Fisher–Hartwig expansion for Toeplitz determinants and the spectrum of a single-particle reduced density matrix for one-dimensional free fermions

Dmitri A Ivanov\textsuperscript{1,2} and Alexander G Abanov\textsuperscript{3}

\textsuperscript{1} Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland
\textsuperscript{2} Institute for Theoretical Physics, University of Zurich, 8057 Zurich, Switzerland
\textsuperscript{3} Department of Physics and Astronomy and Simons Center for Geometry and Physics, Stony Brook University, Stony Brook, NY 11794, USA

E-mail: ivanov@itp.phys.ethz.ch

Received 2 July 2013
Published 2 September 2013
Online at stacks.iop.org/JPhysA/46/375005

Abstract
We study the spectrum of the Toeplitz matrix with a sine kernel, which corresponds to the single-particle reduced density matrix for free fermions on the one-dimensional lattice. For the spectral determinant of this matrix, a Fisher–Hartwig expansion in the inverse matrix size has been recently conjectured. This expansion can be verified order by order, away from the line of accumulation of zeros, using the recurrence relation known from the theory of discrete Painlevé equations. We perform such a verification to the tenth order and calculate the corresponding coefficients in the Fisher–Hartwig expansion. Under the assumption of the validity of the Fisher–Hartwig expansion in the whole range of the spectral parameter, we further derive expansions for an equation on the eigenvalues of this matrix and for the von Neumann entanglement entropy in the corresponding fermion problem. These analytical results are supported by a numerical example.

PACS numbers: 05.30.Fk, 03.65.Ud, 05.40.−a
(Some figures may appear in colour only in the online journal)

1. Introduction

Toeplitz matrices, i.e., matrices with entries $a_{i-j}$ depending only on the difference of the column and row indices, play an important role in a wide range of physical and mathematical problems, including problems in statistical mechanics [1–3], random-matrix theory [4, 5], quantum integrable systems [6–13], and nonequilibrium bosonization [14–16]. One is often interested in the asymptotic behavior of the spectrum of such matrices in the limit of a large matrix size $L$, for a given symbol of the matrix.
\[ \sigma(k) = \sum_{m=-\infty}^{+\infty} a_m e^{-ikm}, \quad k \in [-\pi, \pi]. \] (1)

While the leading exponential dependence of the spectral determinant of Toeplitz matrices on their size \( L \) is usually easy to guess on physical grounds (the rigorous result is known as the first Szegő theorem) [17], finding subleading corrections is a nontrivial problem, which continues to be a topic of active research in mathematics and mathematical physics [18–26]. A recent important step in developing the theory of Toeplitz determinants was the proof of the Fisher–Hartwig conjecture for the case of symbols (1) with power-law singularities [27].

In mathematical and physical literature, stronger conjectures about higher-order corrections to the Fisher–Hartwig formula have been proposed [15, 28–34]. In particular, many studies focused on the specific example of the matrix of the sine-kernel form:

\[ a_{i-j} = \begin{cases} \sin k_F (i-j), & i \neq j, \\ \pi (i-j), & i = j, \end{cases} \] (2)

which corresponds to the symbol

\[ \sigma(k) = \begin{cases} 1, & |k| < k_F, \\ 0, & \text{otherwise}. \end{cases} \] (3)

This Toeplitz matrix (with \( k_F \) being the only parameter, apart from the matrix size \( L \)) appears in many problems involving one-dimensional free fermions and closely related systems. The parameter \( k_F \) corresponds to the Fermi wave vector of the fermions. In [34], the higher-order corrections to the spectral determinant of this matrix,

\[ \chi(\kappa, k_F, L) = \det_{1\leq i,j\leq L} [\delta_{ij} + a_{i-j} (e^{2\pi i \kappa} - 1)], \] (4)

were conjectured to form an asymptotic series

\[ \chi(\kappa, k_F, L) = \sum_{j=-\infty}^{+\infty} \chi_*(\kappa + j, k_F, L) \] (5)

where

\[ \chi_*(\kappa, k_F, L) = \exp \left[ 2i \kappa k_f L - 2 \kappa^2 \ln (2L \sin k_f) + \tilde{C}(\kappa) + \sum_{n=1}^{\infty} \tilde{F}_n(\kappa, k_F)(iL)^{-n} \right], \] (6)

\[ \tilde{C}(\kappa) = 2 \ln[G(1 + \kappa)G(1 - \kappa)]. \] (7)

and \( G() \) is the Barnes \( G \) function [35]. We will call the explicitly periodic in \( \kappa \) expansion (5)–(6) the Fisher–Hartwig expansion.

As pointed out in [29], a calculation of the expansion coefficients \( \tilde{F}_n(\kappa, k_F) \) is possible using a recurrence relation from the theory of discrete Painlevé equations [36]. In [29] such a computation has been performed to the second order. In the present work, we extend this calculation to the tenth order and find the coefficients up to \( \tilde{F}_{10}(\kappa, k_F) \). Formally, this procedure allows us to verify, order by order, the periodic form of the expansion (5)–(6) away from the half-line \( \text{Im } e^{2\pi i \kappa} = 0, \text{Re } e^{2\pi i \kappa} < 0 \). At this half-line, the zeros of \( \chi(\kappa) \) accumulate (as \( L \to \infty \)), which prevents a verification of the expansion at this line, even to a finite order. However, the available numerical evidence from earlier works [29, 34, 37] and from this work

4 Our parameter \( \kappa \) coincides with that in [37, 52] and is related to the counting fields \( \lambda \) in [34, 38, 44] and \( \eta \) in [13] by \( 2\pi \lambda = \lambda = \eta \). It is also related to the parameter \( \beta \) in [29] as \( \kappa = -\beta \). Our definition of \( \tilde{F}_n(\kappa, k_F) \) differs from \( F_n(\kappa, k_F) \) in [34] by a factor of \( i^n \), in order to make it a real function. Our definition of \( \tilde{C}(\kappa) \) differs from \( C(\kappa) \) in [52] by \( 2\kappa^2 \ln 2 \), in order to simplify formulas.
(see section 7 below) suggests that the expansion (5)–(6) also extends to this half-line. If we assume this conjectured extension, we can convert the coefficients $\tilde{F}_n(\kappa, k_F)$ into a series expansion for the eigenvalues of the Toeplitz matrix $a_{-j}$ (or, equivalently, for the zeros of the spectral determinant $\chi(\kappa)$). Furthermore, under the same assumption, we can derive the power series for the von Neumann entanglement entropy for free fermions on a segment of the one-dimensional lattice (thus extending the results of [37] to the lattice case).

The paper is organized as follows. In the next section, we summarize the main results, with references to subsequent sections containing detailed formulas and derivations. In section 3, we overview the relation of the spectral problem for the Toeplitz matrix to one-dimensional free fermions. In section 4, we review the recurrence relation used for calculating the coefficients $\tilde{F}_n(\kappa, k_F)$ and present results of such a calculation to the tenth order. In section 5, we use the coefficients $\tilde{F}_n(\kappa, k_F)$ to find the asymptotic expansion of the eigenvalues of the Toeplitz matrix. In section 6, we calculate the expansion for the von Neumann entanglement entropy. In section 7, we support the results of the two preceding sections with a numerical example. Finally, the last section 8 contains several concluding remarks. To avoid lengthy equations, in the main part of the paper we only present the first six orders, and the results for orders seven to ten are given in the appendix.

2. Main results

The main results of this paper assume the conjectured expansion (5)–(6). Under this assumption,

- We compute the coefficients $\tilde{F}_n(\kappa, k_F)$ up to the tenth $(n = 10)$ order. They turn out to be polynomials in $\kappa$ and $\cot k_F$. The explicit expressions for $\tilde{F}_n(\kappa, k_F)$ are given in equations (17) and (18) of section 4 and in equation (A.1) of the appendix. The consistency of this calculation supports the conjecture (5)–(6).
- We write an equation on the spectrum of the matrix (2) in the form of a ‘quasiclassical expansion’ in $1/L$ (equations (21) and (22)). The coefficients of this expansion are again polynomials in $\kappa$ and $\cot k_F$. The expansion is computed to the tenth order in $1/L$ and the coefficients are reported in equations (23) and (24) of section 5 and in equation (A.2) of the appendix.
- We derive the power series for the von Neumann entanglement entropy for free fermions on a segment of length $L$ of an infinite one-dimensional lattice. This expansion is also derived to the tenth order in $1/L$, with the coefficients listed in equation (30) of section 6 and in equation (A.3) of the appendix.
- Finally, we check our results for the spectrum and for the entanglement entropy numerically and find a perfect agreement between our analytic predictions and numerical data (see figures 2 and 3). This numerical evidence strongly supports the conjecture (5)–(6) and our analytical results.

3. Motivation: free fermions in one dimension

Our study of the spectral determinant (4) of the matrix (2) is motivated largely by the problems of full counting statistics (FCS) [38] and entanglement [39, 40] for free fermions on the one-dimensional lattice. In the ground state, the single-particle correlation function is given by the matrix elements (2):

$$\langle \Psi_i | \Psi_j \rangle = a_{i-j},$$

(8)
where $\Psi_i^\dagger$ and $\Psi_j$ are the fermionic creation and annihilation operators on lattice sites $i$ and $j$, respectively. As shown in [41–44], the eigenvalues $p_m$ of this matrix restricted to some segment of the lattice give the set of single-particle occupation numbers, which describe the FCS of fermions on this segment. In particular, the FCS generating function coincides with $\chi(\kappa, k_F, L)$ defined in equation (4) and can be written as

$$\chi(\kappa, k_F, L) = \exp \left( 2\pi i \kappa \sum_{i=1}^{L} \Psi_i^\dagger \Psi_i \right) = \prod_{m=1}^{L} \left( 1 - p_m + p_m e^{2\pi i \kappa} \right).$$

In other words, the statistics of the number of particles on the line segment coincides with that of $L$ levels filled independently with the probabilities $p_m$.

These probabilities may thus be related to the zeros of the spectral determinant (4). The zeros lie on the negative real axis of $\exp[2\pi i \kappa]$ and therefore may be parametrized as

$$\kappa_m = \frac{1}{2} - i \xi_m$$

with real parameters $\xi_m$. The probabilities $p_m$ are, in turn, related to $\xi_m$ as

$$p_m = \frac{1}{1 + e^{2\pi \xi_m}}.$$  

The results of the present paper (in particular, equations (21) and (22)) describe the spectrum of the probabilities $p_m$ not very close to 0 or 1. Such probabilities are relevant for typical fluctuations of the number of particles around its average. At the same time, our results do not provide any information about the probabilities $p_m$ very close to 0 or 1 (i.e., corresponding to large $|\xi_m|$): those probabilities would be relevant for atypical fluctuations, e.g., for the emptiness formation probability [28, 45, 46].

The same spectrum of the probabilities is known to determine the entanglement (von Neumann) entropy of the segment with the rest of the lattice [47–50]:

$$S(k_F, L) = \sum_{m=1}^{L} [ -p_m \ln p_m - (1 - p_m) \ln(1 - p_m)].$$

The probabilities $p_m$ exponentially close to 0 or to 1 give an exponentially small contribution to the entropy and may be neglected. This justifies our derivation of the asymptotic expansion (28) in section 6 (see also [37] for more details).

4. Coefficients of the Fisher–Hartwig expansion

Recurrence relations for the spectral determinant (4) were derived from its connection to the theory of discrete Painlevé equations in [36]. Then, in [29], the procedure of extracting the coefficients of the Fisher–Hartwig expansion was outlined and the first two coefficients computed. We follow the prescription of [29] to compute further coefficients of the Fisher–Hartwig expansion, order by order.

The recurrence relations read:

$$\frac{\chi(\kappa, k_F, L + 1) \chi(\kappa, k_F, L - 1)}{[\chi(\kappa, k_F, L)]^2} = 1 - x_L^2,$$

where $x_L$ obey the relations

$$x_L x_{L-1} - \cos k_F = \frac{1 - x_L^2}{2x_L} [(L + 1)x_{L+1} + (L - 1)x_{L-1}] - \frac{1 - x_{L-1}^2}{2x_{L-1}} [Lx_L + (L - 2)x_{L-2}].$$

(14)
If we assume the Fisher–Hartwig expansion (5)–(6), then, from the relation (13), one finds an expansion for $x_L$ of the form

$$x_L = \frac{\kappa}{L} (r_L - r_L^{-1}) + \sum_{n=2}^{\infty} \frac{Y_n(r_L)}{(r_L - r_L^{-1})^{2n-3}L^n},$$  

where we have defined

$$r_L = (-1)^L \frac{e^{ikF L}}{(2L \sin kF)^{2z}} \frac{\Gamma(1 + \kappa)}{\Gamma(1 - \kappa)}$$

and $Y_n(r_L)$ are Laurent polynomials in $r_L$ with coefficients depending on $\kappa$ and $kF$. Each term $Y_n(r_L)$ can be expressed via the coefficients of the Fisher–Hartwig expansion $\tilde{F}_n$ with $n' = 1, \ldots, n - 1$. By substituting the expansion (15) into the relation (14), we can calculate the coefficients $\tilde{F}_n(\kappa, kF)$ order by order. Remarkably, the number of conditions exceeds the number of the coefficients $\tilde{F}_n(\kappa, kF)$ to be calculated, and the fact that the coefficients $\tilde{F}_n(\kappa, kF)$ satisfy all the conditions simultaneously supports the conjecture of the Fisher–Hartwig expansion. We do not have a proof of this property to all orders, but only observed it in calculating the coefficients $\tilde{F}_n(\kappa, kF)$ to the tenth order.

Note that this procedure is a discrete version of a similar calculation using Painlevé V equation in the continuous ($kF \to 0$) limit [51, 52]. The computations are straightforward, but require tedious manipulations with polynomials and series. We have performed these computations using Mathematica software [53].

As a result, we find that the coefficients $\tilde{F}_n(\kappa, kF)$ are polynomials in $\kappa$ and $\cot kF$:

$$\tilde{F}_n(\kappa, kF) = \sum_{l=0}^{\lfloor \frac{n}{2} \rfloor} P_{n,n-2l}(\kappa) \cot^{n-2l} kF,$$

where all $P_{n,l}(\kappa)$ are polynomials with real rational coefficients. We have calculated these polynomials to the tenth order. To avoid lengthy equations in the main body of the paper, we present below the first six orders, and report the seventh to tenth orders in equation (A.1) of the appendix:

$$P_{11}(\kappa) = 2\kappa^3,$$

$$P_{22}(\kappa) = \frac{5}{7}\kappa^4,$$

$$P_{30}(\kappa) = \frac{4}{5}\kappa^4 + \frac{1}{5}\kappa^2,$$

$$P_{33}(\kappa) = \frac{11}{2}\kappa^3 + \frac{2}{5}\kappa^2,$$

$$P_{31}(\kappa) = \frac{9}{5}\kappa^5 + \frac{1}{5}\kappa^3,$$

$$P_{44}(\kappa) = \frac{63}{4}\kappa^6 + \frac{1}{2}\kappa^4,$$

$$P_{42}(\kappa) = \frac{35}{2}\kappa^6 + \frac{1}{2}\kappa^4,$$

$$P_{50}(\kappa) = \frac{167}{60}\kappa^6 + \frac{25}{24}\kappa^4 + \frac{1}{20}\kappa^2,$$

$$P_{55}(\kappa) = \frac{527}{10}\kappa^7 + 12\kappa^5 + \frac{1}{2}\kappa^3,$$

$$P_{53}(\kappa) = 74\kappa^7 + \frac{77}{3}\kappa^5 + \frac{1}{2}\kappa^3,$$

$$P_{51}(\kappa) = \frac{45}{2}\kappa^7 + \frac{21}{2}\kappa^5 + \frac{1}{2}\kappa^3,$$

$$P_{66}(\kappa) = \frac{3129}{160}\kappa^8 + \frac{1931}{24}\kappa^6 + \frac{25}{16}\kappa^4,$$

$$P_{64}(\kappa) = \frac{2665}{24}\kappa^8 + \frac{339}{36}\kappa^6 + \frac{47}{24}\kappa^4,$$

$$P_{63}(\kappa) = \frac{2385}{16}\kappa^8 + \frac{781}{16}\kappa^6 + \frac{151}{16}\kappa^4,$$

$$P_{61}(\kappa) = \frac{936}{21}\kappa^8 + \frac{371}{36}\kappa^6 + \frac{43}{24}\kappa^4 + \frac{5}{120}\kappa^2.$$

(18)
The leading coefficients $P_{nn}(\kappa)$ reproduce $f_n(\kappa)$ found in [52] in the continuous limit $k_F \to 0$. The coefficients $\tilde{F}_1(\kappa, k_F)$ and $\tilde{F}_2(\kappa, k_F)$ have been previously reported in [29]. The coefficient $\tilde{F}_1(\kappa, k_F)$ was also conjectured in [34].

We also observe several remarkable properties of these coefficients, of which we do not have proofs and formulate them as conjectures (to all orders):

- The polynomial structure of $\tilde{F}_n(\kappa, k_F)$ persists to all orders, with the largest degree in $\kappa$ being $n + 2$ and the largest degree in $\cot k_F$ being $n$.
- The coefficients $\tilde{F}_1(\kappa, k_F)$ have the parity of $n$ with respect to $\kappa$ and to $\cot k_F$ (separately).
- All the numerical coefficients of these polynomials are real rational numbers. Most probably, they are all positive.
- The terms $\kappa^2$ appear only in the coefficients $P_{2n,0}(\kappa)$. All the other coefficients $P_{nn}$ have the lowest terms $\kappa^3$ or $\kappa^4$.

5. Eigenvalues of the Toeplitz matrix

If we conjecture that the Fisher–Hartwig expansion (5)–(6) holds for any $\kappa$ (including those with half-integer real part, where zeros of $\chi(\kappa, k_F, L)$ accumulate), then we can use it to find the zeros of $\chi(\kappa, k_F, L)$.

If we keep only the two leading branches of the Fisher–Hartwig expansion ($j = 0$ and $j = -1$) and only terms up to $\tilde{C}(\kappa)$ in the exponent (6), then we arrive at the quasiclassical equation for the zeros

$$\psi_0(\xi, k_F, L) \approx \pi \left( m + \frac{1}{2} \right),$$

where we have defined

$$\psi_0(\xi, k_F, L) = k_F L + 2\ln(2L \sin k_F) - 2\arg \Gamma \left( \frac{1}{2} + i \xi \right),$$

$\Gamma()$ denotes the gamma function, and we use the parametrization (10). This approximation was also derived in [37] in the continuous limit and in [54] using a relation to spheroidal functions [55].

Higher corrections in $1/L$ and higher Fisher–Hartwig branches may be incorporated in the quasiclassical approximation (19) in terms of a power series in $1/L$:

$$\Phi(\xi, k_F, L) = \pi \left( m + \frac{1}{2} \right),$$

where

$$\Phi(\xi, k_F, L) = \psi_0(\xi, k_F, L) + \sum_{n=1}^{\infty} \frac{X_n(\xi, k_F)}{L^n}$$

(22)

(the quantity $\Phi(\xi, k_F, L)$ was introduced earlier in [37], where the first term in the sum (22) was computed in the continuous limit). We do not have a proof of this series, but we have checked it explicitly to the tenth order. The coefficients $X_n(\xi, k_F)$ are found to have a polynomial form of the same type as $\tilde{F}_n(\kappa, k_F)$:

$$X_n(\xi, k_F) = \sum_{l=0}^{\lfloor \frac{n}{2} \rfloor} Q_{n-n-2l}(\xi) \cot^{n-2l} k_F.$$  

(23)

For $n$ up to six, the coefficients are:

$$Q_{11}(\xi) = 3\xi^2 - \frac{1}{3},$$
$$Q_{22}(\xi) = -5\xi^3 + \frac{5}{3}\xi,$$
$$Q_{20}(\xi) = -\frac{5}{3}\xi^3 + \frac{5}{6}\xi.$$
\( Q_{33}(\xi) = \frac{55}{2} \xi^4 - \frac{57}{8} \xi^2 + \frac{37}{16} \),
\( Q_{31}(\xi) = \frac{45}{4} \xi^4 - \frac{51}{8} \xi^2 + \frac{13}{4} \),
\( Q_{44}(\xi) = -\frac{189}{8} \xi^5 + \frac{85}{2} \xi^3 - 239 \xi \),
\( Q_{42}(\xi) = -\frac{105}{2} \xi^5 + 50 \xi^3 - \frac{155}{8} \xi \),
\( Q_{40}(\xi) = -\frac{163}{16} \xi^5 + \frac{107}{8} \xi^3 - \frac{1019}{8} \xi \),
\( Q_{55}(\xi) = \frac{3680}{27} \xi^6 - \frac{4139}{16} \xi^4 + 15661 \xi^2 - \frac{1009}{1280} \),
\( Q_{53}(\xi) = \frac{2591}{4} \xi^6 - \frac{1515}{4} \xi^4 + \frac{1229}{16} \xi^2 - \frac{85}{64} \),
\( Q_{51}(\xi) = \frac{315}{4} \xi^6 - \frac{1085}{16} \xi^4 + \frac{1773}{64} \xi^2 - \frac{139}{256} \),
\( Q_{66}(\xi) = -\frac{3129}{8} \xi^7 + \frac{25450}{16} \xi^5 - \frac{102949}{192} \xi^3 + \frac{7245}{256} \xi \),
\( Q_{64}(\xi) = -\frac{2655}{8} \xi^7 + \frac{22323}{16} \xi^5 - \frac{31745}{32} \xi^3 + \frac{7093}{128} \xi \),
\( Q_{62}(\xi) = -\frac{2385}{8} \xi^7 + \frac{20979}{64} \xi^5 - \frac{3209}{64} \xi^3 + \frac{7799}{256} \xi \),
\( Q_{60}(\xi) = -\frac{944}{27} \xi^7 + \frac{1279}{12} \xi^5 - \frac{1661}{36} \xi^3 + \frac{13261}{4032} \xi \),
\( m = 1 \) (24)
and the seventh to tenth orders are presented in equation (A.2) of the appendix. From observing the polynomial structure of the coefficients, we conjecture that the equations (21)–(22) holds uniformly for all \( \xi \) in the window
\( |\xi| < \Xi \).

Finally remark that the sum of all the probabilities (11) must give the total average number of particles, i.e.,
\[
\sum_{\xi_m} \frac{1}{1 + e^{\xi_m}} = \frac{k_F L}{\pi}.
\]

This condition allows us identify the integer index \( m \) in equation (21) with the sequential number of the root \( \xi_m \) in the increasing order starting with \( m = 0 \).

6. Von Neumann entanglement for one-dimensional free fermions

Similarly to the roots of \( \chi(\kappa, k_F, L) \), we can calculate the expansion for the von Neumann entanglement entropy (12). The whole discussion of [37] applies to the lattice case, with the only difference in the coefficients \( F_n(\kappa, k_F) \). In particular, if the conjecture about the polynomial structure of the coefficients \( F_n(\kappa, k_F) \) (with respect to \( \kappa \)) is valid, then the statement of [37] about the power-law expansion of the entropy (without oscillating terms) extends directly to the lattice case. A straightforward calculation along the lines of [37] produces the expansion
\[
S(k_F, L) = \frac{1}{3} \ln(2L \sin k_F) + \gamma + \sum_{n=1}^{\infty} \delta_{2n}(k_F) L^{-2n}.
\]
Figure 1. The spectrum of the matrix (2) at $k_F = \pi/3$ and $L = 500$ in $p_m$ (empty squares, left axis) and $\xi_m$ (solid circles, right axis) parametrizations. The two parametrizations are related by equation (11). The roots $p_m$ and $\xi_m$ are enumerated in decreasing and increasing order, respectively, starting with $m = 0$. 

where

$$\Upsilon = -\frac{2}{\pi} \int_{-\infty}^{+\infty} d\xi \Re \psi \left( \frac{1}{2} + i\xi \right) \left( \ln[2 \cosh(\pi \xi)] - \pi \xi \tanh[\pi \xi] \right)$$

is a numerical constant ($\psi()$ is the digamma function: the logarithmic derivative of $\Gamma()$), and $\tilde{s}_2(k_F)$ are polynomials. A calculation to the tenth order gives:

$$\tilde{s}_2(k_F) = -\frac{1}{12} \cot^2 k_F - \frac{1}{120},$$

$$\tilde{s}_4(k_F) = -\frac{31}{96} \cot^4 k_F - \frac{5}{16} \cot^2 k_F - \frac{47}{1728},$$

$$\tilde{s}_6(k_F) = -\frac{7007}{17280} \cot^6 k_F - \frac{247}{120} \cot^4 k_F - \frac{301}{144} \cot^2 k_F - \frac{403}{2016},$$

and the coefficients $\tilde{s}_4(k_F)$ and $\tilde{s}_6(k_F)$ are presented in equation (A.3) of the appendix. The logarithmic term is well-known from the conformal-field-theory considerations [47], the $\Upsilon$ term was computed earlier in [57], the $\tilde{s}_2(k_F)$ is known from [29, 58], and the leading orders in $\tilde{s}_2(k_F)$, $\tilde{s}_4(k_F)$, and $\tilde{s}_6(k_F)$ were reported in the continuous limit in [37].

An alternative way of calculating the expansion (28) is by using the expansion (22)–(24) for $\Phi(\xi, k_F, L)$. Indeed, it follows from the discussion of [37] that the von Neumann entropy can be calculated as

$$S(k_F, L) = \int_{-\infty}^{+\infty} \frac{\pi \xi}{\cosh^2(\pi \xi)} \Phi(\xi, k_F, L),$$

which immediately gives the coefficients $\tilde{s}_2n$ once the coefficients $X_{2n}$ are known.

7. Numerical illustration

Since the results presented in this paper are not proven in a rigorous way, but rely on the conjecture of the Fisher–Hartwig expansion and of the structure of the expansion coefficients, we find it helpful to check them against numerical data. For such a test, we take the wave vector $k_F = \pi/3$ (which corresponds to the filling fraction 1/3). We perform an exact diagonalization of large matrices (2) with the use of LAPACK library [59] compiled to work with 128-bit-precision floating-point numbers, together with the quadmath C library.

An example of the spectrum found in this way is plotted in figure 1 in both $p_m$ and $\xi_m$ parametrizations. Note that we enumerate $p_m$ in decreasing and $\xi_m$ in increasing order, starting
Figure 2. The absolute value of $\delta \phi_N$, the left-hand side of equation (25), as a function of the eigenvalue number for the matrix with $k_F = \pi/3$ and $L = 500$. The plots correspond to $N = 0$ to $N = 10$, from top to bottom. The non-smoothness of the plots in the central part of the graph is not a numerical noise, but related to changes of sign of $\delta \phi_N$.

Figure 3. The absolute value of the remainder in the expansion (28) terminated at order $N$ for the matrix with $k_F = \pi/3$ and several values $L$ ranging from 100 to 500.

with $m = 0$. The normalization condition (27) guarantees that $p_n$ crosses over from 1 to 0 at $n \approx k_F L/\pi$.

Next, we test the expansion for the eigenvalue equation (21)–(22). We denote by $\delta \phi_N$ the left-hand side of equation (25). In figure 2, we plot $|\delta \phi_N|$ as a function of $n$ (the number of eigenvalue) for the same example of $k_F = \pi/3$ and $L = 500$, using the coefficients $X_n(\xi, k_F)$ listed in equations (23) and (24). From the exponential decay of $\delta \phi_N$ with increasing $N$, we see that the coefficients are correct.

Finally, we also test the expansion of the von Neumann entanglement entropy (28). Denote by $\delta S_N$ the difference between the exact value of the entropy $S(k_F, L)$ and the right-hand side of equation (28) with the sum truncated at $N$ terms. The absolute value of $\delta S_N$ is plotted in figure 3 for the case of $k_F = \pi/3$ and several different values of $L$. From the exponential decay of $\delta S_N$ with increasing $N$, we see that the coefficients are correct.

Our numerical test confirms the analytical expressions for the matrix eigenvalues and the entanglement entropy. Note that the higher-order coefficients (starting with the fourth order) contain contributions from several Fisher–Hartwig branches. We are therefore confident that the original conjecture about the validity of the Fisher–Hartwig expansion for all values of $\kappa$ holds.
8. Conclusion

In this paper, we employ the conjectured Fisher–Hartwig expansion for the sine-kernel Toeplitz matrix for calculating the expansion coefficients. Furthermore, we translate those results into finite-size corrections for the von Neumann entanglement entropy and for the quasiclassical-type equation on the spectrum.

We hope that these results will serve as a useful reference for future studies of Toeplitz determinants. Besides, they provide a strong support to the conjectured Fisher–Hartwig expansion in the periodic form (5)–(6). While it is not proven, our calculation to the tenth order leaves no doubt in its validity in the case of the sine kernel (2).

Our study also outlines further challenges in the theory of Toeplitz determinants. In particular, we find the following open questions deserving future consideration:

- Proving the Fisher–Hartwig expansion (5)–(6), at least in the case of the sine kernel (2) and possibly in a general case of a Toeplitz matrix with Fisher–Hartwig singularities. Furthermore, one could attempt an even more general extension to determinants of the form \( \det(1 + AB) \) where A and B are local operators in the coordinate and momentum space, respectively: the leading Fisher–Hartwig asymptotics for such determinants was studied in [16] in the context of nonequilibrium bosonization.

- Exploring the decomposition into Fisher–Hartwig branches (5): can one extend such a decomposition to finite values of \( L \) [with \( \chi_\ast(\kappa, k_F, L) \) defined at any finite \( L \), and not as a formal asymptotic series (6)]?

- In the case of the sine kernel (2), proving the polynomial structure of the coefficients \( \tilde{F}_n(\kappa, k_F) \) to all orders, as well as the properties of those polynomials conjectured in section 4. Such a proof would be most probably related to the integrability of the corresponding Painlevé equations.

Acknowledgments

DI thanks I Protopopov, A Mirlin, P Schmitteckert and S Winitzki for discussions and the Simons Center for Geometry and Physics for hospitality. The work of AGA was supported by the NSF under grant no. DMR-1206790.

Appendix. Seventh to tenth orders

We present here the coefficients of the expansions (17), (23), and (28) in orders seven to ten.

\[
P_{77}(\kappa) = \frac{175045}{224} \kappa^9 + \frac{8263}{16} \kappa^7 + \frac{2155}{32} \kappa^5 + \frac{45}{56} \kappa^3,
\]
\[
P_{75}(\kappa) = \frac{49755}{32} \kappa^9 + \frac{19175}{16} \kappa^7 + \frac{5699}{32} \kappa^5 + \frac{19}{2} \kappa^3,
\]
\[
P_{73}(\kappa) = \frac{88735}{96} \kappa^9 + \frac{13585}{16} \kappa^7 + \frac{4909}{32} \kappa^5 + \frac{59}{2} \kappa^3,
\]
\[
P_{71}(\kappa) = \frac{4765}{32} \kappa^9 + \frac{2721}{16} \kappa^7 + \frac{1317}{32} \kappa^5 + \frac{9}{8} \kappa^3,
\]
\[
P_{88}(\kappa) = \frac{422565}{128} \kappa^{10} + \frac{414915}{128} \kappa^8 + \frac{98575}{128} \kappa^6 + \frac{4183}{128} \kappa^4,
\]
\[
P_{86}(\kappa) = \frac{723283}{96} \kappa^{10} + \frac{265959}{32} \kappa^8 + \frac{70011}{32} \kappa^6 + \frac{9761}{96} \kappa^4,
\]
\[
P_{84}(\kappa) = \frac{356007}{64} \kappa^{10} + \frac{44829}{64} \kappa^8 + \frac{135565}{64} \kappa^6 + \frac{7165}{64} \kappa^4,
\]
\[
P_{82}(\kappa) = \frac{44825}{32} \kappa^{10} + \frac{65967}{32} \kappa^8 + \frac{23907}{32} \kappa^6 + \frac{1587}{32} \kappa^4,
\]
\[
P_{90}(\kappa) = \frac{353777}{32} \kappa^{10} + \frac{42761}{32} \kappa^8 + \frac{102449}{32} \kappa^6 + \frac{6527}{1152} \kappa^4 + \frac{7}{120} \kappa^2,
\]
\[
P_{90}(\kappa) = \frac{139825}{96} \kappa^{11} + \frac{180872}{9} \kappa^9 + \frac{246729}{32} \kappa^7 + \frac{25483}{48} \kappa^5 + 7 \kappa^3.
\]
\[ P_{77}(\kappa) = 149.997 \kappa^{11} + 907.199 \kappa^9 + 189.241 \kappa^7 + 39.147 \kappa^5 + 99.2 \kappa^3. \]
\[ P_{95}(\kappa) = 265.689 \kappa^{11} + 881.143 \kappa^9 + 2059.487 \kappa^7 + 676.061 \kappa^5 + 551.3 \kappa^3. \]
\[ P_{93}(\kappa) = 11.414 \kappa^{11} + 1053.763 \kappa^9 + 2093.57 \kappa^7 + 2146.5 \kappa^5 + 229 \kappa^3. \]
\[ P_{91}(\kappa) = 36.597 \kappa^{11} + 40.129 \kappa^9 + 50.457 \kappa^7 + 2085 \kappa^5 + 19 \kappa^3. \]
\[ P_{10,10}(\kappa) = 564.149 \kappa^{12} + 1979.539 \kappa^{10} + 2246.875 \kappa^8 + 1996.7 \kappa^6 + 6795 \kappa^4. \]
\[ P_{10,8}(\kappa) = 381.51 \kappa^{12} + 244.735 \kappa^{10} + 1510.074 \kappa^8 + 2812.389 \kappa^6 + 101805 \kappa^4. \]
\[ Q_{77}(\xi) = 15.757.405 \xi^8 + 60.205 \xi^6 + 2703.025 \xi^4 + 4328.955 \xi^2 + 82.221, \]
\[ Q_{75}(\xi) = 447.79 \xi^8 + 1288.133 \xi^6 + 5770.025 \xi^4 + 1383.957 \xi^2 + 274.07, \]
\[ Q_{73}(\xi) = 264.205 \xi^8 + 792.827 \xi^6 + 3753.895 \xi^4 + 256.667 \xi^2 + 202.123, \]
\[ Q_{71}(\xi) = 42.885 \xi^8 + 134.211 \xi^6 + 587.615 \xi^4 + 1931.011 \xi^2 + 449.965, \]
\[ Q_{88}(\xi) = 2112.825 \xi^8 + 1957.401 \xi^6 + 49.541.793 \xi^4 + 10152.729 \xi^2 + 3276, \]
\[ Q_{86}(\xi) = 3616.415 \xi^8 + 571.261 \xi^6 + 2986.667 \xi^4 + 10195.649 \xi^2 + 82906.601, \]
\[ Q_{84}(\xi) = 1784.035 \xi^8 + 1730.154 \xi^6 + 4727.731 \xi^4 + 10711.015 \xi^2 + 10.384, \]
\[ Q_{82}(\xi) = 224.125 \xi^8 + 56.685 \xi^6 + 6594.816 \xi^4 + 1585.615 \xi^2 + 2318.257 \xi^2, \]
\[ Q_{80}(\xi) = 53777 \xi^8 + 11290 \xi^6 + 20245 \xi^4 + 3258.089 \xi^2 + 8925.299 \xi^2, \]
\[ Q_{99}(\xi) = 15.380.761 \xi^8 + 97.119.635 \xi^6 + 546.571.316 \xi^4 + 1483.130 \xi^2 + 191.313 \xi^2 + 569.473 \xi^2, \]
\[ Q_{97}(\xi) = 169.496 \xi^8 + 320.548 \xi^6 + 7275.679 \xi^4 + 99.152.045 \xi^2 + 69.407 \xi^2 + 2785 \xi^2, \]
\[ Q_{95}(\xi) = 29.233.579 \xi^8 + 116.094.807 \xi^6 + 137.306.011 \xi^4 + 309.409.139 \xi^2 + 1024, \]
\[ Q_{93}(\xi) = 62.777 \xi^8 + 5137.695 \xi^6 + 3188.441 \xi^4 + 19048.154 \xi^2 + 3680.047 \xi^2 + 1944337 \xi^2 + 12288, \]
\[ Q_{91}(\kappa) = 402.567 \kappa^8 + 8573.175 \kappa^6 + 5298.242 \kappa^4 + 3646.515 \kappa^2 + 3058711 \kappa^2 + 1461187, \]
\[ Q_{10,10}(\xi) = -798.447 \xi^{11} + 304.191 \xi^9 + 450.692 \xi^7 + 1754.196.861 \xi^5 + 1024, \]
\[ Q_{10,8}(\xi) = -1144.533 \xi^{11} + 434.663 \xi^9 + 337.710.603 \xi^7 + 2711.784.825 \xi^5 + 312, \]
\[ Q_{10,6}(\xi) = -2306.631 \xi^{11} + 466.926 \xi^9 + 7336.103 \xi^7 + 3055.729095 \xi^5 + 512, \]
\[ Q_{10,4}(\xi) = -1032.79 \xi^{11} + 3271.345 \xi^9 + 170.842.821 \xi^7 + 371.988.813 \xi^5 + 128, \]
\[ Q_{10,2}(\xi) = -8381 \xi^{11} + 20127.475 \xi^9 - 1208.847 \xi^7 - 554.032.432 \xi^5 + 120, \]
\[ Q_{10,0}(\xi) = -264031 \xi^{11} + 3147.805 \xi^9 - 240.49 \xi^7 + 962.191 \xi^5 - 4808.631 \xi^3 + 35.042.939 \xi. \]
\[ \delta_8(k_F) = -\frac{2578531}{15360} \cot^8 k_F - \frac{1398467}{3840} \cot^6 k_F - \frac{388885}{1536} \cot^4 k_F - \frac{45031}{768} \cot^2 k_F - \frac{77197}{33792}, \]
\[ \delta_{10}(k_F) = -\frac{11035941}{107542} \cot^{10} k_F - \frac{50826283}{17928} \cot^8 k_F - \frac{5797407}{1280} \cot^6 k_F - \frac{14343081}{1280} \cot^4 k_F. \]

(A.3)

References

[1] Montroll E W, Potts R B and Ward J C 1963 Correlations and spontaneous magnetization of the two-dimensional Ising model J. Math. Phys. 4 308
[2] McCoy B and Wu T 1967 Theory of Toeplitz determinants and spin correlations of the two-dimensional Ising model: II Phys. Rev. 155 438–52
[3] Basor E 2006 Toeplitz determinants and statistical mechanics Encyclopedia of Mathematical Physics vol 5 (Amsterdam: Elsevier) p 244
[4] Tracy C A and Widom H 1993 Introduction to random matrices Geometric and Quantum Aspects of Integrable Systems (Springer Lecture Notes in Physics) vol 424 ed G F Helmnick (Berlin: Springer) p 103
[5] Widom H 1994 Random Hermitian matrices and (nonrandom) Toeplitz matrices Toeplitz: Operators and Related Topics (Oper. Theory Adv. Appl. vol 71) ed E Basor and I Gohberg (Basel: Birkhäuser) p 9
[6] 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
[7] Its A L, Izergin A G and Korepin V E 1990 Long-distance asymptotics of temperature correlators of the impenetrable Bose gas Commun. Math. Phys. 130 471
[8] Its A R, Izergin A G, Korepin V E and Varzugin G G 1992 Large time and distance asymptotics of field Correlation function of impenetrable bosons at finite temperature Physica D 54 351
[9] Its A R, Izergin A G, Korepin V E and Slavnov N A 1993 Temperature correlations of quantum spins Phys. Rev. Lett. 70 1704
[10] Deift P A, Its A R and Zhou X 1997 A Riemann–Hilbert approach to asymptotics problems arising in the theory of random matrix models and also in the theory of integrable statistical mechanics Ann. Math. 146 149
[11] Göhmann F, Izergin A G, Korepin V E and Pronko A G 1998 Time and temperature dependent correlation functions of the one-dimensional impenetrable electron gas Int. J. Mod. Phys. B 12 2409
[12] Fuji Y and Wadati M 2000 Operator-valued Riemann–Hilbert problem for correlation functions of the XXZ spin chain J. Phys. A: Math. Gen. 33 1351
[13] Cheianov V V and Zvonarev M 2004 Zero temperature correlation functions for the impenetrable fermion gas J. Phys. A: Math. Gen. 37 2261
[14] Gutman D B and Mirlian A D 2010 Bosonization out of equilibrium Europhys. Lett. 90 37003
[15] Gutman D B, Gefen Y and Mirlian A D 2010 Bosonization of one-dimensional fermions out of equilibrium Phys. Rev. B 81 085436
[16] Gutman D B, Gefen Y and Mirlian A D 2011 Non-equilibrium LD many-body problems and asymptotic properties of Toeplitz determinants J. Phys. A: Math. Theor. 44 165003
[17] Protopopov I, Gutman D B and Mirlian A D 2012 Correlations in non-equilibrium Luttinger liquid and singular Fredholm determinants arXiv:1212.0708
[18] Szego G 1915 Ein Grenzwertsatz über die Toeplitzschen Determinanten einer reellen positiven Funktion Math. Ann. 76 490
[19] Szege G 1952 On certain Hermitian forms associated with the Fourier series of a positive function Commun. Sém. Math. Univ. Lund Suppl. 1952 228
[20] Fisher M E and Hartwig R E 1968 Toeplitz determinants, some applications, theorems and conjectures Adv. Chem. Phys. 15 333
[21] Basor E L 1978 Asymptotic formulas for Toeplitz determinants Trans. Am. Math. Soc. 239 33
[22] Basor E and Widom H 1983 Toeplitz and Wiener–Hopf determinants with piecewise continuous symbols J. Funct. Anal. 50 387
[23] Basor E L and Tracy C A 1991 The Fisher–Hartwig conjecture and generalizations Physica A 177 167
[24] Böttcher A, Silbermann B and Widom H 1994 A continuous analogue of the Fisher–Hartwig formula for piecewise continuous symbols J. Funct. Anal. 122 222
[25] Ehrenreich H 2001 A status report on the asymptotic behavior of Toeplitz determinants with Fisher–Hartwig singularities Operator Theory: Adv. Appl. 124 217
[26] Böttcher A and Silbermann B 2006 Analysis of Toeplitz Operators (Springer Monographs in Mathematics) 2nd edn (Berlin: Springer)
Ivanov D A, Abanov A G and Cheianov V V 2013 Counting free fermions on a line: a Fisher–Hartwig asymptotic expansion for the Toeplitz determinant in the double-scaling limit J. Phys. A: Math. Theor. **46** 085003

Slepian D 1965 Some asymptotic expansions for prolate spheroidal wave functions J. Math. Phys. **44** 99

Slepian D 1978 Prolate spheroidal wave functions, Fourier analysis, and uncertainty—V: the discrete case Bell Syst. Tech. J. **57** 1371

Slepian D 1983 Some comments on Fourier analysis, uncertainty, and modeling SIAM Rev. **25** 379

Peschel I 2004 Reduced density matrices and entanglement entropy in free lattice models J. Phys. A: Math. Theor. **42** 504003

Jin B-Q and Korepin V 2004 Quantum spin chain, Toeplitz determinants and the Fisher–Hartwig conjecture J. Stat. Phys. **116** 79

Calabrese P, Mintchev M and Vicari E 2011 Entanglement entropy of one-dimensional gases Phys. Rev. Lett. **107** 020601

Calabrese P, Mintchev M and Vicari E 2011 The entanglement entropy of one-dimensional systems in continuous and homogeneous space J. Stat. Mech. **P09028**

Anderson E et al 1999 LAPACK Users' Guide 3rd edn (Philadelphia, PA: SIAM)