad \left. + \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} \left| \theta - \frac{\pi}{2} \right|^{2\Re\beta} \left| \theta - \frac{3\pi}{2} \right|^{-2\Re\beta} d\theta \right) \\ &= \frac{e^{\pi|\Im\beta|} 3}{\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \left| \theta - \frac{\pi}{2} \right|^{2|\Re\beta|} \left| \theta + \frac{\pi}{2} \right|^{-2|\Re\beta|} d\theta \\ &\leq e^{\pi|\Im\beta|} 3 \int_0^\pi t^{-2|\Re\beta|} dt \\ &\leq 3 \frac{e^{\pi|\Im\beta|} \pi^{1-2|\Re\beta|}}{1-2|\Re\beta|}. \end{aligned}$$

Therefore by the Cauchy–Schwartz inequality we get

$$\begin{aligned} \left| \sum_{l=m+1}^\infty g_l d_l \right| &\leq \frac{2}{\pi} \sum_{l=m+1}^\infty \frac{1}{l} |d_l| \leq \frac{2}{\pi} \sqrt{\sum_{l=m+1}^\infty \frac{1}{l^2}} \sqrt{\frac{1}{2\pi} \int_{-\pi}^\pi |\mathcal{D}(e^{i\theta})|^2 d\theta} \\ &\leq \frac{2}{\pi} \sqrt{\int_m^\infty \frac{1}{x^2} dx} \sqrt{\frac{1}{2\pi} \int_{-\pi}^\pi |\mathcal{D}(e^{i\theta})|^2 d\theta} \\ &\leq \frac{2}{\pi} m^{-1/2} e^{\frac{\pi}{2}|\Im\beta|} \sqrt{3} \sqrt{\frac{1}{1-2|\Re\beta|}} \pi^{\frac{1}{2}-|\Re\beta|} = O(m^{-1/2}) \end{aligned}$$

as $m \rightarrow \infty$, uniformly in λ on compact subsets of $\mathbb{C} \setminus [-1, 1]$. □

Before we proceed with computing the contribution coming from $R - I$, we need some auxiliary calculations about the integral $\widetilde{f_{m,1}}$ defined in (4.19), and the local parametrices appearing in the analysis of R in [16].

6. Estimation of $\widetilde{f_{m,1}}$

We start with the following proposition.

Proposition 6.1. *We have*

$$e^{-mu} = (1 - u)^m + O\left(\frac{1}{m}\right)$$

as $m \rightarrow \infty$, uniformly in $u \in [0, 1]$.

Proof. As $\ln(1 - u) < -u$ ($0 < u < 1$), we have $e^{-mu} > (1 - u)^m$ ($0 < u \leq 1$). Note that

$$\frac{d}{du}(e^{-mu} - (1 - u)^m) = m((1 - u)^{m-1} - e^{-mu}) = 0 \iff -mu = (m - 1)\ln(1 - u) \quad (0 \leq u \leq 1).$$

Since $\ln(1 - u)$ is concave, we have at most two stationary points, and clearly one of them is $u = 0$. Simple calculations show that for $u = \frac{1}{m}$ the derivative is positive, and that for $u = \frac{3}{m}$

it is negative, therefore there is a second stationary point $\frac{1}{m} < \widetilde{u}_m < \frac{3}{m}$ ($m \in \mathbb{N}$, $m > 5$). It is then obvious that for all $u \in [0, 1]$ we have

$$\begin{aligned} 0 \leq e^{-mu} - (1 - u)^m &\leq e^{-m\widetilde{u}_m} - (1 - \widetilde{u}_m)^m = e^{-m\widetilde{u}_m}(1 - e^{m(\ln(1-\widetilde{u}_m)+\widetilde{u}_m)}) \\ &= O(1)(1 - e^{O(m\widetilde{u}_m^2)}) = O(1)(1 - e^{O(1/m)}) = O\left(\frac{1}{m}\right) \end{aligned}$$

as $m \rightarrow \infty$. □

We proceed with the estimation of $\widetilde{f}_{m,1}(z) = (-1)^M \int_0^z \frac{y^{2M+2}}{1+y^2} dy$ when z is close to the cut $[-i, i]$.

Lemma 6.2. *As $m \rightarrow \infty$, we have the following estimates which are uniform in z and t :*

(a)

$$\widetilde{f}_{m,1}(z) = O(2^{-m}) \quad \left(|z| \leq \frac{1}{2}\right),$$

(b)

$$\widetilde{f}_{m,1}(it) = O\left(e^{-\frac{1}{2}\sqrt{m}} \frac{1}{\sqrt{m}}\right) \quad \left(-1 + \frac{1}{\sqrt{m}} \leq t \leq 1 - \frac{1}{\sqrt{m}}\right)$$

(c)

$$\widetilde{f}_{m,1}(it) = \frac{1}{2i} \int_{m(1-t)}^{\infty} \frac{e^{-\zeta}}{\zeta} d\zeta + O\left(\frac{1}{m} \ln m\right) = O(1) \quad \left(1 - \frac{1}{\sqrt{m}} \leq t \leq 1 - \frac{1}{m}\right)$$

and $\widetilde{f}_{m,1}(-it) = O(1)$.

Proof. (a) is obvious. Note that $\widetilde{f}_{m,1}$ is an odd function, therefore it is enough to prove (b) and (c) for $t \geq 0$. For $0 \leq t \leq 1 - \frac{1}{m}$ we have

$$\widetilde{f}_{m,1}(it) = \frac{(-1)^M}{2i} \int_0^{it} \frac{y^{2M+2}}{y-i} dy - \frac{(-1)^M}{2i} \int_0^{it} \frac{y^{2M+2}}{y+i} dy = \frac{(-1)^M}{2i} I_1(t) - \frac{(-1)^M}{2i} I_2(t),$$

where $I_1(t)$ and $I_2(t)$ are the first and second integrals, respectively. By substituting $y = ix$ and keeping in mind that $m \in \{2M + 1, 2M + 2\}$, we get for all $0 \leq t \leq 1 - \frac{1}{m}$ that

$$|I_2(t)| = \int_0^t \frac{x^{2M+2}}{x+1} dx \leq \int_0^t x^{2M+2} dx = \frac{t^{2M+3}}{2M+3} \leq \frac{(1 - \frac{1}{m})^{2M+3}}{2M+3} \leq \frac{(1 - \frac{1}{m})^m}{m} = O\left(\frac{1}{m}\right)$$

as $m \rightarrow \infty$. We also obtain that if $0 \leq t \leq 1 - \frac{1}{\sqrt{m}}$, then

$$\begin{aligned} |I_2(t)| \leq |I_1(t)| &= \int_0^t \frac{x^{2M+2}}{1-x} dx \leq \sqrt{m} \int_0^{1-\frac{1}{\sqrt{m}}} x^{2M+2} dx \leq \frac{1}{\sqrt{m}} \left(1 - \frac{1}{\sqrt{m}}\right)^m \\ &= O\left(\frac{1}{\sqrt{m}} e^{-\frac{1}{2}\sqrt{m}}\right) \end{aligned}$$

as $m \rightarrow \infty$, which proves (ii).

Now, let $1 - \frac{1}{\sqrt{m}} \leq t \leq 1 - \frac{1}{m}$, then

$$\begin{aligned} I_1(t) &= (-1)^M \int_0^t \frac{x^{2M+2}}{1-x} dx = (-1)^M \int_{1-\frac{1}{\sqrt{m}}}^t \frac{x^{2M+2}}{1-x} dx + O\left(\frac{1}{\sqrt{m}} e^{-\frac{1}{2}\sqrt{m}}\right) \\ &= (-1)^M \int_{1-t}^{\frac{1}{\sqrt{m}}} \frac{(1-u)^{2M+2}}{u} du + O\left(\frac{1}{\sqrt{m}} e^{-\frac{1}{2}\sqrt{m}}\right) \\ &= (-1)^M \int_{1-t}^{\frac{1}{\sqrt{m}}} \frac{e^{-(2M+2)u} + O\left(\frac{1}{m}\right)}{u} du + O\left(\frac{1}{\sqrt{m}} e^{-\frac{1}{2}\sqrt{m}}\right) \\ &= (-1)^M \int_{1-t}^{\frac{1}{\sqrt{m}}} \frac{e^{-(2M+2)u}}{u} du + O\left(\frac{1}{m}\right) \int_{1-t}^{\frac{1}{\sqrt{m}}} \frac{1}{u} du + O\left(\frac{1}{\sqrt{m}} e^{-\frac{1}{2}\sqrt{m}}\right) \\ &= (-1)^M \int_{1-t}^{\frac{1}{\sqrt{m}}} \frac{e^{-(2M+2)u}}{u} du + O\left(\frac{1}{m} \ln m\right) = (-1)^M \int_{(2M+2)(1-t)}^{\frac{2M+2}{\sqrt{m}}} \frac{e^{-\zeta}}{\zeta} d\zeta + O\left(\frac{1}{m} \ln m\right) \end{aligned}$$

as $m \rightarrow \infty$, uniformly in t . What remains to prove is that the latter integral is $\int_{m(1-t)}^{\infty} \frac{e^{-\zeta}}{\zeta} d\zeta + O\left(\frac{1}{m} \ln m\right)$ as $m \rightarrow \infty$, uniformly in t , which follows from the following calculations:

$$\int_{\frac{2M+2}{\sqrt{m}}}^{\infty} \frac{e^{-\zeta}}{\zeta} d\zeta \leq \int_{\frac{2M+2}{\sqrt{m}}}^{\infty} e^{-\zeta} d\zeta = e^{-\frac{2M+2}{\sqrt{m}}} \leq e^{-\sqrt{m}}$$

and

$$\int_{m(1-t)}^{(2M+2)(1-t)} \frac{e^{-\zeta}}{\zeta} d\zeta = (2M+2-m)(1-t) \frac{e^{-m(1-t)}}{m(1-t)} \leq \frac{e^{-1}}{m}.$$

□

Now, we estimate near i .

Lemma 6.3. *Let $0 < c < 1 < C$, then the following holds as $m \rightarrow \infty$, uniformly in $\frac{c}{m} \leq |z - i| \leq \frac{C}{m}$, $z \notin [i, i\infty)$:*

$$\widetilde{f}_{m,1}(z) = \frac{1}{2i} \int_1^{\infty} \frac{e^{-\zeta}}{\zeta} d\zeta - \frac{1}{2i} \int_1^{im(z-i)} \frac{e^{-\zeta}}{\zeta} d\zeta + O\left(\frac{1}{m} \ln m\right) = O(1), \quad (6.1)$$

where the path for the second integral lies in $\zeta \in \mathbb{C} \setminus (-\infty, 0]$, $c \leq |\zeta| \leq C$, as shown in figure 3.

Proof. Notice that for all $c < |u| < C$ we have

$$\begin{aligned} \left(1 - \frac{u}{m}\right)^{2M+2} - e^{-u} &= e^{(2M+2)\ln(1-u/m)} - e^{-u} = e^{(2M+2)(-u/m + O(m^{-2}))} - e^{-u} \\ &= e^{-u} \left(e^{-(2M+2-m)u/m + (2M+2)O(m^{-2})} - 1 \right) \\ &= e^{-u} \left(e^{O(1/m)} - 1 \right) = O\left(\frac{1}{m}\right). \end{aligned}$$

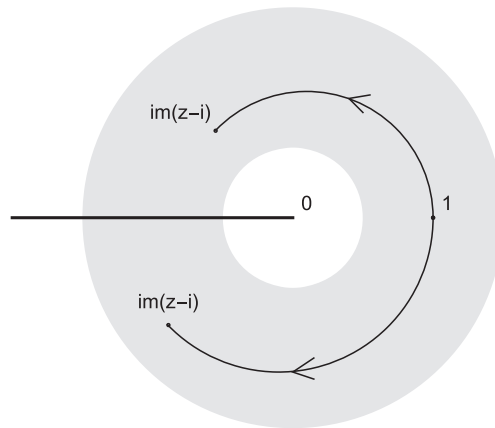


Figure 3. The contour of integration in (6.1).

Therefore, using the substitution $y = i(1 - \frac{u}{m})$, $u = im(y - i)$, we obtain

$$\begin{aligned} \widetilde{f_{m,1}}(z) &= \widetilde{f_{m,1}}(i(1 - \frac{1}{m})) + (-1)^M \int_{i(1-\frac{1}{m})}^z \frac{y^{2M+2}}{1+y^2} dy \\ &= \frac{1}{2i} \int_1^\infty \frac{e^{-\zeta}}{\zeta} d\zeta + O\left(\frac{1}{m} \ln m\right) + \frac{(-1)^M}{2i} \int_{i(1-\frac{1}{m})}^z \frac{y^{2M+2}}{y-i} + O(1) dy \\ &= \frac{1}{2i} \int_1^\infty \frac{e^{-\zeta}}{\zeta} d\zeta - \frac{1}{2i} \int_1^{im(z-i)} \frac{(1-\frac{u}{m})^{2M+2}}{u} du + O\left(\frac{1}{m} \ln m\right) \\ &= \frac{1}{2i} \int_1^\infty \frac{e^{-\zeta}}{\zeta} d\zeta - \frac{1}{2i} \int_1^{im(z-i)} \frac{e^{-u}}{u} + \frac{O(\frac{1}{m})}{u} du + O\left(\frac{1}{m} \ln m\right) \\ &= \frac{1}{2i} \int_1^\infty \frac{e^{-\zeta}}{\zeta} d\zeta - \frac{1}{2i} \int_1^{im(z-i)} \frac{e^{-\zeta}}{\zeta} d\zeta + O\left(\frac{1}{m} \ln m\right). \end{aligned}$$

□

We note that one can similarly estimate near $-i$.

7. The local parametrics

In this section we shall compute how the local paramterices look like, with paying special attention to those parts that depend on m . As the two cases are very similar, we shall only examine the parametrix P_1 around i in detail. As in (4.12) and (4.23)–(4.24) in [16] we have

$$\zeta = m \ln \frac{z}{i} \quad (z \in U_1) \tag{7.1}$$

and

$$P_1(z) = E(z)\Psi_1(\zeta)F_1(z)^{-\sigma_3} z^{\pm m\sigma_3/2} \quad (z \in U_1), \tag{7.2}$$

where $\pm = +$ when $|z| < 1$, and $\pm = -$ when $|z| > 1$. By equations (4.18)–(4.22) in [16], one easily sees that the auxiliary function $F_1(z)$ is constant in U_1 , and its value is

$$F_1(z) = F_1 := \sqrt{(\lambda - 1)e^{i\pi\beta}} = \sqrt{(\lambda + 1)e^{-i\pi\beta}} \quad (z \in U_1). \tag{7.3}$$

The function $E(z)$ is analytic in a neighbourhood of U_1 and is defined in (4.47)–(4.50) in [16]. What is important for our considerations is that

$$E(z) = \begin{pmatrix} 0 & E_{12}(z) \\ E_{21}(z) & 0 \end{pmatrix} = m^{-\beta\sigma_3} i^{\frac{m}{2}\sigma_3} \tilde{E}(z) = m^{-\beta\sigma_3} i^{\frac{m}{2}\sigma_3} \begin{pmatrix} 0 & \tilde{E}_{12}(z) \\ \tilde{E}_{21}(z) & 0 \end{pmatrix}, \tag{7.4}$$

where $\tilde{E}(z)$ is independent of m and analytic in a neighbourhood of U_1 . Furthermore,

$$E_{12}(z) = i^{\frac{m}{2}} \mathcal{D}(z) \zeta^{-\beta} F_1^{-1} e^{i\pi\beta}, \quad \tilde{E}_{12}(z) = \mathcal{D}(z) \left(\ln \frac{z}{i} \right)^{-\beta} F_1^{-1} e^{i\pi\beta} \quad (|z| < 1)$$

and

$$E_{21}(z) = -i^{-\frac{m}{2}} \mathcal{D}(z)^{-1} \zeta^\beta F_1 e^{-2i\pi\beta}, \quad \tilde{E}_{21}(z) = -\mathcal{D}(z)^{-1} \left(\ln \frac{z}{i} \right)^\beta F_1 e^{-2i\pi\beta} \quad (|z| < 1).$$

The function $\Psi_1(\zeta)$ is an auxiliary function which is the main ingredient in constructing the local parametrix in [16], and which is given explicitly in terms of the confluent hypergeometric function $\psi(a, c; \zeta)$. We recall the details now. Let the contours $\Gamma_1, \dots, \Gamma_8$ be defined as in figure 4. In particular, each of them is a half line starting or ending at 0. Furthermore, $\Gamma_k \cup \Gamma_{k+4}$ is a line ($k = 1, 2, 3, 4$), and when $k = 1, 3$, these unions are the imaginary and real axes, respectively. These contours divide the complex plane into 8 sectors, denoted by I, II, \dots , VIII as shown in figure 4. The function $\Psi_1(\zeta)$ is analytic in $\mathbb{C} \setminus \bigcup_{k=1}^8 \Gamma_k$, and is uniquely defined by

$$\Psi_1(\zeta) = \Psi_1^{(I)}(\zeta) = \begin{pmatrix} \psi(\beta, 1; \zeta) e^{i\pi 2\beta} e^{-\zeta/2} & -\psi(1 - \beta, 1, e^{-i\pi} \zeta) e^{i\pi\beta} e^{\zeta/2} \frac{\Gamma(1 - \beta)}{\Gamma(\beta)} \\ -\psi(1 + \beta, 1; \zeta) e^{i\pi\beta} e^{-\zeta/2} \frac{\Gamma(1 + \beta)}{\Gamma(-\beta)} & \psi(-\beta, 1, e^{-i\pi} \zeta) e^{\zeta/2} \end{pmatrix} \quad (\zeta \in I),$$

and the following jump condition

$$\Psi_{1,+}(\zeta) = \Psi_{1,-}(\zeta) J_k(\zeta) \quad (\zeta \in \Gamma_k),$$

where the jump matrices J_k are constant and are given by

$$J_1 = \begin{pmatrix} 0 & e^{-i\pi\beta} \\ -e^{i\pi\beta} & 0 \end{pmatrix}, \quad J_2 = J_8 = \begin{pmatrix} 1 & 0 \\ e^{i\pi\beta} & 1 \end{pmatrix}, \quad J_3 = J_7 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$J_4 = J_6 = \begin{pmatrix} 1 & 0 \\ e^{-i\pi\beta} & 1 \end{pmatrix}, \quad J_5 = \begin{pmatrix} 0 & e^{i\pi\beta} \\ -e^{-i\pi\beta} & 0 \end{pmatrix},$$

see (4.25)–(4.29) and (4.32) in [16]. Note that the functions $\psi(a, c, \zeta)$ and $\psi(a, c, e^{-i\pi}\zeta)$ are defined on the universal covering of the punctured plane $\zeta \in \mathbb{C} \setminus \{0\}$, and that $\Psi_1^{(I)}(\zeta)$ is the analytic continuation of $\Psi_1|_I$ to $0 < \arg \zeta < 2\pi$.

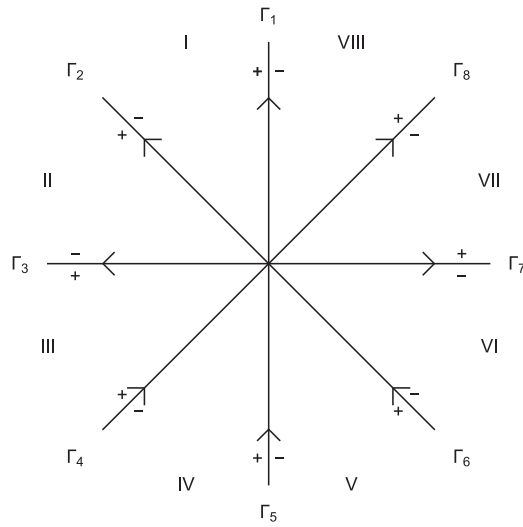


Figure 4. The contour for the local parametrix Ψ_1 .

8. The contribution from $R - I$

Recall that the the integration in (2.12) will be taken over the circle $(1 + \frac{\epsilon}{2})C$, hence from now on we only consider the case when $|\lambda| > 1$, which implies $|\Re\beta| < 1/4$. In this section our aim is to show that for $|\lambda| > 1$ the integral

$$\oint_{|z|=2} (R_{11}(z) - 1) \left(\frac{z-i}{z+i}\right)^\beta \frac{\tilde{f}_m(z)}{z} dz \tag{8.1}$$

introduced in (4.20) converges to 0, and thus the contribution to our inner product coming from $R - I$ is, roughly speaking, negligible. Of course, the contour of integration can be deformed to the outer boundary of the unbounded component of $\mathbb{C} \setminus \Gamma_R$. Since the integrand is analytic outside $\Gamma_R \cup [-i, i]$, the integrals over the other contours shown on figure 5 vanish. Therefore, by a straightforward calculation we obtain the following expression for (8.1) where $\Delta(z) + I$ is the jump in the R -RHP:

$$- \int_{\Gamma_R} (R_+(z) - R_-(z))_{11} \left(\frac{z-i}{z+i}\right)^\beta \frac{\tilde{f}_m(z)}{z} dz + \int_{\gamma_m} (R_{11}(z) - 1) \left(\frac{z-i}{z+i}\right)^\beta \frac{\tilde{f}_m(z)}{z} dz \tag{8.2}$$

$$= - \int_{\Gamma_R} (R_-(z)\Delta(z))_{11} \left(\frac{z-i}{z+i}\right)^\beta \frac{\tilde{f}_m(z)}{z} dz + \int_{\gamma_m} (R_{11}(z) - 1) \left(\frac{z-i}{z+i}\right)^\beta \frac{\tilde{f}_m(z)}{z} dz, \tag{8.3}$$

where γ_m is the union of two circles of radius $1/m$, four line segments and two half-circles of radius $1/2$. More precisely, $\gamma_m = C_m^i \cup [(1 - 1/m)i, i/2]_+ \cup [-i/2, -(1 - 1/m)i]_+ \cup C_m^{-i} \cup [-(1 - 1/m)i, i/2]_- \cup [i/2, (1 - 1/m)i]_- \cup \{z : |z| = 1/2\}$ oriented in the positive direction where $C_m^{\pm i}$ is the circle around $\pm i$ with radius $\frac{1}{m}$, and the line segment $[-i, i]$ is oriented upwards, hence its $-/+$ side is its right/left side.

We shall examine the two integrals in (8.3) separately, starting with the second one.

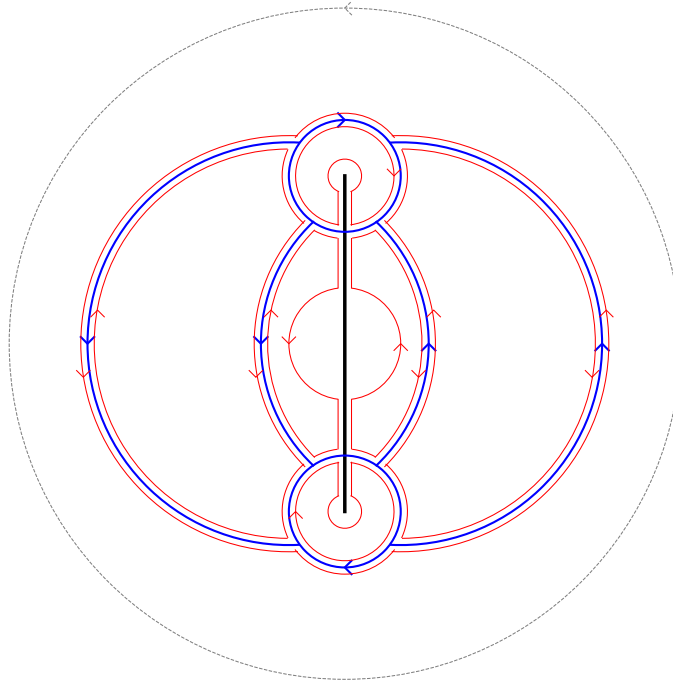


Figure 5. The contour deformation of the dashed circle into the outer thin (red) contour. The contour integrals along the other thin (red) contours vanish.

8.1. The integral over γ_m

Proposition 8.1. We have

$$\int_{\gamma_m} (R_{11}(z) - 1) \left(\frac{z - i}{z + i} \right)^\beta \frac{\tilde{f}_m(z)}{z} dz = O(m^{-1/4}) \quad \text{as } m \rightarrow \infty,$$

which is uniform in λ on compact subsets of $|\lambda| > 1$.

Proof. We know from the standard analysis in the steepest descent method that $\Delta(z) = O(m^{2|\Re\beta|-1})$ and hence $R(z) - I = \frac{1}{2\pi i} \int_{\Gamma_R} \frac{R_-(s)\Delta(s)}{s-z} ds = O(m^{2|\Re\beta|-1})$ as $m \rightarrow \infty$, which is uniform in λ on compact subsets of $|\lambda| > 1$, and in z on $\mathbb{C} \setminus \Gamma_R$ (see e.g. [16], and note that there is some flexibility in choosing the parameters for Γ_R , hence the Cauchy integral does not blow up as z gets closer to Γ_R). Also, elementary observations show that $\left(\frac{z-i}{z+i} \right)^\beta = O(m^{|\Re\beta|})$ as $m \rightarrow \infty$, which is uniform in λ on compact subsets of $|\lambda| > 1$, and in z on γ_m . Therefore, combining the above estimates with lemmas 6.2 and 6.3, we conclude

$$\begin{aligned} \int_{\gamma_m} (R_{11}(z) - 1) \left(\frac{z - i}{z + i} \right)^\beta \frac{\tilde{f}_m(z)}{z} dz &= \int_{\gamma_m} O(m^{2|\Re\beta|-1}) O(m^{|\Re\beta|}) O(1) dz \\ &= O(m^{3|\Re\beta|-1}) = O(m^{-1/4}) \quad \text{as } m \rightarrow \infty. \end{aligned}$$

□

From now on, we estimate the integral over Γ_R from (8.3), which we split into two parts.

8.2. The integrals over $\Sigma_j^{\prime\prime out}$ and Σ_j^{out}

First we deal with the integrals over the lenses.

Proposition 8.2. We have

$$\int_{\Sigma_1^{\prime\prime out} \cup \Sigma_2^{\prime\prime out} \cup \Sigma_1^{out} \cup \Sigma_2^{out}} (R_-(z)\Delta(z))_{11} \left(\frac{z-i}{z+i}\right)^\beta \frac{\tilde{f}_m(z)}{z} dz = O(m^{-1/2}),$$

which is uniform in λ on compact subsets of $|\lambda| > 1$.

Proof. Notice that for $z \in \Sigma_j^{\prime\prime out}$ we have

$$\Delta(z) = \mathcal{D}(z)^{\sigma_3} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ \phi(z)^{-1}z^m & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \mathcal{D}(z)^{-\sigma_3} = \begin{pmatrix} 0 & * \\ 0 & 0 \end{pmatrix}. \tag{8.4}$$

Thus $(R_-(z)\Delta(z))_{11} = 0$, and we conclude that

$$\int_{\Sigma_j^{\prime\prime out}} (R_-(z)\Delta(z))_{11} \left(\frac{z-i}{z+i}\right)^\beta \frac{\tilde{f}_m(z)}{z} dz = 0 \quad (j = 1, 2). \tag{8.5}$$

Next, for $z \in \Sigma_j^{out}$ we have

$$\Delta(z) = \mathcal{D}(z)^{\sigma_3} \begin{pmatrix} 0 & 0 \\ \phi(z)^{-1}z^{-m} & 0 \end{pmatrix} \mathcal{D}(z)^{-\sigma_3} = \phi(z)^{-1}z^{-m} \begin{pmatrix} z-i \\ z+i \end{pmatrix}^{-2\beta} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

Note that

$$\left| \frac{\tilde{f}_m(z)}{z^{m+1}} \right| \leq \left| \frac{f_m(z)}{z^{m+1}} \right| + \frac{1}{2} \left| \frac{\ln \frac{z-i}{z+i}}{z^{m+1}} \right| \leq \sum_{\ell=1}^m |z|^{\ell-m-1} + O(1) = \frac{1-|z|^{-m}}{|z|-1} + O(1) = O(1)$$

as $m \rightarrow \infty$, uniformly in z on $\Sigma_1^{out} \cup \Sigma_2^{out}$. Therefore,

$$\begin{aligned} \int_{\Sigma_j^{out}} (R_-(z)\Delta(z))_{11} \left(\frac{z-i}{z+i}\right)^\beta \frac{\tilde{f}_m(z)}{z} dz &= \int_{\Sigma_j^{out}} \phi(z)^{-1} \left(\frac{z-i}{z+i}\right)^{-\beta} R_{12,-}(z) \frac{\tilde{f}_m(z)}{z^{m+1}} dz \\ &= \int_{\Sigma_j^{out}} O(1) O(m^{2|\Re\beta|-1}) O(1) dz = O(m^{-1/2}) \end{aligned} \tag{8.6}$$

as $m \rightarrow \infty$ ($j = 1, 2$), which is uniform in λ on compact subsets of $|\lambda| > 1$. □

Finally, we estimate the integrals over the circles.

8.3. The integrals over the circles ∂U_1 and ∂U_2

We shall only examine the integral over ∂U_1 and note that the case of ∂U_2 is very similar. We will deform the contour ∂U_1 inside the disk U_1 . Recall the jump condition (4.14), and that the jump there $P_1(z)N(z)^{-1} = \Delta(z) + I$ is analytic only in a neighbourhood of $U_1 \setminus (\Sigma_1 \cup \Sigma_2 \cup \Sigma_1^{\prime\prime} \cup \Sigma_2^{\prime\prime})$. The disk U_1 is cut into five components by $[-i, i] \cup \Sigma_1 \cup \Sigma_2 \cup \Sigma_1^{\prime\prime} \cup \Sigma_2^{\prime\prime}$, on all of which the integrand is analytic and continuous up to the boundaries, except

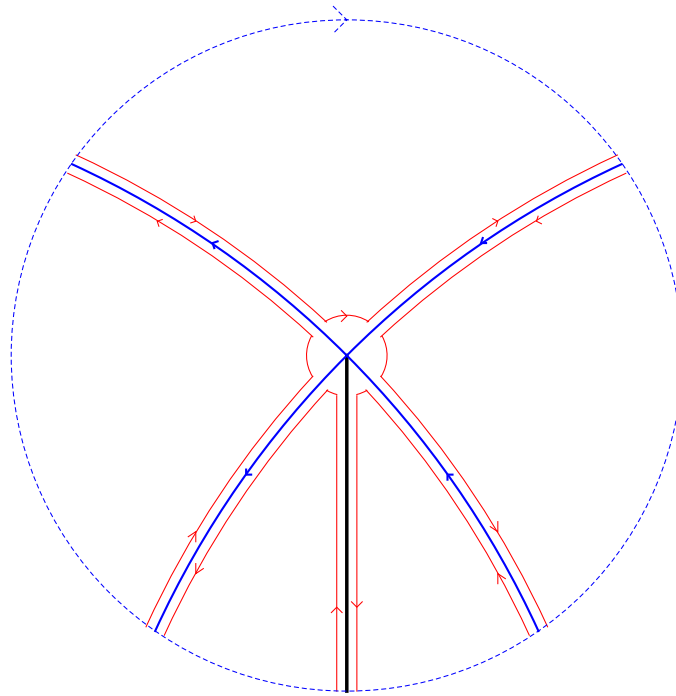


Figure 6. The contour deformation of ∂U_1 .

maybe at i . Therefore, we can deform the five arcs in the way shown in figure 6, and obtain the following:

$$\begin{aligned}
 & \int_{\partial U_1} (R_-(z)\Delta(z))_{11} \left(\frac{z-i}{z+i}\right)^\beta \frac{\tilde{f}_m(z)}{z} dz \\
 &= - \int_{\gamma_m \cap U_1} (R(z)\Delta(z))_{11} \left(\frac{z-i}{z+i}\right)^\beta \frac{\tilde{f}_m(z)}{z} dz \\
 &+ \int_{\Sigma_1^{i,m} \cup \Sigma_2^{i,m} \cup \Sigma_1^{\prime i,m} \cup \Sigma_2^{\prime i,m}} (R(z) [\Delta_+(z) - \Delta_-(z)])_{11} \left(\frac{z-i}{z+i}\right)^\beta \frac{\tilde{f}_m(z)}{z} dz, \tag{8.7}
 \end{aligned}$$

where γ_m was defined just after (8.3), and $\Sigma_j^{i,m} = \Sigma_j \cap U_1 \cap \{z : |z-i| > 1/m\}$, $\Sigma_j^{\prime i,m} = \Sigma_j'' \cap U_1 \cap \{z : |z-i| > 1/m\}$.

First, we handle the integral over $\gamma_m \cap U_1$.

Proposition 8.3. *We have*

$$\int_{\gamma_m \cap U_1} (R(z)\Delta(z))_{11} \left(\frac{z-i}{z+i}\right)^\beta \frac{\tilde{f}_m(z)}{z} dz = O\left(m^{-1/4}\right) \quad \text{as } m \rightarrow \infty, \tag{8.8}$$

uniformly in λ on compact subsets of $|\lambda| > 1$. Moreover, the same estimation holds for U_2 .

Proof. We have

$$N(z)^{-1} = \begin{cases} \left(\frac{z-i}{z+i}\right)^{-\beta\sigma_3} & |z| > 1, \\ \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \phi(z)^{-\sigma_3} \left(\frac{z-i}{z+i}\right)^{-\beta\sigma_3} & |z| < 1, \end{cases}$$

hence we obtain $N(z)^{-1} = O(m^{|\Re\beta|})$ as $m \rightarrow \infty$, uniformly in z on C_i^m and in λ on compact subsets of $|\lambda| > 1$. Using (7.1)–(7.4) we also obtain the following:

$$P_1(z) = m^{-\beta\sigma_3} O(1) \Psi_1 \left(m \ln \frac{z}{i}\right) O(1) = m^{-\beta\sigma_3} O(1) = O(m^{|\Re\beta|}) \quad \left(|z-i| = \frac{1}{m}\right)$$

as $m \rightarrow \infty$, uniformly in z and in λ on compact subsets of $|\lambda| > 1$. Hence $\Delta(z) = P_1(z)N(z)^{-1} - I = O(m^{2|\Re\beta|})$, and therefore

$$\int_{C_i^m} (R(z)\Delta(z))_{11} \left(\frac{z-i}{z+i}\right)^\beta \frac{\tilde{f}_m(z)}{z} dz = \int_{C_i^m} O(m^{2|\Re\beta|}) O(m^{|\Re\beta|}) dz = O(m^{-1/4})$$

as $m \rightarrow \infty$, uniformly in λ on compact subsets of $|\lambda| > 1$.

Next we show that, by the formulae in section 7, we have the following for $z \in \text{II} \cup \text{III}$:

$$\begin{aligned} P_1(z)N(z)^{-1} - I &= E(z)\Psi_1(\zeta)F_1^{-\sigma_3}z^{\frac{m}{2}\sigma_3} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \mathcal{D}(z)^{-\sigma_3} - I \\ &= \begin{pmatrix} 0 & E_{12}(z) \\ E_{21}(z) & 0 \end{pmatrix} \Psi_1^{(I)}(\zeta) \begin{pmatrix} 1 & 0 \\ e^{i\pi\beta} & 1 \end{pmatrix} F_1^{-\sigma_3}z^{\frac{m}{2}\sigma_3} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \mathcal{D}(z)^{-\sigma_3} - I \\ &= F_1 z^{-\frac{m}{2}} \begin{pmatrix} * & E_{12}(z)\Psi_{1,22}^{(I)}(\zeta) \\ * & E_{21}(z)\Psi_{1,12}^{(I)}(\zeta) \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \mathcal{D}(z)^{-\sigma_3} - I \\ &= F_1 z^{-\frac{m}{2}} \mathcal{D}(z)^{-1} \begin{pmatrix} E_{12}(z)\Psi_{1,22}^{(I)}(\zeta) & * \\ E_{21}(z)\Psi_{1,12}^{(I)}(\zeta) & * \end{pmatrix} - I \\ &= F_1 z^{-\frac{m}{2}} \mathcal{D}(z)^{-1} \begin{pmatrix} i^{\frac{m}{2}} \mathcal{D}(z) \zeta^{-\beta} F_1^{-1} e^{i\pi\beta} \Psi_{1,22}^{(I)}(\zeta) & * \\ -i^{-\frac{m}{2}} \mathcal{D}(z)^{-1} \zeta^\beta F_1 e^{-2i\pi\beta} \Psi_{1,12}^{(I)}(\zeta) & * \end{pmatrix} - I \\ &= \begin{pmatrix} e^{i\pi\beta} e^{-\zeta/2} \zeta^{-\beta} \Psi_{1,22}^{(I)}(\zeta) - 1 & * \\ -i^{-m} \mathcal{D}(z)^{-2} F_1^2 e^{-2i\pi\beta} e^{-\zeta/2} \zeta^\beta \Psi_{1,12}^{(I)}(\zeta) & * \end{pmatrix} \\ &= \begin{pmatrix} (e^{-i\pi} \zeta)^{-\beta} \psi(-\beta, 1, e^{-i\pi} \zeta) - 1 & * \\ i^{-m} \mathcal{D}(z)^{-2} (e^{-i\pi} \zeta)^\beta \psi(1 - \beta, 1, e^{-i\pi} \zeta) \frac{\Gamma(1 - \beta)}{\Gamma(\beta)} F_1^2 & * \end{pmatrix}. \end{aligned}$$

In the above we have concentrated on the first column only. Denote the radius of U_1 by ε . Then,

$$\begin{aligned} &\int_{(\gamma_m \cap U_1) \setminus C_i^m} (R(z)\Delta(z))_{11} \left(\frac{z-i}{z+i}\right)^\beta \frac{\tilde{f}_m(z)}{z} dz \\ &= \int_{(1-\varepsilon)i}^{(1-1/m)i} (R(z) (P_1(z)N(z)^{-1} - I))_{11} O(m^{|\Re\beta|}) \frac{dz}{z} \end{aligned}$$

$$\begin{aligned}
 &= \int_{(1-\varepsilon)i}^{(1-1/m)i} R_{11}(z) \left((e^{-i\pi} \zeta)^{-\beta} \psi(-\beta, 1, e^{-i\pi} \zeta) - 1 \right) O\left(m^{|\Re \beta|}\right) \frac{dz}{z} \\
 &\quad + \int_{(1-\varepsilon)i}^{(1-1/m)i} R_{12}(z) \mathcal{D}(z)^{-2} (e^{-i\pi} \zeta)^\beta \psi(1-\beta, 1, e^{-i\pi} \zeta) O\left(m^{|\Re \beta|}\right) \frac{dz}{z}. \quad (8.9)
 \end{aligned}$$

Finally, by substituting $\xi = e^{-i\pi} \zeta$, $\frac{dz}{z} = -\frac{d\xi}{\xi}$, and using the large ξ asymptotics of the confluent hypergeometric function and the usual estimates for R and \mathcal{D} , we obtain

$$\begin{aligned}
 &= \int_{-m \ln(1-1/m)}^{-m \ln(1-\varepsilon)} (\xi^{-\beta} \psi(-\beta, 1, \xi) - 1) O\left(m^{|\Re \beta|}\right) \frac{d\xi}{\xi} \\
 &\quad + \int_{-m \ln(1-1/m)}^{-m \ln(1-\varepsilon)} \xi^\beta \psi(1-\beta, 1, \xi) O\left(m^{5|\Re \beta|-1}\right) \frac{d\xi}{\xi} \\
 &= O\left(m^{|\Re \beta|-1}\right) \int_1^{-m \ln(1-\varepsilon)} \xi^{-1} d\xi + O\left(m^{5|\Re \beta|-2}\right) \int_1^{-m \ln(1-\varepsilon)} \xi^{2\Re \beta-1} d\xi \\
 &= O\left(m^{|\Re \beta|-1} \ln m\right) + O\left(m^{5|\Re \beta|-2}\right) \int_1^{-m \ln(1-\varepsilon)} \xi^{-1/2} d\xi = O\left(m^{-1/4}\right) \quad \text{as } m \rightarrow \infty.
 \end{aligned}$$

□

As last step, we consider the integrals over $\Sigma_j^{i,m}$ and $\Sigma_j^{ii,m}$ ($j = 1, 2$).

Proposition 8.4. *We have*

$$\int_{\Sigma_1^{i,m} \cup \Sigma_2^{i,m} \cup \Sigma_1^{ii,m} \cup \Sigma_2^{ii,m}} (R(z) [\Delta_+(z) - \Delta_-(z)])_{11} \left(\frac{z-i}{z+i}\right)^\beta \tilde{f}_m(z) \frac{dz}{z} = O(m^{-1/4}). \quad (8.10)$$

as $m \rightarrow \infty$, uniformly in λ on compact subsets of $|\lambda| > 1$.

Proof. First, we notice that the integral in (8.7) over $\Sigma_j^{ii,m}$ ($j = 1, 2$) vanishes. Indeed, we have $\Delta_+(z) - \Delta_-(z) = (P_{1,+}(z) - P_{1,-}(z)) N(z)^{-1}$ and the jump of P_1 is exactly the same as that of S . Therefore, similarly as in (8.4) we obtain that $(R(z) [\Delta_+(z) - \Delta_-(z)])_{11} = 0$.

In the rest of the proof, we shall only deal with the integral over $\Sigma_1^{i,m}$, and note that the other integral over $\Sigma_2^{i,m}$ can be handled very similarly, since the local parametrix does not jump along Γ_7 . Note that for $z \in \Sigma_1^{i,m}$ we have

$$\begin{aligned}
 \Delta_+(z) - \Delta_-(z) &= (P_{1,+}(z) - P_{1,-}(z)) N(z)^{-1} = P_{1,-}(z) \begin{pmatrix} 0 & 0 \\ \phi(z)^{-1} z^{-m} & 0 \end{pmatrix} \mathcal{D}(z)^{-\sigma_3} \\
 &= m^{-\beta \sigma_3} i^{\frac{m}{2} \sigma_3} \begin{pmatrix} 0 & \tilde{E}_{12}(z) \\ \tilde{E}_{21}(z) & 0 \end{pmatrix} \Psi_{1,-}(\zeta) F_1^{-\sigma_3} z^{-m \sigma_3/2} \begin{pmatrix} 0 & 0 \\ \phi(z)^{-1} z^{-m} & 0 \end{pmatrix} \mathcal{D}(z)^{-\sigma_3} \\
 &= m^{-\beta \sigma_3} i^{\frac{m}{2} \sigma_3} \begin{pmatrix} 0 & \tilde{E}_{12}(z) \\ \tilde{E}_{21}(z) & 0 \end{pmatrix} \Psi_{1,-}(\zeta) \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \phi(z)^{-\sigma_3} F_1^{\sigma_3} z^{-m \sigma_3/2} \mathcal{D}(z)^{-\sigma_3} \\
 &= m^{-\beta \sigma_3} i^{\frac{m}{2} \sigma_3} \begin{pmatrix} 0 & \tilde{E}_{12}(z) \\ \tilde{E}_{21}(z) & 0 \end{pmatrix} \begin{pmatrix} \Psi_{1-,12}(\zeta) & 0 \\ \Psi_{1-,22}(\zeta) & 0 \end{pmatrix} \phi(z)^{-1} z^{-m/2} \mathcal{D}(z)^{-1} F_1
 \end{aligned}$$

$$\begin{aligned}
 &= m^{-\beta\sigma_3} i^{\frac{m}{2}\sigma_3} \begin{pmatrix} \tilde{E}_{12}(z)\Psi_{1-,22}(\zeta) & 0 \\ \tilde{E}_{21}(z)\Psi_{1-,12}(\zeta) & 0 \end{pmatrix} \phi(z)^{-1} z^{-m/2} \mathcal{D}(z)^{-1} F_1 \\
 &= \begin{pmatrix} m^{-\beta} i^{\frac{m}{2}} \tilde{E}_{12}(z)\Psi_{1-,22}(\zeta) & 0 \\ m^{\beta} i^{-\frac{m}{2}} \tilde{E}_{21}(z)\Psi_{1-,12}(\zeta) & 0 \end{pmatrix} \phi(z)^{-1} z^{-m/2} \left(\frac{z-i}{z+i}\right)^{-\beta} F_1.
 \end{aligned}$$

Thus, the integral over $\Sigma_1^{i,m}$ has the following form:

$$\int_{\Sigma_1^{i,m}} R_{11}(z) m^{-\beta} i^{\frac{m}{2}} \tilde{E}_{12}(z)\Psi_{1-,22}(\zeta) \phi(z)^{-1} z^{-m/2} F_1 \tilde{f}_m(z) \frac{dz}{z} \tag{8.11}$$

$$+ \int_{\Sigma_1^{i,m}} R_{12}(z) m^{\beta} i^{-\frac{m}{2}} \tilde{E}_{21}(z)\Psi_{1-,12}(\zeta) \phi(z)^{-1} z^{-m/2} F_1 \tilde{f}_m(z) \frac{dz}{z}. \tag{8.12}$$

Note that we have

$$\Psi_1(\zeta) = \Psi_1^{(I)}(\zeta) J_1^{-1} J_8^{-1} = \Psi_1^{(I)}(\zeta) \begin{pmatrix} 1 & -e^{-i\pi\beta} \\ e^{i\pi\beta} & 0 \end{pmatrix} = \begin{pmatrix} * & -e^{-i\pi\beta} \Psi_{1,11}^{(I)}(\zeta) \\ * & -e^{-i\pi\beta} \Psi_{1,21}^{(I)}(\zeta) \end{pmatrix} \quad (\zeta \in \text{VII}).$$

Therefore, if we use the estimation $|\frac{f_m(z)}{z^m}| \leq \sum_{\ell=1}^m \frac{|z|^{-\ell-m}}{\ell} \leq \sum_{\ell=1}^m \frac{1}{\ell}$ ($|z| > 1$), the integral (8.11) becomes

$$\begin{aligned}
 &\int_{\Sigma_1^{i,m}} O(m^{-\Re\beta}) \Psi_{1-,22}(\zeta) z^{-m/2} \tilde{f}_m(z) \frac{dz}{z} \\
 &= \int_{\Sigma_1^{i,m}} O(m^{-\Re\beta}) \Psi_{1,21}^{(I)}(\zeta) z^{-m/2} \left(f_m(z) - \frac{1}{2i} \ln \frac{z-i}{z+i} \right) \frac{dz}{z} \\
 &= \int_{\Sigma_1^{i,m}} O(m^{-\Re\beta}) \psi(1+\beta, 1; \zeta) \frac{f_m(z) - \frac{1}{2i} \ln \frac{z-i}{z+i}}{z^m} \frac{dz}{z} \\
 &= \int_{\Sigma_1^{i,m}} O(m^{-\Re\beta} \ln m) \psi(1+\beta, 1; \zeta) \frac{dz}{z}, \\
 &= \int_{\Gamma_8 \cap \{\zeta: 1+O(1/m) \leq |\zeta| \leq Cm\}} O(m^{-\Re\beta} \ln m) \zeta^{-1-\beta} \frac{d\zeta}{m} \\
 &= O(m^{-\Re\beta} m^{-1} (m^{1/4} + 1) \ln m) = O(m^{-1/2}),
 \end{aligned}$$

where $C > 0$ is a constant, $\frac{dz}{z} = \frac{d\zeta}{m}$, and we used the large ζ asymptotics of $\psi(1+\beta, 1; \zeta)$. The other integral (8.12) can be estimated somewhat similarly as follows:

$$\begin{aligned}
 &\int_{\Sigma_1^{i,m}} O(m^{-1+2|\Re\beta|}) m^{\beta} \Psi_{1,12}(\zeta) z^{-m/2} \tilde{f}_m(z) \frac{dz}{z} \\
 &= \int_{\Sigma_1^{i,m}} O(m^{-1+2|\Re\beta|}) m^{\beta} \Psi_{1,11}^{(I)}(\zeta) z^{-m/2} \tilde{f}_m(z) \frac{dz}{z} \\
 &= \int_{\Sigma_1^{i,m}} O(m^{-1+2|\Re\beta|}) m^{\beta} \psi(\beta, 1; \zeta) \frac{\tilde{f}_m(z)}{z^m} \frac{dz}{z}
 \end{aligned}$$

$$\begin{aligned}
 &= \int_{\Gamma_8 \cap \{\zeta: 1+O(1/m) \leq |\zeta| \leq Cm\}} O\left(m^{-1+2|\Re\beta|} \ln m\right) \left(\frac{\zeta}{m}\right)^{-\beta} \frac{d\zeta}{m} \\
 &= O\left(m^{-1+2|\Re\beta|} \ln m\right) \int_0^C t^{-\Re\beta} dt = O\left(m^{-1+2|\Re\beta|} \ln m\right) = O\left(m^{-1/2}\right).
 \end{aligned}$$

□

With the above proof we have finished proving lemma 3.2, which we use in the next section.

9. Calculating the mutual information

In this section we prove theorem 2.1, that is, we calculate (2.12). We start with a lemma.

Lemma 9.1. *We have*

$$\left| \tan\left(\frac{\pi}{2}\beta\right) \right| < 1 \quad (\lambda \in \mathbb{C} \setminus [-1, 1]).$$

Proof. This is a simple geometric observation. Consider the parallelogram on the complex plane with vertices $0, e^{i\frac{\pi}{2}\beta}, e^{-i\frac{\pi}{2}\beta}$ and $e^{i\frac{\pi}{2}\beta} + e^{-i\frac{\pi}{2}\beta}$. Notice that $|\arg(e^{\pm i\frac{\pi}{2}\beta})| < \pi/4$, hence the angle in the parallelogram at 0 is less than $\pi/2$. Therefore $|e^{i\frac{\pi}{2}\beta} - e^{-i\frac{\pi}{2}\beta}| < |e^{i\frac{\pi}{2}\beta} + e^{-i\frac{\pi}{2}\beta}|$, which completes the proof. □

Integration by parts gives the following for all $\varepsilon > 0$ and $m, n \in \mathbb{N}$:

$$\begin{aligned}
 &\frac{-1}{2\pi i} \oint_{\Gamma_\varepsilon} e(1 + \varepsilon, \lambda) \frac{d}{d\lambda} \ln \widehat{D}(\lambda) d\lambda = \frac{1}{2\pi i} \oint_{\Gamma_\varepsilon} \ln \widehat{D}(\lambda) \frac{d}{d\lambda} e(1 + \varepsilon, \lambda) d\lambda \\
 &= \frac{1}{2\pi i} \oint_{\Gamma_\varepsilon} \ln\left(1 - \langle \vec{\mathfrak{G}}_1, \vec{\mathfrak{g}}_1 \rangle \langle \vec{\mathfrak{G}}_2, \vec{\mathfrak{g}}_2 \rangle\right) \frac{d}{d\lambda} e(1 + \varepsilon, \lambda) d\lambda \\
 &= \frac{1}{2\pi i} \oint_{\Gamma_\varepsilon} \ln\left(1 - \left[i \tan\left(\frac{\pi}{2}\beta\right) + O(m^{-1/4})\right] \left[i \tan\left(\frac{\pi}{2}\beta\right) + O(n^{-1/4})\right]\right) \frac{d}{d\lambda} e(1 + \varepsilon, \lambda) d\lambda \\
 &= \frac{1}{2\pi i} \oint_{\Gamma_\varepsilon} \ln\left(1 + \tan^2\left(\frac{\pi}{2}\beta\right) + O(m^{-1/4} + n^{-1/4})\right) \frac{d}{d\lambda} e(1 + \varepsilon, \lambda) d\lambda.
 \end{aligned}$$

Therefore, equation (2.12) becomes

$$\begin{aligned}
 &\lim_{\varepsilon \searrow 0} \frac{1}{2\pi i} \oint_{\Gamma_\varepsilon} \ln\left(1 + \tan^2\left(\frac{\pi}{2}\beta\right)\right) \frac{d}{d\lambda} e(1 + \varepsilon, \lambda) d\lambda \\
 &= \lim_{\varepsilon \searrow 0} \frac{-1}{2\pi i} \oint_{\Gamma_\varepsilon} e(1 + \varepsilon, \lambda) \frac{d}{d\lambda} \ln\left(1 + \tan^2\left(\frac{\pi}{2}\beta\right)\right) d\lambda, \tag{9.1}
 \end{aligned}$$

where we used integration by parts. Note that

$$\frac{d}{d\lambda} \ln\left(1 + \tan^2\left(\frac{\pi}{2}\beta\right)\right) = \frac{d}{d\beta} \ln\left(1 + \tan^2\left(\frac{\pi}{2}\beta\right)\right) \frac{d\beta}{d\lambda} = -i \tan\left(\frac{\pi}{2}\beta\right) \frac{1}{1 - \lambda^2}.$$

Hence, equation (9.1) becomes

$$\lim_{\varepsilon \searrow 0} \frac{1}{2\pi} \oint_{\Gamma_\varepsilon} e(1 + \varepsilon, \lambda) \tan\left(\frac{\pi}{2}\beta\right) \frac{1}{1 - \lambda^2} d\lambda.$$

Note that by Cauchy's theorem there is a flexibility in choosing Γ_ε . We observe that for $|\lambda - 1| = \frac{\varepsilon}{2}$ we have $e(1 + \varepsilon, \lambda) = -\frac{1+\varepsilon+\lambda}{2} \ln \frac{1+\varepsilon+\lambda}{2} - \frac{1+\varepsilon-\lambda}{2} \ln \frac{1+\varepsilon-\lambda}{2} = O(\varepsilon) + O(\varepsilon \ln \varepsilon) = O(\varepsilon \ln \varepsilon)$ as $\varepsilon \searrow 0$. Therefore, if C_1^ε denotes the circle around 1 with radius $\frac{\varepsilon}{2}$, then

$$\lim_{\varepsilon \searrow 0} \frac{1}{2\pi} \oint_{C_1^\varepsilon} e(1 + \varepsilon, \lambda) \tan\left(\frac{\pi}{2}\beta\right) \frac{1}{1 - \lambda^2} d\lambda = \lim_{\varepsilon \searrow 0} \oint_{C_1^\varepsilon} O(\ln \varepsilon) d\lambda = 0.$$

We similarly get that the integral over C_{-1}^ε converge to 0. Therefore, by the Lebesgue dominant convergence theorem, we conclude that (9.1) is equal to the following:

$$\begin{aligned} & \lim_{\varepsilon \searrow 0} \frac{1}{2\pi} \int_{-1+\frac{\varepsilon}{2}}^{1-\frac{\varepsilon}{2}} e(1 + \varepsilon, \lambda) \left[\tan\left(\frac{\pi}{2}\beta_+\right) - \tan\left(\frac{\pi}{2}\beta_-\right) \right] \frac{1}{1 - \lambda^2} d\lambda \\ &= \frac{1}{2\pi} \int_{-1}^1 e(1, \lambda) \left[\tan\left(\frac{\pi}{2}\beta_+\right) - \tan\left(\frac{\pi}{2}\beta_-\right) \right] \frac{1}{1 - \lambda^2} d\lambda, \end{aligned} \tag{9.2}$$

where the interval $[-1, 1]$ is oriented from the right to the left, hence its $+/-$ sides are its below/upper sides. Note that $\lambda \mapsto \beta$ transforms $\mathbb{C} \setminus [-1, 1]$ onto $\mathbb{C} \setminus (-\infty, 0]$. Also, if $(-\infty, 0]$ is oriented from the left to right, then the $+$ side of $[-1, 1]$ is mapped onto the $+$ side of $(-\infty, 0]$. In particular,

$$\beta_\pm = \frac{1}{2\pi i} \left(\ln \left| \frac{\lambda + 1}{\lambda - 1} \right| \pm \pi i \right) = \frac{1}{2\pi i} \left(\ln \left(\frac{1 + \lambda}{1 - \lambda} \right) \pm \pi i \right) \quad (\lambda \in (-1, 1)),$$

and hence a straightforward calculation shows that

$$\tan\left(\frac{\pi}{2}\beta_+\right) - \tan\left(\frac{\pi}{2}\beta_-\right) = 2\sqrt{1 - \lambda^2} \quad (\lambda \in (-1, 1)).$$

Now, plugging in the above into (9.2) we obtain

$$\begin{aligned} & \frac{-1}{\pi} \int_{-1}^1 \left(\frac{1 + \lambda}{2} \ln \frac{1 + \lambda}{2} + \frac{1 - \lambda}{2} \ln \frac{1 - \lambda}{2} \right) \frac{1}{\sqrt{1 - \lambda^2}} d\lambda \\ &= \frac{-1}{\pi} \int_{-1}^1 \sqrt{\frac{1 + \lambda}{1 - \lambda}} \ln \frac{1 + \lambda}{2} d\lambda \\ &= \frac{-2}{\pi} \int_0^1 \sqrt{\frac{t}{1 - t}} \ln t dt = \frac{-8}{\pi} \int_0^1 \frac{v^2}{\sqrt{1 - v^2}} \ln v dv \\ &= \frac{8}{\pi} \left(\int_0^1 \sqrt{1 - v^2} \ln v dv - \int_0^1 \frac{\ln v}{\sqrt{1 - v^2}} dv \right) = 2 \ln 2 - 1. \end{aligned}$$

Above we performed two substitutions $2t = 1 + \lambda$ and $t = v^2$. Since the last two special integrals are well known to be equal to $-\frac{\pi}{8} - \frac{\pi}{4} \ln 2$ and $-\frac{\pi}{2} \ln 2$, respectively, the proof of theorem 2.1 is complete.

10. Conclusions

Understanding entanglement in bipartite systems is of fundamental importance in quantum information, but at the same time it is often fraught with technical difficulties. One of the

major reasons that makes it such a challenging problem is that even in simple systems the calculations are rather involved and often it is impossible to perform a rigorous analysis. Over the past twenty years a lot of research on bipartite entanglement has focussed on one-dimensional quantum lattice models, because they are amenable to a certain degree of mathematical manipulations. Originally, the interest concentrated on the entanglement entropy of a single interval of contiguous spins with the rest of the chain [1, 10, 18, 21–23, 25, 27–30, 33, 38] but more recently physicists have directed their research on the computation of the entanglement entropy of disjoint blocks [2, 3, 11–13, 17, 26, 32].

In this article we study a quadratic form of Fermi operators and compute the von Neumann entropy of two disjoint intervals separated by one lattice site. The major contribution of this paper is a rigorous analysis of the asymptotic limit of the entropy as the size of the intervals tends to infinity. More precisely, let $P = P_1 \cup P_2$, where $P_1 = \{1, \dots, m\}$ and $P_2 = \{m + 2, \dots, m + n + 1\}$. Write $S(\rho_P^{(m)})$ and $S(\rho_P^{(n)})$ for the entropies of the blocks of fermions at P_1 and P_2 , respectively; denote by $S(\rho_P)$ the entanglement entropy between P and the rest of the chain. The quantity $S(\rho_P^{(m)})$ was computed in [25]. We prove that the *mutual entropy* between P_1 and P_2

$$S(\rho_P^{(m)}) + S(\rho_P^{(n)}) - S(\rho_P) \rightarrow 2 \ln 2 - 1, \quad (10.1)$$

as $m, n \rightarrow \infty$. The proof is based on the Riemann–Hilbert method and involves computing the asymptotics of a Toeplitz determinant as well as extracting precise information on the asymptotic behaviour of the inverse of a Toeplitz matrix. Besides the intrinsic physical importance of the problem, the mathematical result is of interest in its own right. The asymptotic analysis of Toeplitz determinants has a long history and is still an area of active research. The ultimate goal would be to compute rigorously the entanglement entropy of two disjoint gaps separated by an arbitrary number of lattice sites. Unfortunately, this is still beyond our present ability.

ORCID iDs

G P Gehér  <https://orcid.org/0000-0003-1499-3229>

F Mezzadri  <https://orcid.org/0000-0002-4572-5617>

References

- [1] Amico L, Osterloh A, Plastina F, Fazio R and Palma G M 2004 Dynamics of entanglement in one-dimensional spin systems *Phys. Rev. A* **69** 022304
- [2] Alba V, Tagliacozzo L and Calabrese P 2010 Entanglement entropy of two disjoint blocks in critical Ising models *Phys. Rev. B* **81** 060411
- [3] Ares F, Esteve J and Falceto F 2014 Entanglement of several block in Fermionic chains *Phys. Rev. A* **90** 062321
- [4] Au-Yang H and Jacques H H 1987 Perk critical correlations in a $/$ -invariant inhomogeneous Ising model *Physica A* **144** 44–104
- [5] Baik J, Deift P and Johansson K 1999 On the distribution of the length of the longest increasing subsequence of random permutations *J. Am. Math. Soc.* **12** 1119–78
- [6] Baik J, Deift P and Suidan T 2016 *Combinatorics and Random Matrix Theory, Graduate Studies in Mathematics* vol 172 (Providence, RI: American Mathematical Society)
- [7] Basor E L 1979 A localization theorem for Toeplitz determinants *Indiana Univ. Math. J.* **28** 975–83
- [8] Basor E L and Ehrhardt T 2017 Asymptotic formulas for determinants of a special class of Toeplitz + Hankel matrices *Large Truncated Toeplitz Matrices, Toeplitz Operators, and Related*

- Topics (Operator Theory: Advances and Applications vol 259)* (Berlin: Birkhäuser/Springer) pp 125–54
- [9] Bennett C H, Bernstein H J, Popescu S and Schumacher B 1996 Concentrating partial entanglement by local operations *Phys. Rev. A* **53** 2046–52
 - [10] Calabrese P and Cardy J 2004 Entanglement entropy and quantum field theory *J. Stat. Mech.* **P06002**
 - [11] Calabrese P, Cardy J and Tonni E 2009 Entanglement entropy of two disjoint intervals in conformal field theory *J. Stat. Mech.* **P11001**
 - [12] Calabrese P, Cardy J and Tonni E 2011 Entanglement entropy of two disjoint intervals in conformal field theory: II *J. Stat. Mech.* **P01021**
 - [13] Cardy J 2013 Some results on the mutual information of disjoint regions in higher dimensions *J. Phys. A: Math. Theor.* **46** 285402
 - [14] Chelkak D, Hongler C and Mahfouf R 2020 Magnetization in the zig-zag layered Ising model and orthogonal polynomials (arXiv:1904.09168)
 - [15] Deift P 1999 Integrable operators *Differential Operators and Spectral Theory (American Mathematical Society Translations Series 2 vol 189)* (Providence, RI: American Mathematical Society) pp 69–84
 - [16] Deift P, Its A R and Krasovsky I 2011 Asymptotics of Toeplitz, Hankel, and Toeplitz+Hankel determinants with Fisher-Hartwig singularities *Ann. Math.* **174** 1243–99
 - [17] Fagotti M and Calabrese P 2010 Entanglement entropy in two disjoint blocks of XY chains *J. Stat. Mech.* **P04016**
 - [18] Furukawa S, Pasquier V and Shiraishi J 2009 Mutual information and boson radius in a $c = 1$ critical system in one dimension *Phys. Rev. Lett.* **102** 170602
 - [19] Gharakhloo R and Its A 2009 A Riemann-Hilbert approach to asymptotic analysis of Toeplitz+Hankel determinants (arXiv:1909.00963)
 - [20] Its A R, Izergin A G, Korepin V E and Slavnov N A 1990 Differential equations for quantum correlation functions *Int. J. Mod. Phys. B* **4** 1003–37
 - [21] Its A R, Jin B-Q and Korepin V E 2005 Entanglement in the XY spin chain *J. Phys. A: Math. Gen.* **38** 2975–90
 - [22] Its A R, Jin B-Q and Korepin V E 2007 Entropy of XY spin chain and block Toeplitz determinants *Universality and Renormalization* vol 50 (Providence, RI: American Mathematical Society) pp 151–83 Fields Inst. Commun.
 - [23] Its A R, Mezzadri F and Mo M Y 2008 Entanglement entropy in quantum spin chains with finite range interaction *Commun. Math. Phys.* **284** 117–85
 - [24] Its A, Tracy C and Widom H 2001 Random words, Toeplitz determinants and integrable systems. II *Physica D* **152–153** 199–224
 - [25] Jin B-Q and Korepin V E 2004 Quantum spin chain, Toeplitz determinants and the Fisher-Hartwig conjecture *J. Stat. Phys.* **116** 79–95
 - [26] Jin B-Q and Korepin V E 2011 Entanglement entropy for disjoint subsystems in XX spin chain in chain (arXiv:1104.1004)
 - [27] Keating J P and Mezzadri F 2004 Random matrix theory and entanglement in quantum spin chains *Commun. Math. Phys.* **252** 543–79
 - [28] Keating J P and Mezzadri F 2005 Entanglement in quantum spin chains, symmetry classes of random matrices, and conformal field theory *Phys. Rev. Lett.* **94** 050501
 - [29] Keating J P, Mezzadri F and Novaes M 2006 Comb entanglement in quantum spin chains *Phys. Rev. A* **74** 012311
 - [30] Korepin V E 2004 Universality of entropy scaling in one dimensional gapless models *Phys. Rev. Lett.* **92** 096402
 - [31] Lieb E, Schultz T and Mattis D 1961 Two soluble models of an antiferromagnetic chain *Ann. Phys., NY* **16** 407–66
 - [32] Molina-Vilaplana J and Sodano P 2011 Holographic view on quantum correlations and mutual information between disjoint blocks of a quantum critical system *J. High Energy Phys.* **JHEP10(2011)011**
 - [33] Osborne T J and Nielsen M A 2002 Entanglement in a simple quantum phase transition *Phys. Rev. A* **66** 032110
 - [34] Osterloh A, Amico L, Falci G and Fazio R 2002 Scaling of entanglement close to a quantum phase transition *Nature* **416** 608–10

- [35] Rangamani M and Takayanagi T 2017 *Holographic Entanglement Entropy (Lecture Notes in Physics vol 931)* (Cham: Springer)
- [36] Szegő G 1915 Ein Grenzwertsatz über die Toeplitzschen Determinanten einer reellen positiven Funktion *Math. Ann.* **76** 490–503
- [37] Szegő G 1952 On certain Hermitian forms associated with the Fourier series of a positive function *Comm. Sém. Math. Univ. Lund [Medd. Lunds Univ. Mat. Sem.]* **1952** 228–38
- [38] Vidal G, Latorre J I, Rico E and Kitaev A 2003 Entanglement in quantum critical phenomena *Phys. Rev. Lett.* **90** 227902