Fisher–Hartwig expansion for the transverse correlation function in the XX spin-1/2 chain

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 23 September 2013
Accepted for publication 4 November 2013
Published 3 December 2013

Abstract
Motivated by the recent results on the asymptotic behavior of Toeplitz determinants with Fisher–Hartwig singularities, we develop an asymptotic expansion for transverse spin correlations in the XX spin-1/2 chain. The coefficients of the expansion can be calculated to any given order using the relation to discrete Painlevé equations. We present explicit results up to the 11th order and compare them with a numerical example.

Keywords: Fisher–Hartwig conjecture, Toeplitz matrices, spin chains, full counting statistics, Painleve equations
PACS numbers: 71.10.Pm, 02.30.Mv, 75.10.Pq

1. Introduction

The spin-1/2 XX chain described by the Hamiltonian
\[ H = \sum_{i=-\infty}^{+\infty} \left[ -J(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + h \sigma_i^z \right] \] (1)

(where \(\sigma_i^\alpha\) are Pauli matrices associated with the spin at the site \(i\)) is one of the simplest examples of exactly solvable spin systems: by a Jordan–Wigner transformation it can be mapped onto free fermions, which gives a complete solution for the ground state and for the excitations [1] (this model is also equivalent to the Tonks–Girardeau gas of hard-core bosons on a one-dimensional lattice [2]). Computing correlation functions is, however, a more
difficult task, since transverse spin operators (or, equivalently, the boson operators in the Tonks–Girardeau gas) are nonlocal in terms of fermions. In particular, already the leading-order asymptotic behavior of the ground-state transverse correlations

\[ \langle \sigma_i^+ \sigma_{i+L}^- \rangle \propto L^{-1/2}, \quad L \to \infty \tag{2} \]

requires a nontrivial calculation\(^4\). One of the possible approaches to this correlation function is to re-express it as a Toeplitz determinant of a Fisher–Hartwig type by using the fermionic representation [1, 3, 4]. The asymptotic behavior of such determinants continues to be the subject of active studies in mathematics and mathematical physics [5–13]. In particular, some corrections to the leading asymptotic behavior of the correlation function (2) have been computed [14–17]\(^5\).

In this paper, we extend this approach by demonstrating that all the corrections to equation (2) can be computed order by order using the recent results on a closely related Toeplitz determinant for statistics of free fermions [18, 19]. Furthermore, those corrections may be combined into a double sum explicitly periodic in the ‘counting parameter’ (equations (14)–(15) below): this double-sum form was dubbed the Fisher–Hartwig expansion in [19].

Note that while our calculation can be performed analytically to any order, it does not constitute a rigorous proof: in fact, the results of [18, 19] on which it is based still have the status of conjecture. The available analytical and numerical evidence [10, 19–21] leaves no doubt as to the validity of this conjecture (see a more detailed discussion of this in section 5); however, we find it helpful to check our analytical results against numerical evaluations of the determinants. Such a check provides additional support to the conjecture and verifies analytical manipulations performed with Mathematica software [22] (see section 4 for details).

The paper is organized as follows. In section 2, we report our analytical results on the Fisher–Hartwig expansion of the relevant Toeplitz determinant. In section 3, we apply these results to the case of transverse spin correlations in the XX chain. In section 4, we compare the analytical results with a numerical example. Finally, in section 5, we discuss the assumptions used in our calculations and the implications of our results. The appendix contains expressions for some of the expansion coefficients.

### 2. Main results

The Hamiltonian (1) can be diagonalized via the Jordan–Wigner transformation [1]

\[ \sigma_i^+ = \Psi_i^\dagger \exp \left( i \pi \sum_{j<i} \Psi_j^\dagger \Psi_j \right), \]

\[ \sigma_i^- = \exp \left( i \pi \sum_{j<i} \Psi_j^\dagger \Psi_j \right) \Psi_i, \]

\[ \sigma_i^z = 2 \Psi_i^\dagger \Psi_i - 1. \tag{3} \]

In terms of the fermionic operators \( \Psi_i^\dagger \) and \( \Psi_i \), the Hamiltonian (1) represents free spinless fermions on a one-dimensional lattice with \( J \) being the hopping amplitude and \( h \) corresponding to the chemical potential. The ground state of such a system is a Fermi sea where all the states below the Fermi wave vector \( k_F = \arccos(h/2J) \) are filled (here we assume that \( |h| < 2J \); otherwise the ground state is a trivial fully polarized state corresponding to \( k_F = 0 \) or \( k_F = \pi \)).

\(^4\) Probably, the easiest way of deriving the leading term (2) is to use the bosonization technique [32].

\(^5\) The expansion coefficients in [14, 15] contain typos which were corrected later in [16, 17].
The parameter $k_F$ ranges between 0 and $\pi$ and fully describes the ground state. The average density of fermions in the ground state is $k_F/\pi$, which corresponds to $\langle \sigma_z^i \rangle = 2k_F/\pi - 1$.

We will be interested in the transverse spin correlation function (2). For our purposes, it will be more convenient to introduce a more general correlation function involving a ‘counting parameter’ $\kappa$:

$$\Sigma(\kappa, k_F, L) = \left\langle \left( \sum_{1 \leq j \leq L-1} \Psi_j^\dagger \Psi_j \right) \Psi_L \right\rangle,$$  

where the average is taken over the ground state in an infinite system. Then, by the Jordan–Wigner transformation, the transverse spin correlation function is a particular case of this definition:

$$\langle \sigma_+^i \sigma_-^{i+1} \rangle = \Sigma \left( \kappa = \frac{1}{2}, k_F, L \right).$$

Note that $\Sigma(\kappa, k_F, L)$ is explicitly periodic in $\kappa$ with period 1, since the number of fermions $\sum_{1 \leq j \leq L-1} \Psi_j^\dagger \Psi_j$ is integer.

Using the Wick theorem, the correlation function (4) can be expressed as [1, 3]

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

where

$$a_{i-j} = \langle \Psi_j^\dagger \Psi_i \rangle = \begin{cases} \sin \frac{k_F(i-j)}{\pi} & i \neq j, \\
\frac{k_F}{\pi} & i = j \end{cases}$$

and

$$\delta_{i-j} = \begin{cases} 0, & i \neq j, \\
1, & i = j \end{cases}.$$

The determinant in equation (6) is very similar to that studied in [19] for the correlation function

$$\chi(\kappa, k_F, L) = \left\langle \left( \sum_{1 \leq j \leq L} \Psi_j^\dagger \Psi_j \right) \right\rangle = \det_{1 \leq i, j \leq L} [(e^{2\pi i \kappa} - 1)a_{i-j} + \delta_{i-j}].$$

Namely, up to an overall sign, the Toeplitz matrices (6) and (9) differ only by a shift by one row (or, equivalently, by one column). The determinants of such Toeplitz matrices may therefore be related using the Desnanot–Jacobi identity [23, 24] (also known as the Lewis Carroll identity [25], which is a particular case of the Muir relations [26]):

$$[\chi(\kappa, k_F, L)]^2 - [(1 - e^{2\pi i \kappa})\Sigma(\kappa, k_F, L)]^2 = \chi(\kappa, k_F, L - 1)\chi(\kappa, k_F, L + 1).$$

This relation determines $\Sigma(\kappa, k_F, L)$ up to a sign, once $\chi(\kappa, k_F, L)$ is known. The sign of $\Sigma(\kappa, k_F, L)$ may, in turn, be fixed independently from the known main asymptotics (2).6

We can now use the asymptotic expansion for $\chi(\kappa, k_F, L)$ derived in [19]:

$$\chi(\kappa, k_F, L) = \sum_{j=-\infty}^{+\infty} \chi_0(\kappa + j, k_F, L),$$

where $\chi_0(k, k_F, L)$ is

$$x_L = \left( 1 - e^{2\pi i \kappa} \right) \Sigma(\kappa, k_F, L)/\chi(\kappa, k_F, L).$$

6 Remarkably, the quantity $x_L$ studied in [10, 19] and obeying the discrete version of Painlevé equations is given by the ratio of the two determinants $x_L = (1 - e^{2\pi i \kappa})\Sigma(\kappa, k_F, L)/\chi(\kappa, k_F, L).$
The coefficients \( H_j(\tilde{\kappa}, k_F) \) can be calculated from the coefficients \( \tilde{F}_n(\kappa, k_F) \) order by order. We have calculated the first ten orders using Mathematica software [22]. The first six coefficients are

\[
\begin{align*}
H_1(\tilde{\kappa}, k_F) &= (\tilde{\kappa}^2 - \frac{1}{4}) \cdot 2\tilde{\kappa} \cot k_F, \\
H_2(\tilde{\kappa}, k_F) &= (\tilde{\kappa}^2 - \frac{1}{4}) \left( \frac{3}{5} \tilde{\kappa}^2 - \frac{1}{4} \right) \cot^2 k_F + \frac{1}{8} \tilde{\kappa}^2, \\
H_3(\tilde{\kappa}, k_F) &= (\tilde{\kappa}^2 - \frac{1}{4}) \left( \frac{11}{5} \tilde{\kappa}^2 - \frac{3}{8} \right) \cot^3 k_F + \left( \frac{3}{8} \tilde{\kappa}^2 - \frac{1}{8} \right) \cot k_F, \\
H_4(\tilde{\kappa}, k_F) &= (\tilde{\kappa}^2 - \frac{1}{4}) \left( \frac{63}{16} \tilde{\kappa}^4 - \frac{11}{16} \tilde{\kappa}^2 - \frac{1}{16} \right) \cot^4 k_F \\
&\quad + \left( \frac{35}{2} \tilde{\kappa}^4 + \frac{1}{2} \tilde{\kappa}^2 - \frac{1}{4} \right) \cot^2 k_F + \frac{47}{32} \tilde{\kappa}^4 + \frac{29}{16} \tilde{\kappa}^2 - \frac{1}{16}, \\
H_5(\tilde{\kappa}, k_F) &= (\tilde{\kappa}^2 - \frac{1}{4}) \left( \frac{527}{10} \tilde{\kappa}^5 + \frac{17}{10} \tilde{\kappa}^3 - \frac{67}{2} \tilde{\kappa} \right) \cot^3 k_F \\
&\quad + (74 \tilde{\kappa}^5 + 7 \tilde{\kappa}^3 - \frac{11}{8} \tilde{\kappa}) \cot k_F + \left( \frac{45}{7} \tilde{\kappa}^5 + \frac{9}{7} \tilde{\kappa}^3 - \frac{17}{35} \tilde{\kappa} \right) \cot k_F, \\
H_6(\tilde{\kappa}, k_F) &= (\tilde{\kappa}^2 - \frac{1}{4}) \left( \frac{1329}{16} \tilde{\kappa}^6 + \frac{6271}{102} \tilde{\kappa}^4 - \frac{1769}{102} \tilde{\kappa}^2 - \frac{539}{510} \right) \cot^6 k_F \\
&\quad + \left( \frac{2655}{8} \tilde{\kappa}^6 + \frac{2563}{32} \tilde{\kappa}^4 - \frac{1155}{128} \tilde{\kappa}^2 - \frac{221}{512} \right) \cot^4 k_F \\
&\quad + \left( \frac{2385}{16} \tilde{\kappa}^6 + \frac{3341}{64} \tilde{\kappa}^4 - \frac{1025}{256} \tilde{\kappa}^2 - \frac{353}{1024} \right) \cot^2 k_F \\
&\quad + \frac{236}{125} \tilde{\kappa}^6 + \frac{241}{125} \tilde{\kappa}^4 - \frac{47}{125} \tilde{\kappa}^2 - \frac{2}{125}. \tag{17}
\end{align*}
\]

The coefficients \( H_j(\tilde{\kappa}, k_F) \) to \( H_{10}(\tilde{\kappa}, k_F) \) are listed in the appendix.

The expansion (14)–(15), together with the algorithm for computing the coefficients \( H_j(\tilde{\kappa}, k_F) \) (starting from the coefficients \( \tilde{F}_n(\kappa, k_F) \)), constitutes the main result of this work. The algorithm for calculating \( \tilde{F}_n(\kappa, k_F) \) using discrete Painlevé equations was reported earlier in [19]. Combined together, these results provide an algorithm for calculating the expansion for \( \Sigma(\kappa, k_F, L) \) to any given order. The transverse spin correlations can be obtained by setting \( \kappa = 1/2 \) in all the formulas (so that the summation in expansion (14)–(15) is performed over all integer \( \tilde{\kappa} \)).

We note several properties of the coefficients \( H_j(\tilde{\kappa}, k_F) \). Similarly to \( \tilde{F}_n(\kappa, k_F) \), they are polynomials in \( \tilde{\kappa} \) and \( \cot k_F \) with rational coefficients. These polynomials have degrees \((n+2)\) and \( n \) in \( \tilde{\kappa} \) and \( \cot k_F \), respectively, and are of a fixed parity in each of these variables (even for even \( n \) and odd for odd \( n \)). Moreover, they are all divisible by \( (\tilde{\kappa}^2 - 1/4) \); this property must persist to all orders, since it guarantees that expansion (14)–(15) reproduces the fermionic correlation function (7) in the limit \( \kappa \to 0 \).
3. Transverse spin correlations in the XX chain

We now specify to the case of the transverse spin correlation function (5). In this case, all the powers of $L^{-1}$ in expansion (14)–(15) are integer, and the expansion may be rewritten in the form

$$\langle \sigma^+_{i} \sigma^-_{i+L} \rangle = e^{C_{x}(0)} \sqrt{\frac{\sin k_F}{2L}} \sum_{j=-\infty}^{+\infty} (2 \sin k_F)^{-2j} e^{2i j k_F L} \sum_{n=0}^{\infty} \frac{\alpha_{jn}(k_F)}{(iL)^n}.$$ (18)

This form of expansion has already been established in [14]. The coefficients $\alpha_{jn}(k_F)$ can be calculated in a simple manner from the coefficients $H_n(\tilde{\kappa}, k_F)$. Note that at any given order $n$, the coefficients $\alpha_{jn}(k_F)$ are nonzero only for $|j| \leq \sqrt{n}/2$. The explicit form of the coefficients $\alpha_{jn}(k_F)$ for $n$ up to 11 is given in the appendix.

The beginning of expansion (18) reads

$$\langle \sigma^+_{i} \sigma^-_{i+L} \rangle = e^{C_{x}(0)} \sqrt{\frac{\sin k_F}{2L}} \left( 1 - \frac{\cos^2 k_F + 4 \cos(2k_F L)}{32(L \sin k_F)^2} - \frac{3 \cos k_F \sin(2k_F L)}{16(L \sin k_F)^3} + \cdots \right).$$ (19)

The leading order gives the asymptotic behavior (2) with the correct coefficient [14–17]:

$$e^{C_{x}(0)} = [G(1/2)G(3/2)]^2 = 2^{1/6} e^{1/2} A^{-6},$$ (20)

where $A = 1.282\,427\,1291\ldots$ is the Glaisher–Kinkelin constant. The subsequent coefficients $\alpha_{jn}$ reproduce, in particular, the corrections calculated in [16, 17].

4. Numerical illustration

We illustrate our analytic calculation with a numerical example of the correlation function (5). We have chosen the Fermi wave vector $k_F = \pi/3$ (corresponding to the $z$ polarization equal to 1/3 of the full polarization) and have numerically calculated the corresponding determinants for distance $L$ up to 400. In our numerics, we have used the LAPACK library [27] compiled to work with 128-bit floating-point numbers, together with the quadmath C library.

In figure 1 we plot the difference $\Delta_N(k_F, L)$ between the left-hand side of equation (18) and its right-hand side with the sum over $n$ restricted to $n \leq N$. These results show that, even though our analytical calculations involved a non-rigorous analytic continuation of the asymptotic series to half-integer values of $\kappa$, such an analyticity, in fact, holds. A similar conclusion was also reached in [10, 19–21] for the expansion of $\chi(\kappa, k_F, L)$.

5. Discussion

In this paper, we apply the earlier results of [19] on the Toeplitz determinants with the sine kernel to deriving a Fisher–Hartwig expansion for the correlation function (4) (including the transverse spin correlations (5) as a particular case). The expansion is not rigorously proven and remains a conjecture supported by several arguments.

Away from the line $\text{Re} \kappa = j + 1/2$ (with an integer $j$), this expansion may be verified order by order using the methods of [10, 19] (and of [18] in the continuous limit $k_F \to 0$). The verification was actually performed to the 10th order in the lattice case and to the 15th order in the continuous limit, and this leaves little doubt about the validity of the general form of the expansion to all orders.

On the line $\text{Re} \kappa = j + 1/2$ (relevant for the case of the transverse correlations in the XX model), the situation is more delicate. In this case, the expansion cannot even be rigorously
Figure 1. The difference $\Delta_N$ between the left-hand side of equation (18) and its right-hand side with the sum over $n$ restricted to $n \leq N$ is plotted as a function of $L$. The value of $k_F$ is $\pi/3$. The upper line is the spin correlations (the left-hand side of equation (18)), and the other data correspond, top to bottom, to $N = 0$ to $N = 11$ (excluding $N = 1$, since there are no first-order terms in expansion (18)).

derived to any order, but is obtained by an analytic continuation from other values of $\kappa$. This is not a mathematically justified procedure, and therefore our results at $\text{Re} \, \kappa = j + 1/2$ are additionally based on the assumption that expansion (11)–(12) of $\chi(\kappa, k_F, L)$ is analytically continuable, term by term, across the line $\text{Re} \, \kappa = j + 1/2$ (see [18, 19]). The corresponding analytic continuation for expansion (14)–(15) of $\Sigma(\kappa, k_F, L)$ follows from this assumption, together with the Lewis Carroll identity (10). At this point it is not clear how to prove this assumption. However, available numerical studies ([10, 19–21] and this paper) indicate that, in the examples and to the orders considered, the analytic continuation of the expansions to the line $\text{Re} \, \kappa = j + 1/2$ is indeed possible.

These conjectures present a challenge to future mathematical studies of Toeplitz determinants. Besides proving them, an interesting question remains if they are valid for other Toeplitz determinants with Fisher–Hartwig singularities, or, even more generally, for pseudodifferential operators with discontinuous symbols [28]. Transferring some of the results on the Fisher–Hartwig expansion to spectral properties of such operators would have implications in extending the Widom conjecture [29] to a wider class of functions. In particular, this may lead to extracting subleading corrections to the von Neumann entanglement entropy for free fermions in higher dimensions (similarly to the one-dimensional case [19, 21]).

Another use of the present results may be in application to one-dimensional bosonization (describing the low-energy fermionic degrees of freedom in terms of bosonic fields) [30]. While the subleading bosonization terms (responsible for the discreteness of fermionic particles) are model dependent [31], it might be possible to fix them for the specific model (free fermions on a chain) by using expansions for correlation functions obtained from Toeplitz determinants.

Acknowledgments

We thank V Fock for bringing to our attention the Lewis Carroll identity for determinants. The work of AGA was supported by the NSF under grant no. DMR-1206790.
Appendix

The coefficients \( H_i(\bar{\kappa}, k_F) \) in orders 7 to 10 are

\[
H_7(\bar{\kappa}, k_F) = \left( \kappa^2 - \frac{1}{3} \right) \left[ \left( \frac{175,045}{228} \right) \kappa^7 + \frac{25,105}{896} \kappa^5 - \frac{51,889}{3584} \kappa^3 - \frac{8243}{2048} \kappa \right] \cot^7 k_F
\]

\[
+ \left( \frac{49,755}{32} \kappa^7 + \frac{90,319}{128} \kappa^5 - \frac{10,991}{512} \kappa^3 - \frac{21,563}{2048} \kappa \right) \cot^5 k_F
\]

\[
+ \left( \frac{88,735}{96} \kappa^7 + \frac{202,627}{384} \kappa^5 - \frac{35}{1336} \kappa^3 - \frac{18,361}{2048} \kappa \right) \cot^3 k_F
\]

\[
+ \left( \frac{4765}{32} \kappa^7 + \frac{14,281}{128} \kappa^5 + \frac{3031}{512} \kappa^3 - \frac{4669}{2048} \kappa \right) \cot k_F
\]

\[
H_8(\bar{\kappa}, k_F) = \left( \kappa^2 - \frac{1}{3} \right) \left[ \left( \frac{422,565}{128} \kappa^8 + \frac{1079,898}{512} \kappa^6 + \frac{235,859}{2048} \kappa^4 \right.ight.
\]

\[
- \frac{407,593}{8192} \kappa^2 \left. \right] \cot^8 k_F
\]

\[
+ \left( \frac{723,283}{96} \kappa^8 + \frac{2134,807}{384} \kappa^6 + \frac{659,881}{1536} \kappa^4 - \frac{281,377}{2048} \kappa^2 - \frac{1945}{512} \right) \cot^6 k_F
\]

\[
+ \left( \frac{356,807}{64} \kappa^8 + \frac{1234,703}{256} \kappa^6 + \frac{545,033}{1024} \kappa^4 - \frac{520,155}{4096} \kappa^2 - \frac{17025}{1024} \right) \cot^4 k_F
\]

\[
+ \left( \frac{44,825}{32} \kappa^8 + \frac{186,653}{128} \kappa^6 + \frac{121,011}{512} \kappa^4 + \frac{83,617}{2048} \kappa^2 - \frac{1665}{1024} \right) \cot^2 k_F
\]

\[
+ \left( \frac{353,777}{7680} \kappa^8 + \frac{1874,177}{128} \kappa^6 + \frac{954,679}{192} \kappa^4 - \frac{252,007}{12288} \kappa^2 - \frac{1697}{8192} \right)
\]

\[
H_9(\bar{\kappa}, k_F) = \left( \kappa^2 - \frac{1}{3} \right) \left[ \left( \frac{1398,251}{96} \kappa^9 + \frac{2759,869}{192} \kappa^7 + \frac{263,645}{96} \kappa^5 \right.ight.
\]

\[
- \frac{383,007}{1024} \kappa^3 \left. \right] \cot^9 k_F
\]

\[
+ \left( \frac{149,997}{8} \kappa^9 + \frac{329,653}{16} \kappa^7 + \frac{144,741}{128} \kappa^5 - \frac{135,021}{1024} \kappa^3 - \frac{150,545}{1024} \right) \cot^7 k_F
\]

\[
+ \left( \frac{2656,689}{80} \kappa^9 + \frac{6574,367}{160} \kappa^7 + \frac{442,443}{40} \kappa^5 \right. \frac{257377}{256} \kappa^3 - \frac{719,261}{4096} \kappa^1 \left. \right) \cot^5 k_F
\]

\[
+ \left( \frac{1144}{4} \kappa^9 + \frac{64}{32} \kappa^7 + \frac{81,147}{16} \kappa^5 \right. \frac{21,971}{64} \kappa^3 - \frac{22,669}{256} \kappa^1 \left. \right) \cot^3 k_F
\]

\[
+ \left( \frac{36,979}{32} \kappa^9 + \frac{222,547}{64} \kappa^7 + \frac{24,549}{32} \kappa^5 \right. \frac{21,459}{1024} \kappa^3 - \frac{123,653}{8192} \kappa^1 \left. \right) \cot k_F
\]

\[
H_{10}(\bar{\kappa}, k_F) = \left( \kappa^2 - \frac{1}{3} \right) \left[ \left( \frac{266,149}{4} \kappa^{10} + \frac{60,326,939}{640} \kappa^8 \right. \right.
\]

\[
- \frac{181,763}{320} \kappa^6 \left. \right] \cot^{10} k_F
\]

\[
+ \left( \frac{381}{2} \kappa^{10} + \frac{588}{2} \kappa^8 + \frac{15,122,545}{128} \kappa^6 \right. \frac{442,507}{512} \kappa^4 \left. \right)
\]

\[
- \frac{608,297}{2048} \kappa^2 \left. \right] \cot^8 k_F
\]

\[
+ \left( \frac{786,877}{2048} \kappa^{10} + \frac{21,302,633}{128} \kappa^8 + \frac{19,058,315}{128} \kappa^6 \right. \frac{9023}{4} \kappa^4 \left. \right)
\]

\[
- \frac{786,877}{2048} \kappa^2 \left. \right] \cot^6 k_F
\]

\[
+ \left( \frac{344,253}{4} \kappa^{10} + \frac{517,573}{32} \kappa^8 + \frac{657,703}{8} \kappa^6 + \frac{810,981}{256} \kappa^4 \right. \frac{2264,409}{1024} \kappa^2 \left. \right]
\]

\[
- \frac{457,181}{8192} \kappa^2 \left. \right] \cot^4 k_F
\]

\[
+ \left( \frac{279,971}{2} \kappa^{10} + \frac{380,704}{128} \kappa^8 + \frac{452,815}{128} \kappa^6 \right. \frac{5181}{4} \kappa^4 \left. \right) \frac{2064,369}{4096} \kappa^2 \left. \right]
\]

\[
- \frac{512,839}{32} \kappa^2 \left. \right] \cot^2 k_F
\]

\[
+ \left( \frac{264,031}{660} \kappa^{10} + \frac{1055,183}{1056} \kappa^8 \right. \frac{15,531,919}{21120} \kappa^6 \left. \right) \frac{2831,701}{28,160} \kappa^4 \right)
\]

\[
- \frac{492,119}{2} \kappa^2 \left. \right] \frac{22,528}{2048} \kappa^2 \left. \right]
\]

\[
- \frac{2301}{1024} \kappa^2 \left. \right] \left. \right) (A.1)
We also list all nonzero coefficients $a_{jn}(k_F)$ for $n \leq 11$. Only coefficients with $j \geq 0$ are presented because of the symmetry $a_{-jn}(k_F) = (-1)^j a_{jn}(k_F)$:

\[
\begin{align*}
\alpha_{00}(k_F) &= 1, & \alpha_{02}(k_F) &= \frac{1}{12} \cot^2 k_F, \\
\alpha_{12}(k_F) &= \frac{1}{2}, & \alpha_{13}(k_F) &= \frac{3}{8} \cot k_F, \\
\alpha_{04}(k_F) &= \frac{3}{128} \cot^4 k_F + \frac{1}{32} \cot^2 k_F + \frac{1}{128}, \\
\alpha_{14}(k_F) &= \frac{9}{128} \cot^2 k_F + \frac{1}{4}, \\
\alpha_{15}(k_F) &= \frac{453}{256} \cot^3 k_F + \frac{153}{128} \cot k_F, \\
\alpha_{06}(k_F) &= \frac{2007}{65536} \cot^6 k_F + \frac{225}{2048} \cot^4 k_F + \frac{247}{2048} \cot^2 k_F + \frac{1}{64}, \\
\alpha_{16}(k_F) &= \frac{42633}{8192} \cot^6 k_F + \frac{2341}{256} \cot^2 k_F + \frac{363}{512}, \\
\alpha_{17}(k_F) &= \frac{293895}{16384} \cot^5 k_F + \frac{98325}{4096} \cot^3 k_F + \frac{2011}{1024} \cot k_F, \\
\alpha_{08}(k_F) &= \frac{258107}{8192} \cot^8 k_F + \frac{1863}{2048} \cot^6 k_F + \frac{773267}{768} \cot^4 k_F + \frac{467}{1024} \cot^2 k_F + \frac{849}{16384}, \\
\alpha_{18}(k_F) &= \frac{18582471}{262144} \cot^6 k_F + \frac{970029}{8192} \cot^4 k_F + \frac{428337}{8192} \cot^2 k_F + \frac{1985}{512}, \\
\alpha_{28}(k_F) &= \frac{9}{256}, \\
\alpha_{19}(k_F) &= \frac{165603555}{642408} \cot^7 k_F + \frac{168581145}{2048} \cot^5 k_F + \frac{12465711}{32768} \cot^3 k_F + \frac{2052147}{32768} \cot^1 k_F, \\
\alpha_{20}(k_F) &= \frac{135}{256} \cot k_F, \\
\alpha_{0,10}(k_F) &= \frac{1006360955}{12288435456} \cot^{10} k_F + \frac{63442485}{4194304} \cot^8 k_F + \frac{44944731}{2097152} \cot^6 k_F \\
&\quad + \frac{3662175}{1024} \cot^4 k_F + \frac{1026407}{262144} \cot^2 k_F + \frac{1151}{3072}, \\
\alpha_{1,10}(k_F) &= \frac{5256685915}{33554432} \cot^{10} k_F + \frac{1918340595}{524288} \cot^8 k_F + \frac{48020101}{65536} \cot^6 k_F \\
&\quad + \frac{2592324661}{1048576} \cot^4 k_F + \frac{4529519}{131072}, \\
\alpha_{2,10}(k_F) &= \frac{4306558132175}{98304}, \quad \alpha_{1,11}(k_F) = \frac{574231373145}{6710864} \cot^9 k_F + \frac{813554621335}{807045685} \cot^7 k_F \\
&\quad + \frac{44340528815}{1048576} \cot^5 k_F + \frac{219859555}{262144} \cot^3 k_F, \\
\alpha_{2,11}(k_F) &= \frac{368658192}{16384} \cot^9 k_F + \frac{62505}{65536} \cot k_F. 
\end{align*}
\]

(A.2)

References

[1] Lieb E, Schultz T and Mattis D 1961 Two soluble models of an antiferromagnetic chain Ann. Phys. 16 407

[2] Girardeau M 1960 Relationship between systems of impenetrable bosons and fermions in one dimension J. Math. Phys. 1 516

[3] Schultz T D 1963 Note on the one-dimensional gas of impenetrable point-particle bosons J. Math. Phys. 4 666

[4] McCoy B M 1968 Spin correlation functions of the X-Y model Phys. Rev. 173 531

[5] Fisher M E and Hartwig R E 1968 Toeplitz determinants, some applications, theorems and conjectures Adv. Chem. Phys. 15 333

[6] Basor E I and Morrison K E 1994 The Fisher–Hartwig conjecture and Toeplitz eigenvalues Linear Algebra Appl. 202 129

[7] Ehrenhardt T 2001 A status report on the asymptotic behavior of Toeplitz determinants with Fisher–Hartwig singularities Recent Advances in Operator Theory (Operator Theory: Advances and Applications vol 124) p 217

[8] Basor E 2006 Toeplitz determinants and statistical mechanics Encyclopedia of Mathematical Physics vol 5 (Amsterdam: Elsevier) p 244

[9] Kozlowski K K 2008 Truncated Wiener–Hopf operators with Fisher–Hartwig singularities arXiv:0805.3902

Kitanine N, Kozlowski K K, Maillet J M, Slavnov N A and Terras V 2007 Riemann–Hilbert method to a generalized sine kernel and applications Commun. Math. Phys. 291 691

Kitanine N, Kozlowski K K, Maillet J M, Slavnov N A and Terras V 2009 Algebraic Bethe ansatz approach to the asymptotic behavior of correlation functions J. Stat. Mech. P04003

Kozlowski K K 2010 Riemann–Hilbert approach to the time-dependent generalized sine kernel arXiv:1011.5897
[10] Calabrese P and Essler F H L 2010 Universal corrections to scaling for block entanglement in spin-1/2 XX chains J. Stat. Mech. P08029
[11] Gutman D B, Gefen Y and Mirlin A D 2011 Non-equilibrium 1D many-body problems and asymptotic properties of Toeplitz determinants J. Phys. A: Math. Theor. 44 165003
[12] Deift P, Its A and Krasovsky I 2011 Asymptotics of Toeplitz, Hankel, and Toeplitz + Hankel determinants with Fisher–Hartwig singularities Ann. Math. 174 1243
[13] Krasovsky I 2011 Aspects of Toeplitz determinants Boundaries and Spectra of Random Walks (Progress in Probability vol 64) ed D Lenz, P Sobieczky and W Woess (Basel: Birkhäuser) p 305
[14] Vaidya H G and Tracy C A 1979 One-particle reduced density matrix of impenetrable bosons in one dimension at zero temperature Phys. Rev. Lett. 42 3
Vaidya H G and Tracy C A 1979 One particle reduced density matrix of impenetrable bosons in one dimension at zero temperature J. Math. Phys. 20 2291
[15] Jimbo M, Miwa T, Möri Y and Sato M 1980 Density matrix an impenetrable Bose gas and the fifth Painlevé transcendent Physica D 1 80
[16] Creamer D B, Thacker H B and Wilkinson D 1981 Some exact results for the two-point function of an integrable quantum field theory Phys. Rev. D 23 3081
[17] Gangardt D M 2004 Universal correlations of trapped one-dimensional impenetrable bosons J. Phys. A: Math. Gen. 37 9335
Gangardt D M and Shlyapnikov G V 2006 Off-diagonal correlations of lattice impenetrable bosons in one dimension New J. Phys. 8 167
[18] 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
[19] Ivanov D A and Abanov A G 2013 Fisher–Hartwig expansion for Toeplitz determinants and the spectrum of a single-particle reduced density matrix for one-dimensional free fermions arXiv:1306.5017
Abanov A G, Ivanov D A and Qian Y 2011 Quantum fluctuations of one-dimensional free fermions and Fisher–Hartwig formula for Toeplitz determinants J. Phys. A: Math. Theor. 44 485001
[21] Suesstrunk R and Ivanov D A 2012 Free fermions on a line: asymptotics of the entanglement entropy and entanglement spectrum from full counting statistics Europhys. Lett. 100 60009
[22] Wolfram Research, Inc. 2010 Mathematica, Version 8.0 (Champaign, IL: Wolfram Research Inc.)
[23] Muir T 1906 The Theory of Determinants in the Historical Order of Development vol 1 (London: Macmillan)
[24] Brualdi R A and Schneider H 1983 Determinantal identities: Gauss, Schur, Cauchy, Sylvester, Kronheimer, Jacobi, Binet, Laplace, Muir, and Cayley Linear Algebra Appl. 52–53 769
[25] Dodgson C L 1866 Condensation of determinants Proc. R. Soc. Lond. 15 150
[26] Muir T 1883 The law of extensible minors in determinants Trans. R. Soc. Edinb. 30 1
[27] Anderson E et al 1999 LAPACK Users’ Guide 3rd edn (Philadelphia, PA: Society for Industrial and Applied Mathematics)
[28] Sobolev A V 2010 Quasi-classical asymptotics for pseudo-differential operators with discontinuous symbols: Widom’s conjecture Funkt. Anal. Pril. 44 86 (in Russian)
Sobolev A V 2010 Funct. Anal. Appl. 44 313 (Engl. transl.)
[29] Widom H 1982 On a class of integral operators with discontinuous symbol Operator Theory: Advances and Applications (Toeplitz Centennial vol 4) (Basel: Birkhäuser) p 477
[30] Stone M 1994 Bosonization (Singapore: World Scientific)
[31] Haldane F D M 1981 Effective harmonic-fluid approach to low-energy properties of one-dimensional quantum fluids Phys. Rev. Lett. 47 1840
[32] Luther A and Peschel I 1975 Calculation of critical exponents in two dimensions from quantum field theory in one dimension Phys. Rev. B 12 3908