Universal parity effects in the entanglement entropy of XX chains with open boundary conditions

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Abstract. We consider the Rényi entanglement entropies in the one-dimensional XX spin-chains with open boundary conditions in the presence of a magnetic field. In the case of a semi-infinite system and a block starting from the boundary, we derive rigorously the asymptotic behavior for large block sizes on the basis of a recent mathematical theorem for the determinant of Toeplitz plus Hankel matrices. We conjecture a generalized Fisher-Hartwig form for the corrections to the asymptotic behavior of this determinant that allows the exact characterization of the corrections to the scaling at order $o(\ell^{-1})$ for any $n$. By combining these results with conformal field theory arguments, we derive exact expressions also in finite chains with open boundary conditions and in the case when the block is detached from the boundary.
1. Introduction

The interest in quantifying the entanglement in the ground state of extended quantum systems has risen sharply in the last decade [1]. Remarkably, the results of many investigations allowed a deeper and more precise characterization of many-body systems. Furthermore, many surprising connections between fields and techniques apparently disconnected emerged.

In this paper we will consider the Rényi entanglement entropies in the XX chain with open boundary conditions (OBC). As we will review, the leading asymptotic behavior of the entanglement entropy can be deduced directly from known results in conformal field theory (CFT) joined with available exact calculations for the chain with periodic boundary conditions (PBC). However, the open chain presents subleading oscillatory corrections to the scaling whose first observation dates back to 2006 [2] and that until now resisted to an analytic computation. This study provides a new and unexpected by-product that, for some aspects, is even more interesting that the main result itself. Indeed, in order to arrive to an analytic result for the entanglement entropy in systems with OBC, we faced the problem of calculating leading and subleading behavior of the determinants of matrices that in mathematical literature are known as Toeplitz plus Hankel (i.e. they are composed of a part that depends only on the difference between row and column indexes and another depending only on their sum). Toeplitz matrices have a very long history, culminating with the Fisher-Hartwig (FH) conjecture [3]. This conjecture has been proved (in some particular cases) only many years after its formulation by Basor [4]. The interest in the corrections to this formula led to a generalization known as generalized FH conjecture [5] that has not yet been proved. This formula has been fundamental to provide the corrections to the scaling for the entanglement entropy in systems with PBC [6, 7]. When moving from PBC to OBC, we move from Toeplitz matrices to Toeplitz plus Hankel ones, that is a brand new field of mathematics. The formula generalizing FH has been proved very recently [8] (see also [9]), and there is no conjecture for the subleading terms. Putting together the ingredients of the generalized FH and the recent results for Toeplitz plus Hankel, we conjecture a generalized FH formula for Toeplitz plus Hankel matrices, that we use to determine analytically the corrections to the scaling of the entanglement entropy for OBC.

1.1. Entanglement entropy, conformal field theory, and boundaries

Let us consider an infinite one-dimensional critical system whose scaling limit is described by a CFT of central charge c, and a partition into a finite block of length \(\ell\) and the remainder. The entanglement entropy (the von Neumann entropy \(-\text{Tr}\,\rho_A\log\rho_A\) of the reduced density matrix \(\rho_A\)) for \(\ell\) much larger than the short-distance cutoff \(a\) is asymptotically [10, 11, 12, 13]

\[
S_1 = -\text{Tr}\,\rho_A\ln\rho_A \simeq \frac{c}{3} \ln \frac{\ell}{a} + c'_1 ,
\]

where \(c'_1\) is a non-universal additive constant. A more general measure of the quantum entanglement is provided by the Rényi entropies, that in the conformal situation of before scale like [12, 13]

\[
S_n = \frac{1}{1-n} \ln \text{Tr} \,\rho_A^n \simeq \frac{c}{6} \left(1 + \frac{1}{n}\right) \ln \ell + c'_n ,
\]
where $c'_n$ are other non-universal constants. For $n = 1$, Eq. (2) reproduces $S_1$, but the knowledge of $S_n$ for different $n$ contains more information and characterizes the full spectrum of non-zero eigenvalues of $\rho_A$ [14], that is fundamental to understand the scaling of some numerical algorithms based on matrix product states [15].

For semi-infinite systems, Renyi entropies depend on where the block is placed because of the breaking of translational invariance. When the block starts from the beginning of the semi-infinite chain (see Fig. 1), very general results are available from boundary CFT. The Renyi entropies behave like [12, 13]

$$S_n \simeq \frac{c}{12} \left( 1 + \frac{1}{n} \right) \ln \ell + \tilde{c}'_n,$$

(3)

The constants $\tilde{c}'_n$ are non-universal, but their value is related to $c'_n$ for systems with PBC by the universal relation [12, 16, 2]

$$\tilde{c}'_n - \frac{c'_n}{2} = \log g,$$

(4)

where $\log g$ is the boundary entropy, first discussed by Affleck and Ludwig [17]. $g$ depends only on the boundary CFT and its value is known in the simplest cases. For the XX model with OBC considered here, we have $g = 1$ [17].

When the block of length $\ell$ placed at a distance $\ell_0$ from the boundary (see Fig. 1), the situation is more complicated. In this case, global conformal invariance only gives the general scaling of $S_n$ as

$$S_n = \frac{c}{12} \left( 1 + \frac{1}{n} \right) \log \left( \frac{(2\ell_0 + \ell)^2}{\ell^2\ell_0(\ell + \ell_0)} \right) + \frac{2\tilde{c}'_n}{1 - n} + \frac{\log F_n(x)}{\ell^2},$$

(5)

where $\ell$ is the four-point ratio

$$x = \frac{\ell^2}{(2\ell_0 + \ell)^2}. $$

(6)

This formula can be readily obtained from the entanglement of two disjoint intervals in an infinite system [18, 19], where the points corresponding to the second interval are the mirror images (with respect to the boundary) of the actual interval. The function $F_n(x)$ (normalized such that $F_n(0) = 1$) depends on the full operator content of the theory and must be calculated case by case. The entanglement of two blocks attracted in the last year an enormous interest [18, 19, 20, 21, 22, 23] because of its ability to detect the full operator content of a CFT. However, all the results presented so far are for periodic systems and still little attention has been devoted to the boundary case that we address here in a specific case (that we will see to turn out to be trivial, after the corrections to the scaling have been properly taken into account).
1.2. Beyond CFT

When $S_n(\ell)$ is computed numerically, it has been observed that the asymptotic CFT result is obscured by large, and often oscillatory, corrections to the scaling [2, 6, 24]. In Ref. [6], on the basis of both exact and numerical results, it has been argued that these corrections are in fact universal and encode information about the underlying CFT beyond what is captured by the central charge alone. More precisely, they give access to the scaling dimensions of some of the most relevant operators of the underlying CFT. This conjecture of Ref. [6] has been recently confirmed by using perturbed CFT arguments [25] (and generalized to gapped chains as well [26]). For a Luttinger liquid, the proposed scaling form of $S_n$ is [6, 25]

$$S_n = S_n^{\text{CFT}} + f_n \cos(2k_F\ell)e^{-2K/n},$$  \hspace{1cm} (7)

where $K$ is the scaling dimension of a relevant operator (in general the oscillating factor can be different from $\cos(2k_F\ell)$ or even be absent, as it happens for the Ising model [7, 27]). The constant $f_n$ is a non-universal quantity that has been determined exactly only for XX and Ising models [6, 7]. It is worth mentioning that in the known PBC cases $f_1$ turns out to be zero, i.e. for the entanglement entropy there are no unusual corrections. This is also the case for all the numerical computations presented so far, but this fact still lacks of a general proof.

On the basis of universality [6] and directly by CFT [25], it has been argued that in the case of OBC, the exponent governing the corrections is half of the PBC one (i.e. $K/n$ replaces $2K/n$ in Eq. (7)), as compatible with all numerical computations available [2, 28, 29]. It is important to mention that with OBC, unusual corrections are also present for $n \to 1$ [2]. In this manuscript, we present a first analytic computation of these corrections to the scaling for systems with OBC.

We anticipate here the main result of the manuscript for the Rényi entanglement entropy of a block starting from the boundary of a semi-infinite system

$$S_n(\ell) = \frac{1}{12} \left(1 + \frac{1}{n}\right) \ln \left[2(2\ell + 1)\sin k_F\right] + \frac{E_n}{2}$$

$$+ \frac{2\sin[k_F(2\ell + 1)]}{1 - n} \left[2(2\ell + 1)\sin k_F\right]^{-1/n} \frac{\Gamma\left(\frac{1}{2} + \frac{1}{n}\right)}{\Gamma\left(\frac{1}{2} - \frac{1}{n}\right)} + o(\ell^{-1/n}),$$  \hspace{1cm} (8)

that is compatible with the general Luttinger liquid prediction [6, 25] with $K = 1$. Notice that away from half-filling ($k_F = \pi/2$), the oscillations have different forms compared to the PBC case. While this formula is correct only to order $o(\ell^{-1/n})$, in the following we will present the full expansion up to the order $o(\ell^{-1})$, for any finite value of $n$. In the case of $n \to \infty$, the corrections become logarithmic and are also exactly calculated. CFT is also used to infer exact analytic formulas for finite systems with two open boundaries.

1.3. Organization of the manuscript

The remainder of this paper is organized as follows. We first present known results for the XX model and the calculation of corrections to the scaling with PBC in Sec. 2. In Sec. 3 we derive the asymptotic behavior of Rényi entropies, while in the Sec. 4 we calculate analytically the first correction to the scaling and a family of the subleading ones that, independently of $n$, give the correct behavior at $o(\ell^{-1})$. In Sec. 5 we generalize the results to finite systems. In Sec. 6 we consider the case of a block...
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disconnected from the boundary. Finally in Sec. 7, we summarize our main results and discuss problems deserving further investigations.

2. Entanglement entropy in the XX model

The Hamiltonian of the XX model for a semi-infinite chain with an open boundary is

\[ H = -\sum_{l=1}^{\infty} \left( \frac{1}{2} [\sigma^x_l \sigma^x_{l+1} + \sigma^y_l \sigma^y_{l+1}] - h \sigma^z_l \right), \]

(9)

where \( \sigma^x, \sigma^y, \sigma^z \) are the Pauli matrices at site \( l \). The Jordan-Wigner transformation

\[ c_l = \left( \prod_{m<l} \sigma^z_m \right) \left( \frac{\sigma^x_l + i \sigma^y_l}{2} \right), \]

(10)

maps this model to a quadratic Hamiltonian of spinless fermions

\[ H = -\sum_{l=1}^{\infty} c_{l+1}^\dagger c^\dagger_l c_l + 2h \left( c^\dagger_l c_l - \frac{1}{2} \right). \]

(11)

Here \( h \) represents the chemical potential for the spinless fermions \( c_l \), which satisfy canonical anti-commutation relations \( \{c_l, c^\dagger_m\} = \delta_{l,m} \). The Hamiltonian (11) is diagonal in momentum space and for \( |h| < 1 \) the ground-state is a partially filled Fermi sea with Fermi-momentum

\[ k_F = \arccos |h|. \]

(12)

In the following we will always assume that \( |h| < 1 \) so that we are dealing with a gapless theory.

Using Wick theorem, the reduced density matrix of a block \( A = [\ell_0, \ell_0 + \ell] \) composed of \( \ell \) contiguous sites in the ground state of the Hamiltonian (9) can be written as

\[ \rho_A = \text{det} \, C \exp \left( \sum_{j,l \in A} \left[ \ln(C^{-1} - 1) \right]_{jl} c^\dagger_j c_l \right), \]

(13)

where the correlation matrix \( C \) has matrix elements defined by

\[ C_{nm} = \langle c^\dagger_m c_n \rangle \]

(14)

In the ground-state of the open semi-infinite Hamiltonian (9), the elements of the correlation matrix are [31]

\[ C_{nm} = \frac{\sin(k_F(n-m))}{\pi(n-m)} - \frac{\sin(k_F(n+m))}{\pi(n+m)}, \]

(15)

and the PBC result is recovered when \( n, m \to \infty \) while keeping their distance \( n-m \) finite, i.e. far from the boundary as the physical intuition suggests. The first half of this expression (Toeplitz part) is the same as in systems with periodic boundary conditions, while the second part (Hankel type) is direct consequence of the non-translational invariant terms introduced by the boundary.

As a real symmetric matrix, \( C \) can be diagonalized by an orthogonal transformation

\[ R CR^T = \delta_{mn}(1 + \nu_m)/2, \]

(16)
and the eigenvalues depend both on $\ell$ and $\ell_0$. The reduced density matrix $\rho_A$ is uncorrelated in the transformed basis, so that the Rényi entropies can be expressed in terms of the eigenvalues $\nu_l$ as

$$S_n(\ell_0, \ell) = \sum_{l=1}^{\ell} e_n(\nu_l), \quad \text{with} \quad e_n(x) = \frac{1}{1-n} \ln \left[ \left( \frac{1+x}{2} \right)^n + \left( \frac{1-x}{2} \right)^n \right].$$

(17)

More details about this procedure can be found in, e.g., Refs. [11, 30, 31]. The above construction refers to the block entanglement of fermionic degrees of freedom. However, the Jordan-Wigner transformation, although non local, mixes only spins inside the block. As well known, this ceases to be the case when two or more disjoint intervals are considered [21, 32] and other techniques need to be employed [33] in order to recover CFT predictions [18, 19, 21]. Furthermore, also in the case of XX chains with different boundary conditions (e.g. fixed) the Jordan-Wigner string would spoil the correspondence between spins and fermions for an interval detached from the boundary (i.e. $\ell_0 \neq 0$). It is a peculiarity of OBC that the reduced density matrix of any interval at any distance from the boundary is the same for spins and fermions.

The representation (17) is particularly convenient for numerical computations: the eigenvalues $\nu_m$ of the $\ell \times \ell$ correlation matrix $C$ are determined by standard linear algebra methods and $S_n(\ell)$ is then computed using Eq. (17). All the numerical computations presented in the following have been obtained in this way.

The sum in Eq. (17) can be put in the form of an integral on the complex plane [34], introducing the determinant

$$D_\ell(\lambda) = \det \left( (\lambda + 1)I - 2C \right) \equiv \det(\lambda).$$

(18)

In the eigenbasis of $C$ the determinant is simply a polynomial of degree $\ell$ in $\lambda$ with zeros $\{\nu_j| j = 1, \ldots, \ell\}$, i.e.

$$D_\ell(\lambda) = \prod_{j=1}^{\ell} (\lambda - \nu_j).$$

(19)

This implies that the Rényi entropies have the integral representation

$$S_n(\ell) = \frac{1}{2\pi i} \oint d\lambda \frac{\ln D_\ell(\lambda)}{d\lambda},$$

(20)

where the contour of integration encircles the segment $[-1,1]$. In the PBC case and in the thermodynamic limit ($L \to \infty$), Fisher-Hartwig conjecture allows to obtain the asymptotic large $\ell$ behavior of $S_n(\ell)$ [34]. The generalized Fisher-Hartwig conjecture permits the computation of all harmonic corrections [6, 7], while non-harmonic corrections can be computed only exploiting random matrices techniques [7]. In next subsection, we report the Fisher-Hartwig approach to PBC, in order to fix the notation and to understand the needed ingredients for OBC.

2.1. The asymptotic result for periodic boundary condition.

For PBC, the correlation matrix in the limit $L \to \infty$ is

$$C_{nm} = \frac{\sin(k_F(n-m))}{\pi(n-m)}.$$  

(21)

The matrix $G$ in Eq. (18) is a $\ell \times \ell$ Toeplitz matrix, i.e. its elements depend only on the difference between row and column indices $G_{jk} = g_{j-k}$. In this case, it is possible to
use the (generalized) Fisher-Hartwig conjecture to calculate the asymptotic behavior of \(D_\ell(\lambda)\) and hence the Rényi entropies [34, 7]. The standard FH calculation proceeds as follows. We define the symbol of the Toeplitz matrix the Fourier transform \(g(\theta)\) of \(g_l\)

\[
g_l = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{i\theta} g(\theta),
\]

that in our case takes the form

\[
g(\theta) = \begin{cases} 
\lambda + 1 & \theta \in [k_F, 2\pi - k_F] \\
\lambda - 1 & \theta \in [0, k_F] \cup [2\pi - k_F, 2\pi] .
\end{cases}
\]

On the interval \([0, 2\pi]\) the function \(g(\theta)\) has two discontinuities at \(\theta_1 = k_F\) and \(\theta_2 = 2\pi - k_F\). In order to employ the Fisher-Hartwig conjecture one needs to express \(g(\theta)\) in the form

\[
g(\theta) = f(\theta) \prod_{r=1}^R e^{ib_r [\theta - \theta_r - \pi \text{sgn}(\theta - \theta_r)]} (2 - 2 \cos(\theta - \theta_r))^{a_r},
\]

where \(R\) is an integer, \(a_r, b_r\) and \(\theta_r\) are constants and \(f(\theta)\) is a smooth function with winding number zero. The Fisher-Hartwig conjecture then states that the large-\(\ell\) asymptotic behavior of the Toeplitz determinant is

\[
D_\ell \sim F[f(\theta)]^\ell \left( \prod_{j=1}^R \ell^{a_j^2 - k_j^2} \right) E,
\]

where \(F[f(\theta)] = \exp\left(\frac{1}{2\pi} \int_{0}^{2\pi} d\theta \ln f(\theta)\right)\) and \(E\) is a known function of \(f(\theta), a_r, b_r,\) and \(\theta_r\). In our case it is straightforward to express the symbol in the canonical form (24). As \(g(\theta)\) has two discontinuities in \([0, 2\pi]\) we have \(R = 2\). By comparison, we have

\[
a_{1,2} = 0, \\
b_2 = -b_1 = \beta_\lambda + m, \\
f(\theta) = f_0 = (\lambda + 1)e^{-2ib_2k_F} = (\lambda + 1)e^{-2ik_Fm}e^{-2ik_\beta},
\]

where \(m\) is an arbitrary integer number, that labels the different inequivalent representations of the symbol \(g(\theta)\), see [4], and

\[
\beta = \frac{1}{2\pi i} \log \left[ \frac{\lambda + 1}{\lambda - 1} \right] - \pi \leq \arg \left[ \frac{\lambda + 1}{\lambda - 1} \right] < \pi.
\]

Jin and Korepin employed the Fisher-Hartwig conjecture for the \(m = 0\) representation and obtained the following result for the large-\(\ell\) asymptotics of \(D_\ell(\lambda)\) [34]

\[
D_{\ell}^{JK}(\lambda) \sim \left( \lambda + 1 \right) \left( \frac{\lambda + 1}{\lambda - 1} \right)^{-\frac{k_F}{2}} \left( 2\ell |\sin k_F| \right)^{-2\beta^2(\lambda)} \left( 1 + \beta_\lambda \right) G^2(1 - \beta_\lambda),
\]

where \(G(x)\) is the Barnes G-function [36]. Inserting (28) into (20) and carrying out the integral leads to the result for the asymptotic behaviour of the Rényi entropy

\[
S^{JK}_n(\ell) = \frac{1}{6} \left( 1 + \frac{1}{n} \right) \ln(2\ell |\sin k_F|) + E_n,
\]

where the constant \(E_n\) has the integral representation

\[
E_n = \left( 1 + \frac{1}{n} \right) \int_0^\infty \frac{dt}{t} \left[ \frac{1}{1 - n^{-2}} \left( \frac{1}{n \sinh t/n} - \frac{1}{\sinh t} \right) \frac{1}{\sinh t} - \frac{e^{-2t}}{6} \right].
\]
However, when the symbol has several inequivalent representations as in our case, the generalized Fisher-Hartwig conjecture (gFHC) [4] applies and one has to sum over all these representations as
\[
D_\ell(\lambda) \sim \sum_m (f_0(m))^{\ell} \sum_i (b_i(m))^2 E(m),
\]
where all the various FH constants \(f_0, b_i, and E\) depend on \(m\), as shown in Eq. (26).

Then the full result of the generalized Fisher-Hartwig conjecture for the Toeplitz determinant takes the form [7]
\[
D_\ell \sim (\lambda + 1)^{\ell} \frac{\lambda + 1}{\lambda - 1} \sum_{m \in \mathbb{Z}} (2\ell|\sin k_F|)^{-2(\beta + 1)} e^{-2i k_F m \ell} \times [G(m + 1 + \beta \lambda)G(1 - m - \beta \lambda)]^2,
\]
leading after long calculations for the integral (20) to [7]
\[
S_n(\ell) - S_{nK}(\ell) = \frac{2\cos(2k_F \ell)}{1 - n}(2\ell|\sin k_F|)^{-2/n} \left[ \frac{\Gamma(\frac{1}{2} + \frac{1}{2n})}{\Gamma(\frac{1}{2} - \frac{1}{2n})} \right]^2 + o(\ell^{-2/n}).
\]

3. Fisher-Hartwig like conjecture for the semi-infinite chain

We want to use a generalization of the FH conjecture to obtain the determinant in Eq. (18) for large \(\ell\). The matrix \(G\) is not of the Toeplitz form because of the second term in \(C_{nm}\) in Eq. (15). Let us consider a block at distance \(\ell_0\) from the boundary (i.e. starting from the site \(\ell_0 + 1\)). To fix the notation, the matrix \(G\) is an \((\ell + 1) \times (\ell + 1)\) matrix that is a sum of Toeplitz and Hankel matrices with elements of the form
\[
G_{nm} = g_{n-m} - g_{n+m+2\ell_0 + 2}, \quad n, m = 0, 1, \ldots \ell - 1.
\]
Here \(g_{\ell}\) is the same as in Eq. (22). We are not aware of any possible generalization (conjectured or proved) of the FH formula to the case of arbitrary \(\ell_0\). However, very recently a theorem has been proved [8] for some Toeplitz+Hankel matrices, among which those of the form
\[
a_{i-j} - a_{i+j+2},
\]
that applies to our case with \(\ell_0 = 0\), i.e. when the block starts from the boundary.

For the case of a piecewise constant symbol as the one of our interest (cf. Eq. (23)), this theorem was known from longer time [9]. The result in Refs. [8, 9] has a structure similar to the FH formula, with more constants \(a_j, b_j\) corresponding to boundary terms. Such a general formula is not very illuminating and too long to be written in its full glory. We remand the interested reader to the original reference [8]. We specialize this formula to the symbol in Eq. (23), and we obtain the asymptotic behavior of the determinant \(D_\ell(\lambda)\) as
\[
D_\ell(\lambda) \sim e^{i\left(\frac{\pi}{2} - k_F\right)\beta} \left[ (\lambda + 1) \left( \frac{\lambda + 1}{\lambda - 1} \right)^{\frac{k_F}{\beta}} \right]^\ell (4\ell|\sin(k_F)|)^{-3\beta} G(1 - \beta) G(1 + \beta),
\]
where \(\beta\) has been defined in Eq. (27). The result is very similar to the PBC case. The main differences are in the halving of the exponent of \(\ell\), in the factor 4 instead of 2.
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multiplying $\ell$ (both with a clear physical interpretation), in the absence of the square
in the Barnes G function, and in the phase shift in front.

We can now proceed to calculate the integral (20) giving the asymptotic Rényi
entropies. First we notice that the phase shift $e^{i(\frac{\pi}{2} - k_F)\beta}$ in Eq. (41) gives a vanishing
contribution to the entropies, indeed

$$\left(\frac{1}{2} - \frac{k_F}{\pi}\right) \frac{1}{2\pi i} \oint d\lambda e_n(\lambda) \frac{1}{1-\lambda^2} = 0.$$  

(37)

The remaining part of the integral parallels that for PBC, giving

$$S_n(\ell) = \frac{1}{12} \left(1 + \frac{1}{n}\right) \ln(2\ell |\sin k_F|) + \frac{E_n}{2},$$  

(38)

where $E_n$ is defined in Eq. (30).

This result for $S_n$ is exactly what expected from CFT, as reviewed in the
introduction. Both the leading logarithmic term and the subleading constant one are
in agreement with Eq. (3) with $\ln g = 0$. There is then no new physical information
in this expression. However, the present result is based on a mathematical theorem
and so it provides a rigorous confirmation of a general CFT result in a specific lattice
model. The new physical results of this paper are in the following sections.

4. Generalized conjecture for the oscillating corrections to the scaling

We consider now the corrections to the scaling to the asymptotic result derived in
the previous section. Analogously to the PBC case, we need a generalized Fisher-
Hartwig formula that applies to the case of Toeplitz+Hankel matrices. To the best of
our knowledge, this formula does not exist neither conjectured or proved. However,
armed with the general ideas presented above is not difficult to give our own conjecture
for such a determinant: we should only sum on the several different inequivalent
representations of the symbol.

For the symbol in Eq. (23), we conjecture the following formula

$$D_\ell(\lambda) \sim (\lambda + 1)^{\ell} \left(\frac{\lambda + 1}{\lambda - 1}\right)^\frac{k_F\ell}{2} \sum_{m \in \mathbb{Z}} e^{i\frac{\pi}{2}(m+\beta)\ell} \left[4\left(\ell + \frac{1}{2}\right) |\sin k_F| \right]^{-(m+\beta\lambda)^2}$$

$$\times e^{-2\ell k_F(\beta+1)(\ell+1/2)} G(m + 1 + \beta\lambda)G(1 - m - \beta\lambda).$$  

(39)

Most of the above formula is inspired to the gFH Eq. (32) and adapted to the present
case. However, the factor $1/2$ as an additive constant to $\ell$ has been introduced without
any mathematical reason. This factor $1/2$ gives an analytic (i.e. non-harmonic)
correction to $D_\ell(\lambda)$ and we introduced it to reproduce accurately the numerical data.
In Fig. 2 we report the ratio of the numerically calculated $D_\ell(\lambda)$ asymptotic value
with and without the additional $1/2$, showing that the former converges faster. The
data for the resulting entanglement entropy $S_2(\ell)$ (reported in the right panel of Fig.
2) show even more clearly the importance of this factor. In any case, we conjectured
this gFH formula and in doing so we prefer to conjecture an expression that reproduces
numerical data as accurately as possible. A full justification of the factor $1/2$ could
be obtained by generalizing the random matrix results for PBC in Ref. [35], but this
is beyond our knowledge.
The leading corrections to the scaling is obtained by summing only the three
types $m = -1, 0, 1$, obtaining
\begin{align}
D_\ell & \sim D_\ell^{(0)} \left\{ 1 + ie^{-ikFL}e^{-2ikF\ell}L_k^{-1-2\beta}\frac{\Gamma(1+\beta)}{\Gamma(-\beta)} - ie^{ikFL}e^{2ikF\ell}L_k^{-1+2\beta}\frac{\Gamma(1-\beta)}{\Gamma(\beta)} \right\} \\
& \equiv D_\ell^{(0)} (1 + \Psi_\ell(\lambda)) ,
\end{align}
where we isolated the leading term
\begin{equation}
D_\ell^{(0)} \equiv e^{i\frac{\pi}{2-k_F}} \left[ (\lambda + 1)\left(\lambda - 1\right) \right]^{-\frac{1-k_F}{2}} L_k^{-\beta^2} G(1-\beta)G(1+\beta) ,
\end{equation}
we defined $\Psi_\ell(\lambda)$, and $L_k$ for OBC is defined as
\begin{equation}
L_k = 2(2\ell + 1) |\sin(k_F)|.
\end{equation}
We define
\begin{equation}
d_n(\ell) \equiv S_n(\ell) - S_n^{(0)}(\ell) ,
\end{equation}
with
\begin{equation}
S_n^{(0)} = \frac{1}{12} \left( 1 + \frac{1}{n} \right) \ln \left[ 2(2\ell + 1) |\sin k_F| \right] + \frac{E_n}{2} ,
\end{equation}
that includes the additive $1/2$ factor compared to the leading term in Eq. (38). For
large $L_k$ we have
\begin{equation}
d_n(\ell) \sim \frac{1}{2\pi i} \int d\lambda \ e_n(\lambda) \frac{d\ln \left[ 1 + \Psi_\ell(\lambda) \right]}{d\lambda} = \frac{1}{2\pi i} \int d\lambda \ e_n(\lambda) \frac{d\Psi_\ell(\lambda)}{d\lambda} + \ldots
\end{equation}
The contour integral can be written as the sum of two contributions infinitesimally
above and below the interval $[-1, 1]$ respectively, i.e.
\begin{equation}
d_n(\ell) \sim \frac{1}{2\pi i} \left[ \int_{-1+i\epsilon}^{1+i\epsilon} - \int_{-1-i\epsilon}^{1-i\epsilon} \right] d\lambda \ e_n(\lambda) \frac{d\Psi_\ell(\lambda)}{d\lambda} .
\end{equation}
This shows that we only require the discontinuity across the branch cut. The only discontinuous function is $\beta_\lambda$, which for $-1 < x < 1$ behaves as

$$
\beta_{x\pm i\epsilon} = -iw(x) \mp \frac{1}{2}, \quad \text{with} \quad w(x) = \frac{1}{2\pi} \ln \frac{1+x}{1-x}.
$$

(47)

We now change variables from $\lambda$ to $w$

$$
\lambda = \tanh(\pi w), \quad -\infty < w < \infty.
$$

(48)

We have

$$
\left[ L_k^{-1-2\beta} \Gamma(1+\beta) \right]_{\beta=-iw-\frac{1}{2}} - \left[ L_k^{-1-2\beta} \Gamma(1+\beta) \right]_{\beta=-iw+\frac{1}{2}} \simeq L_k^{2iw} \gamma(w),
$$

$$
\left[ L_k^{-1+2\beta} \Gamma(1-\beta) \right]_{\beta=-iw-\frac{1}{2}} - \left[ L_k^{-1+2\beta} \Gamma(1-\beta) \right]_{\beta=-iw+\frac{1}{2}} \simeq - L_k^{-2iw} \gamma(-w),
$$

where we have dropped terms of order $O(L_k^{-2})$ compared to the leading ones and we have defined

$$
\gamma(w) = \frac{\Gamma\left(\frac{1}{2} - iw\right)}{\Gamma\left(\frac{1}{2} + iw\right)}.
$$

(49)

Integrating by parts and using

$$
\frac{d}{dw} \epsilon_n(\tanh(\pi w)) = \frac{\pi n}{1-n} (\tanh(n\pi w) - \tanh(\pi w)),
$$

(50)

we arrive at

$$
d_n(\ell) \sim \frac{in}{2(1-n)} \int_{-\infty}^{\infty} dw (\tanh(\pi w) - \tanh(n\pi w)) \left[ i e^{-ik_F \ell} L_k^{2iw} \frac{\Gamma\left(\frac{1}{2} - iw\right)}{\Gamma\left(\frac{1}{2} + iw\right)} + i e^{ik_F \ell} L_k^{-2iw} \frac{\Gamma\left(\frac{1}{2} + iw\right)}{\Gamma\left(\frac{1}{2} - iw\right)} \right],
$$

(51)

For large $\ell$ the leading contribution to the integral arises from the poles closest to the real axis. These are located at $w_0 = i/2n$ ($w_0 = -i/2n$) for the first (second) term. Evaluating their contributions to the integral gives

$$
d_n(\ell) \sim \frac{2 \sin[k_F(2\ell + 1) - \frac{1}{2}]}{1-n} \left[ \frac{2(2\ell + 1) \sin k_F}{2\ell + 1} \right]^{-1/n} \frac{\Gamma\left(\frac{1}{2} + \frac{1}{2n}\right)}{\Gamma\left(\frac{1}{2} - \frac{1}{2n}\right)},
$$

(52)

In Fig. 3 we report the numerical calculated $S_n(\ell)$ for a semi-infinite chain and for small values of $n = 1, 2, 3$. For these values of $n$, the inclusion of only the first correction to the scaling (as in Eq. (8)) is enough to describe very accurately $S_n(\ell)$ even for relatively small values of $\ell$. The figure shows the correctness also of the $k_F$ dependence of the correction, that is the most important difference compared to PBC. Notice that without the factor $1/2$ introduced by hand in Eq. (39), the correction (52) would be inadequate at order $1/\ell$, as anticipated in Fig. 2.

4.1. Subleading corrections

Eq. (33) describes the asymptotic behavior in the limit $L_k \to \infty$ with $n$ fixed. It provides a good approximation for large, finite $\ell$ as long as $\ln(L_k) \gg n$. For practical purposes it is useful to know the corrections to $S_n(\ell)$ for large $\ell$ but $\ln(L_k)$ not necessarily much larger than $n$. In this regime there are two main sources of corrections to (33). The integral (50) is no longer dominated by the poles closest
to the real axis and contributions from further poles need to be included. These
give rise to corrections proportional to $L_k^{-q/n}$, with $q$ integer. Furthermore, terms
in the expansion of the logarithm in Eq. (45) need to be taken into account. The

We now take both types of corrections into account. The following derivation is
very similar to the one for PBC in Ref. [7]. We first consider the series expansion of
the logarithm in Eq. (45).

$$\ln \left[ 1 + \Psi_{\ell}(\lambda) \right] = \sum_{p=1}^{\infty} \frac{(-1)^{p+1} (\Psi_{\ell}(\lambda))^p}{p}. \quad (53)$$

Recalling the explicit expression (40) for $\Psi_{\ell}(\lambda)$ leads to a binomial sum

$$(\Psi_{\ell}(\lambda))^p = \left( ie^{ik_F e^{-2ik_F \ell}} L_k^{-(1+2\beta)} c_{\beta\lambda} - ie^{-ik_F e^{2ik_F \ell}} L_k^{-(1-2\beta)} c_{-\beta\lambda} \right)^p$$

$$= \sum_{q=0}^{p} \binom{p}{q} (-1)^q e^{ik_F (2q-p)} e^{2ik_F \ell (2q-p)} L_k^{-p} L_k^{-2(p-2q)\beta} c_{\beta\lambda}^{p-q} c_{-\beta\lambda}^q, \quad (54)$$

where we have introduced the shorthand notation $c_\beta = \Gamma(1+\beta)/\Gamma(-\beta).$
When calculating the discontinuity across the branch cut running from $\lambda = -1$ to $\lambda = 1$ all terms other than $q = 0$ and $q = p$ give rise to terms that are subleading in $L_k$. Hence we may approximate

\[
(\Psi_{\ell}(\tanh(\pi w) + i\epsilon))^p - (\Psi_{\ell}(\tanh(\pi w) - i\epsilon))^p \approx \]

\[
i^p e^{-2ik_p(\ell+1/2)p} L_k^{2iwp} c_{-i\omega-1/2} - (-i)^p e^{2ik_p(\ell+1/2)p} L_k^{-2iwp} c_{i\omega-1/2}.
\]  

Plugging this into Eq. (45)

\[d_n(\ell) \sim \sum_{p=1}^{\infty} \frac{(-1)^{p+1}}{p} \frac{in}{2(1-n)} \int_{-\infty}^{\infty} dw (\tanh(\pi w) - \tanh(n\pi w)) \]

\[\times \left[ e^{-2pk_p(\ell+1/2)p} L_k^{2iwp} \gamma_p(w) + (-1)^{p+1} e^{2pk_p(\ell+1/2)p} L_k^{-2iwp} \gamma_p(-w) \right].
\]  

The integral is carried out by contour integration, taking the two terms in square brackets into account separately. The first (second) contribution has simple poles in the upper (lower) half plane at $w_q = i\frac{2q-1}{2n}$ ($w_q = -i\frac{2q-1}{2n}$), where $q$ is a positive integer such that $2q - 1 \neq n, 3n, 5n, \ldots$ for $n \neq 1$. Contour integration then gives

\[d_n(\ell) = \frac{2}{1-n} \sum_{p,q=1}^{\infty} \frac{(-1)^{p+1}}{p} \cos \left( \frac{p(\pi - 2k_F)}{2} - 2pk_p(\ell) \right) L_k^{-\frac{p(2q-1)}{n}} \left( Q_{n,q} \right)^p + \ldots,
\]  

where we defined the constants $Q_{n,q}$ as

\[Q_{n,q} = \frac{\Gamma\left(\frac{1}{2} + \frac{2q-1}{2n}\right)}{\Gamma\left(\frac{1}{2} - \frac{2q-1}{2n}\right)}.
\]  

In the sum over $q$ the special values $2q - 1 \neq n, 3n, 5n, \ldots$ are to be omitted for $n \neq 1$. Eq. (57) shows that there are contributions to the Rényi entropies with oscillation frequencies that are arbitrary multiples of $2k_F$.

At half-filling ($k_F = \pi/2$) certain simplifications occur. For even $\ell$ we find

\[d_n(\ell) \sim \frac{2}{1-n} \left[ (4\ell)^{-\frac{1}{2}} Q_{n,1} + (4\ell)^{-\frac{3}{2}} \frac{Q_{n,1}^2}{2} + (4\ell)^{-\frac{5}{2}} \left( \frac{Q_{n,1}^3}{3} + Q_{n,3} \right) \right] + \ldots,
\]  

while for odd $\ell$ we obtain

\[d_n(\ell) \sim \frac{-2}{1-n} \left[ (4\ell)^{-\frac{1}{2}} Q_{n,1} + (4\ell)^{-\frac{3}{2}} \frac{Q_{n,1}^2}{2} + (4\ell)^{-\frac{5}{2}} \left( \frac{Q_{n,1}^3}{3} + Q_{n,3} \right) \right] + \ldots,
\]  

that are of the same form as for PBC [7] with exponents that are halved. However, we stress that this is true only at half filling, while for generic $k_F$, Eq. (56) shows oscillations different from its PBC counterpart.

In all the above analysis we have ignored contributions to the generalized Fisher-Hartwig conjecture with $|m| > 1$. While these lead to oscillatory contributions with frequencies that are integer multiples of $2k_F$ they are suppressed by additional powers of $\ell^{-1}$ and hence are subleading, even in the case where $n$ is not small.

In Fig. 4 we show the corrections $d_n(\ell)$ for $n = 20$ and 50 with $k_F = \pi/6$ and $\pi/2$ respectively and their comparison with the asymptotic result Eq. (57). Step by step we take into account further terms in the asymptotic expression until we obtain a satisfying agreement with the numerical data. For $n = 20$, 13 terms in Eq. (57) are enough to reproduce the data, while for $n = 50$ we need 41 terms to have the same accuracy. These numbers are larger than the corresponding ones for PBC [7] because the corrections in the present case have smaller exponents.
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4.2. The limit of large \( n \)

It is apparent from (57) that the limit \( n \to \infty \) deserves special attention. \( S_{\infty}(\ell) \) is known in the literature as single copy entanglement [39]. Here it is necessary to sum up an infinite number of contributions in order to extract the large-\( \ell \) asymptotics. It also provides information on the behavior of \( S_n(\ell) \) in the regime \( n \gg \ln L_k, L_k \gg 1 \).

The following derivation parallels the one for PBC in Ref. [7]. In order to investigate the limit \( n \to \infty \) we consider Eq. (56), but now first take the parameter \( n \) to infinity and then carry out the resulting integrals. This gives

\[
d_{\infty}(\ell) \sim \frac{i}{2} \sum_{p=1}^{\infty} \frac{(-1)^p}{p} \int_{-\infty}^{\infty} dw \left( \text{sgn}(w) - \tanh(\pi w) \right)
\times i^p \left[ e^{-2ik_F(\ell+1/2)p} L_k^{2iwp} [\gamma(w)]^p + (-1)^p e^{2ik_F(\ell+1/2)p} L_k^{-2iwp} [\gamma(-w)]^p \right]
= -\sum_{p=1}^{\infty} \frac{(-i)^p}{p} \left[ e^{-2ik_F(\ell+1/2)p} \text{Im} \int_0^{\infty} dw [1 - \tanh(\pi w)] L_k^{2iwp} [\gamma(w)]^p \right]
-(-1)^p e^{2ik_F(\ell+1/2)p} \text{Im} \int_0^{\infty} dw [1 - \tanh(\pi w)] L_k^{-2iwp} [\gamma(-w)]^p .
\]

Using that the first singularity in the upper (lower) half plane occurs at \( w = i/2 \) (\( w = -i/2 \)) we deform the contours to run parallel to the real axis with imaginary parts \( i/4 \) and \( -i/4 \) respectively, i.e. for the first term we use

\[
\int_0^{\infty} dw \ f(w) = \int_0^{i/4} dw \ f(w) + \int_{i/4}^{\infty} dw \ f(w).
\]

It is straightforward to show that the second integral contributes only to order \( O(1/L_k) \) and does not give rise to logarithmic corrections. Hence the leading contribution is of

**Figure 4.** Difference of the Rényi entanglement entropy with its asymptotic value for \( n = 20 \) (left) and 50 (right) with \( k_F = \pi/6 \) and \( \pi/2 \). The exact numerical data are compared with Eq. (57) with increasing number of terms. For \( n = 50 \) we report curves with 1,3,5,9,15,25,41 terms, while for \( n = 20 \) we consider 1,2,3,5,8,13 terms. Increasing the number of terms considered, the expansion (57) becomes accurate even for values of \( \ell \) as small as 2.
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Figure 5. $1/|d_\infty(\ell)|$ with $d_\infty(\ell) = S_\infty(\ell) - S_0^{(0)}(\ell)$ vs $\ell$ in log-linear scale for $k_F = \pi/2$. Corrections to the scaling are logarithmic and perfectly described by Eq. (65) that is represented as two straight lines for $\ell$ even and odd respectively.

The form

$$d_\infty(\ell) \sim \sum_{p=1}^{\infty} \frac{(-i)^p}{p} \left[ e^{-2ik_F(\ell+1/2)p} \text{Re} \int_0^{1/4} dz (1 - i \tan(\pi z)) L_k^{-2zp} (\gamma(iz))^p ight]$$

$$+ (-1)^p e^{2ik_F(\ell+1/2)p} \text{Re} \int_0^{1/4} dz (1 + i \tan(\pi z)) L_k^{-2zp} (\gamma(iz))^p \right]$$

$$= 2 \sum_{p=1}^{\infty} \frac{(-1)^p}{p \cos \left( \frac{p(\pi - 2k_F)}{2} - 2pk_F \ell \right)} \int_0^{1/4} dz e^{-2zp \ln L_k} (\gamma(iz))^p .$$

(62)

For large $L_k$ the dominant contribution to the integral is obtained by expanding $(\gamma(iz))^p$ in a power series around $z = 0$

$$d_\infty(\ell) \sim 2 \sum_{p=1}^{\infty} \frac{(-1)^p}{p} \cos \left( \frac{p(\pi - 2k_F)}{2} - 2pk_F \ell \right) \int_0^{1/4} dz e^{-2zp \ln L_k} (1 + 2pz\Psi(1/2) + \ldots)$$

$$= 2 \sum_{p=1}^{\infty} \frac{(-1)^p}{p^2} \cos \left( \frac{p(\pi - 2k_F)}{2} - 2pk_F \ell \right) \left[ \frac{1}{2 \ln L_k} + \frac{\Psi(1/2)}{2 \ln^2 L_k} + \ldots \right] ,$$

(63)

where $\Psi(z)$ is the digamma function $\Psi(z) = \Gamma'(z)/\Gamma(z)$.

As in the PBC case, at half-filling ($k_F = \pi/2$) this result takes a particularly simple form

$$d_\infty(\ell) \sim \frac{1}{\ln L_k} \sum_{p=1}^{\infty} \frac{(-1)^p(\ell+1)}{p^2} = \begin{cases} \frac{1}{\ln L_k} \frac{\pi^2}{6} & \ell \text{ odd} , \\ \frac{1}{\ln L_k} \frac{\pi^2}{12} & \ell \text{ even} . \end{cases}$$

(64)

Summing some of the subleading terms in (63) to all orders in $(\ln(L_k))^{-1}$ leads to an
expression of the form

\[ d_\infty(\ell) \sim \frac{\pi^2}{12 \ln(bLk)} \begin{cases} 2 & \ell \text{ odd} \\ -1 & \ell \text{ even} \end{cases}, \]  

(65)

where \( b = \exp(-\Psi(1/2)) \approx 7.12429 \). To check this result, in Fig. 5, we report the exact numerical data (only for \( k_F = \pi/2 \)) for \( 1/d_\infty(\ell) \) in log-linear scale, showing explicitly the logarithmic form of the corrections, described very precisely by Eq. (65).

5. Finite systems

The Hamiltonian of a finite XX chain with two open boundaries is

\[ H = -\sum_{l=1}^{L-1} \frac{1}{2} [\sigma_x^l \sigma_x^{l+1} + \sigma_y^l \sigma_y^{l+1}] - h \sum_{l=1}^{L} \sigma_z^l. \]  

(66)

As before, the Hamiltonian is diagonalized by a Jordan-Wigner transformation and Fourier transform. However, we are dealing with a finite chain at fixed magnetic field, that in the language of fermions is fixed chemical potential. In this case, the number of fermions is a non-continuous function of \( L \), because it can assume only integer values. The number of fermions is \( N_F = \lfloor (L+1) |\arccos h| \rfloor \). There is an ambiguity in defining the Fermi momentum and we choose the definition

\[ k_F \equiv \pi N_F = \pi \frac{L}{L+1} |\arccos h|, \]  

(67)

i.e. \( k_F \) is an integer multiple of \( \pi/L \). This definition has the advantage to give \( k_F = \pi/2 \) at half-filling for \( L \) even. However, the correlation matrix \( C \) is better defined in terms of

\[ k_F' = k_F \frac{L}{L+1} + \frac{\pi}{2(L+1)}. \]  

(68)

Notice the following important properties: 1) In the limit \( L \to \infty, k_F = k_F' \); 2) If \( k_F = \pi/2 \), then \( k_F' = \pi/2 \); 3) For \( L \) odd, the ground state is doubly degenerate and both \( k_F \) and \( k_F' \) cannot be equal to \( \pi/2 \). With this definition, we can write the correlation matrix as

\[ C_{nm} = \frac{1}{2(L+1)} \begin{bmatrix} \sin(k_F'(n-m)) & -\sin(k_F'(n+m)) \\ \sin\left(\frac{\pi}{2(L+1)}(n-m)\right) & -\sin\left(\frac{\pi}{2(L+1)}(n+m)\right) \end{bmatrix}. \]  

(69)

From this correlation matrix, it is straightforward to obtain numerical results for \( S_n(\ell) \) also in finite systems. This analysis has been already done with considerable numerical accuracy in Refs. [2, 29] for the Von Neumann entanglement entropy and in Ref. [28] for general \( n \). However, the accurate results for the amplitudes of the corrections to the scaling were not compared with the theoretical predictions not available at that time.

The modification of the leading term in Eq. (8) for finite systems is provided by conformal field theory [12]: the Rényi entropies are given by Eq. (8) where the length of the subsystem \( \ell \) is substituted by the chord distance \( L/\pi \sin(\pi \ell/L) \). However, we would like an expression that takes into account corrections to the scaling and that is accurate at order \( 1/\ell \), while we keep fixed the ratio \( \ell/L \). This is beyond the predictive
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Figure 6. Embedding of the open finite chain in a periodic one. The blue points correspond to the original chain, the red ones are the mirror symmetric sites, while the two yellow points at $x = 0$ and $x = L + 1 \equiv -L - 1$ are “auxiliary sites”. The picture shows a block with $\ell = 2$ in the open chain corresponding to $2\ell + 1 = 5$ in the periodic one.

power of CFT, but an intuitive argument to find a proper modification of Eq. (8) valid in finite size can be given, leading to the expression:

$$S_n(\ell) = \frac{1}{12} \left( 1 + \frac{1}{n} \right) \ln \left[ \frac{4(L + 1)}{\pi} \sin \frac{\pi(2\ell + 1)}{2(L + 1)} | \sin k'_F | \right] + \frac{E_n}{2}$$

$$+ \left[ \frac{4(L + 1)}{\pi} \sin \frac{\pi(2\ell + 1)}{2(L + 1)} | \sin k'_F | \right]^{-1/n} \frac{\Gamma(\frac{1}{2} + \frac{1}{2n})}{\Gamma(\frac{1}{2} - \frac{1}{2n})},$$

(70)

The argument proceeds as follows. While we take the continuum limit from the spin-chain to the CFT, there is a well-known arbitrariness on the exact correspondence between the lattice sites and the coordinate on the continuum space. While for PBC, translational invariance guarantees that we can start the lattice in an arbitrary point, this is no longer true in the presence of boundaries. For a semi-infinite system, the exact result (8) suggests that the first site of the chain should be placed at position $x = 1$ in the continuum theory. Indeed, when building the mirror image (as usually done in boundary CFT), we have a mirror chain starting from $-1$ going up to $-\infty$. This implies that an “auxiliary site” should be introduced at $x = 0$. In this way, we have an infinite chain with a block of length $2\ell + 1$, exactly as Eq. (8) suggests. When we move to a finite chain of length $L$, the mirror construction is graphically depicted in Fig. 6. We clearly have to add another auxiliary site at the other boundary to embed the open chain in a periodic one. The resulting length of the periodic chain is $2(L + 1)$. Thus this argument suggests that from the semi-infinite formula (8), we can obtain a finite-size ansatz by replacing $2\ell + 1$ with the modified chord length $\frac{2(L + 1)}{\pi} \sin \frac{\pi(2\ell + 1)}{2(L + 1)}$. In doing so, we should also keep in mind that the prefactor of the correction $\sin |k'_F(2\ell + 1)|$ is not scaling (as for PBC [6]) and there $\ell$ should be left unchanged. All these ingredients lead to Eq. (70).
In Fig. 7, we report numerical calculated $S_n(\ell)$ for finite systems of different lengths and for different values of $k_F$. In all cases, for $n = 1, 2, 3$, when the first correction describes accurately the numerics for semi-infinite systems, we found perfect agreement between analytical and numerical results, confirming the validity of the non-rigorous argument reported above. Notice that when $k'_F$ is not a simple number, as in the two graphics in the bottom of Fig. 7, the numerical data (points) show apparently strange periodicity. When the asymptotic exact forms are plotted (continuous lines), it is clear that the periodicity is the correct one and the previous effect is only due to the value of $k_F$.

Notice that at $n = 1$, the unusual correction in $\ell^{-1/n}$ and the analytic one coming from expanding $2\ell + 1$ in the leading term are of the same order $1/\ell$ and they have been disentangled in the past [2, 29] only because one is oscillating and the other is not. The presence of the non-oscillating $1/L$ term has been firstly observed and its analytic value guessed in Ref. [2] for $n = 1$. For general $n$, its form has been correctly guessed in Ref. [28]. The oscillatory behavior has also been firstly described in Ref. [2] for $n = 1$, successively its amplitude has been guessed in Ref. [29]. We provided an analytical proof of this sequence of numerical guesses and we gave first analytical expressions for the oscillating corrections to $S_n(\ell)$ for general $n$, that was too complicated to be guessed.
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In Ref. [28], for half-filling and even \( L \), on the basis of numerical results, the Rényi entropies have been parametrized as

\[
S_n = \frac{1}{12} \left( 1 + \frac{1}{n} \right) \left[ \ln[(L + 1) \cos \pi X] + e_n - (-1)^f b_n [L \cos \pi X]^{-1/n} \right],
\]

with \( X = (L/2 - \ell)/(L + 1) \). The numerical values \( b_2 \approx 4.79256 \) and \( b_3 \approx 4.19726 \) have been reported [28]. Eq. (70) is fully compatible with this expression and predicts the value of the amplitude \( b_n \) for any \( n \). The numerical estimates for \( b_n \) in Ref. [28] coincide with the exact values, showing the high numerical accuracy of Ref. [28].

Away from half-filling, in Refs. [28, 29], in order to force a finite-size (or finite-trap) scaling, a new parameter has been introduced to take into account the non-scaling term \( \sin[k'F(2\ell + 1)] \), that is implicit in our definition of \( k_F \). The two representations are equivalent, but we find Eq. (70) clearer.

6. Block disconnected from the boundary

We consider in this section the Rényi entanglement entropies for a block disconnected from the boundary. The numerical calculations are straightforward and can be done exactly in the same way as before just by considering the correlation matrix \( C_{nm} \) starting from a spin different from the first. We stress once again that the calculation of the spin entanglement can be done simply in terms of fermions, as a peculiarity of the chain with open boundary conditions. In the case of two intervals in a PBC chain, the entanglement of spins and fermions are known to be different [21, 32] and also other boundary conditions are generally expected to make spins and fermions inequivalent, so that the calculations should be done following the general method to tackle with the Jordan-Wigner string introduced in Ref. [33].

For simplicity we will consider only systems in the thermodynamic limit (i.e. semi-infinite) and at half filling (\( k_F = \pi/2 \)), but the results are very general. In Fig. 8, we report the function \( F_{2}^{\text{lat}}(x) \) obtained dividing \( \text{Tr}\rho_3^2 \) by the scaling factor in Eq.
Figure 9. Scaling of the finite $\ell$ corrections for $S_n(\ell)$ vs $\ell^{-1/n}$ for $n = 1, 2, 3, 5$. Leading corrections are of the expected form $\propto \ell^{-1/n}$ and the extrapolation to $\ell \to \infty$ clearly gives $F_n(x) = 1$ identically. For large values of $n$, subleading corrections $\propto \ell^{-q/n}$ must be included. (5), i.e.

$$F^{\text{lat}}_n(x) = \frac{\text{Tr} \rho^2}{\ell^n} \left( \frac{(2\ell_0 + \ell)^2}{2\ell_0 (\ell + \ell_0)} \right)^{c/12(n-1/n)}$$

(71)

where $x$ is the 4-point ratio in Eq. (6). Global conformal invariance implies that $F_2(x)$ is a function only of $x$, while in the figure we clearly see different curves for different $\ell$. As usual [18, 21, 33], these differences are due to finite $\ell$ and $\ell_0$ effects that are severe. In Ref. [25], it has been shown that finite $\ell$ corrections are generically of the same form (i.e. governed by the same unusual exponent) independently of the number of blocks (that in the present case generalizes to its location). Notice that the data in Fig. 8 are not asymptotic also because the various curves do not have the conformal symmetry $x \to 1 - x$ [18, 19] (again this is rather common [18, 21, 33] for finite $\ell$).

We can now proceed to the calculation of the asymptotic value of the function $F_n(x)$ for various $n$, by using the fact that corrections to the scaling are of the form $\ell^{-1/n}$. In Fig. 9, we report for $n = 1, 2, 3, 5$ the function $F^{\text{lat}}_n(x)$ at fixed $x$, obtained numerically as explained above, as function of $\ell^{-1/n}$. For large enough $\ell$, the points are aligned on straight lines, confirming the correctness of the finite $\ell$ scaling (increasing $n$, more corrections of the form $\ell^{-q/n}$ must be included to reproduce the numerical data, as obvious). This allows to extrapolate to $\ell \to \infty$. The result is evident from Fig. 9:

$$F_n(x) = 1,$$

(72)
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identically. At first, this can seem very strange when compared with the complicated functions found for two intervals in the XX model with PBC [18, 19, 33]. The simplicity of this result is due to the fact that (in the present case) spins and fermions are equivalent. For PBC free-fermions, the explicit computation shows $F_n(x) = 1$ [40] (as confirmed in some numerical works [41]). This result straightforwardly generalizes to OBC free-fermions [42]. The main peculiarity of OBC is not $F_n(x) = 1$, but the equivalence of fermions and spins.

7. Conclusions

In this manuscript we provided a number of exact results for the asymptotic scaling of the Rényi entanglement entropies in open XX spin-chains. Schematically our results can be summarized as follows.

- In the case of a semi-infinite system and a block starting from the boundary, we derive rigorously the asymptotic behavior for large block sizes on the basis of a recent mathematical theorem for the determinant of Toeplitz plus Hankel matrices. This is given by Eq. (38).
- To obtain the corrections to the scaling to the asymptotic behavior, we conjecture a generalized Fisher-Hartwig form for these determinants. Eq. (57) gives the exact asymptotic behavior of $S_n(\ell)$ at order $o(\ell^{-1})$ for any $n$. Eq. (65) generalizes the result for $n = \infty$, i.e. for the largest eigenvalues of the reduced density matrix.
- By combining these results with conformal field theory arguments, we derive exact expressions also in finite chains with open boundary conditions in Eq. (70).
- In the case of block detached from the boundary, we again use CFT to derive an exact expression for the asymptotic $S_n$ given by Eq. (5) with $F_n(x) = 1$.

All these results have been checked against exact numerical computations. For infinite chains, in Ref. [7], using a combination of methods based on the generalized Fisher-Hartwig conjecture and a recurrence relation connected to the Painlevé VI differential equation, the corrections to $S_n(\ell)$ have been obtained up to order $O(\ell^{-3})$. To the best of our knowledge the recurrence relation obtained in Ref. [35] for an infinite system has not been generalized to a semi-infinite one, although a random matrix description of these chains exists [43, 44].

It would be also very interesting to consider the exact calculation of asymptotic and subleading terms in the Rényi entropies for different boundary conditions and the generalization to the XY model on the lines of Refs. [45, 46]. Finally, the accurate numerical results of Refs. [28, 29] show a very similar structure also for the case of a general confining (trapping) polynomial potential and it is natural to wonder whether exact results can be obtained also in those cases.

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