Entanglement entropy of two disjoint intervals in $c = 1$ theories

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Abstract. We study the scaling of the Rényi entanglement entropy of two disjoint blocks of critical lattice models described by conformal field theories with central charge $c = 1$. We provide the analytic conformal field theory result for the second order Rényi entropy for a free boson compactified on an orbifold describing the scaling limit of the Ashkin–Teller (AT) model on the self-dual line. We have checked this prediction in cluster Monte Carlo simulations of the classical two-dimensional AT model. We have also performed extensive numerical simulations of the anisotropic Heisenberg quantum spin chain with tree tensor network techniques that allowed us to obtain the reduced density matrices of disjoint blocks of the spin chain and to check the correctness of the predictions for Rényi and entanglement entropies from conformal field theory. In order to match these predictions, we have extrapolated the numerical results by properly taking into account the corrections induced by the finite length of the blocks on the leading scaling behavior.

Keywords: conformal field theory (theory), spin chains, ladders and planes (theory), entanglement in extended quantum systems (theory)

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1. Introduction

Let us imagine dividing the Hilbert space $\mathcal{H}$ of a given quantum system into two parts $\mathcal{H}_A$ and $\mathcal{H}_B$ such that $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. When the system is in a pure state $|\Psi\rangle$, the bipartite entanglement between $A$ and its complement $B$ can be measured in terms of the Rényi entropies \[ S_A^{(n)} = \frac{1}{1-n} \log \text{Tr} \rho_A^n, \] where $\rho_A = \text{Tr}_B \rho$ is the reduced density matrix of the subsystem $A$, and $\rho = |\Psi\rangle \langle \Psi|$ is the density matrix of the whole system. The knowledge of $S_A^{(n)}$ as a function of $n$ identifies univocally the full spectrum of non-zero eigenvalues of $\rho_A$ [2], and provides complementary information about the entanglement to that obtained from the von Neumann entanglement.

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entropy $S_A^{(1)}$. Furthermore, the scaling of $S_A^{(n)}$ with the size of $A$ in the ground state of a one-dimensional system is more suited than $S_A^{(1)}$ for understanding whether a faithful representation of the state in terms of a matrix product state can be or cannot be obtained with polynomial resources in the length of the chain [3, 4].

For a one-dimensional critical system whose scaling limit is described by a conformal field theory (CFT), in the case when $A$ is an interval of length $\ell$ embedded in an infinite system, the asymptotic large $\ell$ behavior of the quantities determining the Rényi entropies is [5]–[8]

$$\text{Tr} \rho_A^n \simeq c_n \left( \frac{\ell}{a} \right)^{c(n-1)/6}, \quad \Rightarrow S_A^{(n)} \simeq \frac{c}{6} \left( 1 + \frac{1}{n} \right) \log \frac{\ell}{a} + c'_n,$$

where $c$ is the central charge of the underlying CFT and $a$ is the inverse of an ultraviolet cutoff (e.g. the lattice spacing). The prefactors $c_n$ (and so the additive constants $c'_n$) are non-universal constants (that however satisfy universal relations [9]).

The central charge is a ubiquitous and fundamental feature of a conformal field theory [10], but it does not always identify the universality class of the theory. A relevant class of relativistic massless quantum field theories is the $c = 1$ models, which describe many physical systems of experimental and theoretical interest. The one-dimensional Bose gas with repulsive interaction, the (anisotropic) Heisenberg spin chains, the Ashkin–Teller model and many others are all described (in their gapless phases) by $c = 1$ theories. These are all free bosonic field theories where the boson field satisfies different periodicity constraints, i.e. it is compactified on a specific target space. The two most notable examples are the compactification on a circle (corresponding to the Luttinger liquid field theory) and on a $Z_2$ orbifold (corresponding to the Ashkin–Teller model [11]–[13]). The critical exponents depend in a continuous way on the compactification radius of the bosonic field. A survey of the CFTs compactified on a circle or on a $Z_2$ orbifold is given in figure 1, in a standard representation [12,13]. The horizontal axis is the compactification radius on the circle $r_{\text{circle}}$, while the vertical axis represents the value of the $Z_2$ orbifold compactification radius $r_{\text{orb}}$. The two axes cross in a single point, meaning that the theories at $r_{\text{circle}} = \sqrt{2}$ and at $r_{\text{orb}} = 1/\sqrt{2}$ are the same. (The graph is not a Cartesian plot, i.e. it has no meaning to have one $r_{\text{circle}}$ and one $r_{\text{orb}}$ at the same time.) For some values of $r_{\text{circle}}$ and $r_{\text{orb}}$, we report statistical mechanical models and/or field theories to which they correspond. In the following we will consider the Ashkin–Teller model that on the self-dual line is described by $r_{\text{orb}} \in [\sqrt{2/3}, \sqrt{2}]$ and the XXZ spin chain in zero magnetic field that is described by $r_{\text{circle}} \in [0, 1/\sqrt{2}]$. We mention that different compactifications have been studied [14], but they correspond to more exotic statistical mechanical models and will not be considered here.

According to equations (2), the central charge of the CFT can be extracted from the scaling of both the Rényi and von Neumann entropies. In recent years, this idea has taken over from the previously available techniques of determining $c$, e.g. by measuring the finite-size corrections to the ground state energy of a spin chain [15]. However, the dependence of the scaling of the entropies of a single block on only the central charge prevents us from extracting from them other important parameters of the model such as the compactification radius. It has been shown that instead the entanglement entropies of disjoint intervals are sensitive to the full operator content of the CFT and in particular they depend on the compactification radius and on the symmetries of the target space.

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Figure 1. Survey of \( c = 1 \) theories corresponding to a free boson compactified on a circle (horizontal axis) and on an orbifold (vertical axis) as reported, e.g., in [12]. For some values of \( r_{\text{circle}} \) and \( r_{\text{orb}} \), the corresponding statistical mechanical models are reported. The XXZ spin chain in zero magnetic field lies on the horizontal axis in the interval \( r_{\text{circle}} \in [0, 1/\sqrt{2}] \). The self-dual line of the Ashkin–Teller model lies on the vertical axis in the interval \( r_{\text{orb}} \in [\sqrt{2}/3, \sqrt{2}] \).

Thus they encode information about the underlying conformal field theory of a given critical quantum/statistical system complementary to the knowledge of the central charge present in the scaling of the single block entropies. (Conversely, in 2D systems with conformal invariant wavefunctions, the entanglement entropy of a single region depends on the compactification radius [16].)

This observation boosted an intense theoretical activity aimed at determining Rényi entropies of disjoint intervals both analytically and numerically [17]–[30]. Part of this paper is dedicated to consolidating some of the results already provided in other works where they either have been studied only on very small chains, with the impossibility of properly taking into account the severe finite-size corrections [17] or have been tested in the specific cases of spin chains equivalent to free fermionic models [24, 26]. An important point to recall when dealing with more than one interval is that the Rényi entropies in equation (1) measure only the entanglement of the disjoint intervals with the rest of the system. They do not measure the entanglement of one interval with respect to the other; that instead requires the definition of more complicated quantities because \( A_1 \cup A_2 \) is in a mixed state (see, e.g., [31] for a discussion of this and examples). Furthermore, it must be mentioned that some results about the entanglement of two disjoint intervals are the main ingredient for a recent proposal to ‘measure’ the entanglement entropy [32].

1.1. Summary of some CFT results for the entanglement of two disjoint intervals

We consider the case of two disjoint intervals \( A = A_1 \cup A_2 = [u_1, v_1] \cup [u_2, v_2] \). By global conformal invariance, in the thermodynamic limit, \( \text{Tr} \rho^n_A \) can be written as

\[
\text{Tr} \rho^n_A = c_n^2 \frac{\left| u_1 - u_2 \right| \left| v_1 - v_2 \right|}{\left| u_1 - v_1 \right| \left| u_2 - v_2 \right| \left| v_1 - v_2 \right| \left| u_2 - v_1 \right|} \left( \frac{c}{6} \right)^{(n-1)/n} F_n(x),
\]

where

\[
F_n(x) = \frac{\Gamma \left( \frac{n+1}{n} \right) \Gamma \left( \frac{2n}{n} \right)}{n \Gamma \left( \frac{n+2}{n} \right) \Gamma \left( \frac{2n+1}{n} \right)}
\]

\[
= \frac{\Gamma \left( \frac{n+1}{n} \right)}{n \Gamma \left( \frac{n+2}{n} \right)}
\]

\[
= \frac{1}{n} \binom{2n-1}{n-1}.
\]

The central charge \( c \) is related to the scaling dimensions of the stress tensor.

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where \( x \) is the four-point ratio (for real \( u_j \) and \( v_j \), \( x \) is real)
\[
  x = \frac{(u_1 - v_1)(u_2 - v_2)}{(u_1 - u_2)(v_1 - v_2)}.
\]

The function \( F_n(x) \) is a universal function (after being normalized such that \( F_n(0) = 1 \)) that encodes all the information about the operator spectrum of the CFT and in particular about the compactification radius. \( c_n \) is the same non-universal constant appearing in equations (2).

Furukawa et al [17] calculated \( F_2(x) \) for a free boson compactified on a circle of radius \( \rho_{\text{circle}} \)
\[
  F_2(x) = \frac{\theta_3(\eta \tau) \theta_3(\tau / \eta)}{[\theta_3(\tau)]^2},
\]
where \( \theta_\nu \) are Jacobi theta functions and the (pure-imaginary) \( \tau \) is given by
\[
  x = \left[ \frac{\theta_2(\tau)}{\theta_3(\tau)} \right]^4, \quad \tau(x) = i \frac{2F_1(1/2, 1/2; 1; 1 - x)}{2F_1(1/2, 1/2; 1; x)}.
\]
\( \eta \) is a universal critical exponent related to the compactification radius \( \eta = 2\rho_{\text{circle}}^2 \). This has been extended to general integers \( n \geq 2 \) in [19]
\[
  F_n(x) = \frac{\Theta(0|\eta \Gamma) \Theta(0|\Gamma/\eta)}{[\Theta(0|\Gamma)]^2},
\]
where \( \Gamma \) is an \((n - 1) \times (n - 1)\) matrix with elements [19]
\[
  \Gamma_{rs} = \frac{2\eta}{n} \sum_{k=1}^{n-1} \sin \left( \frac{\pi k}{n} \right) \beta_{k/n} \cos \left( \frac{2\pi k}{n} (r - s) \right),
\]
and
\[
  \beta_y = \frac{2F_1(y, 1 - y; 1; 1 - x)}{2F_1(y, 1 - y; 1; x)}.
\]
\( \eta \) is the same as above, while \( \Theta \) is the Riemann–Siegel theta function
\[
  \Theta(0|\Gamma) = \sum_{m \in \mathbb{Z}^{n-1}} \exp [i \pi m^t \cdot \Gamma \cdot m] .
\]

The analytic continuation of equation (7) to real \( n \) for general values of \( \eta \) and \( x \) (to obtain the von Neumann entanglement entropy) is still an open problem, but results for \( x \ll 1 \) and \( \eta \ll 1 \) are analytically known [19, 30].

The function \( F_n(x) \) is known exactly for arbitrary integral \( n \) also for the critical Ising field theory [30]. However, in the following we will need it only at \( n = 2 \) (i.e. \( F_2(x) \)) for which it assumes the simple form [24]
\[
  F_2^{\text{Is}}(x) = \frac{1}{\sqrt{2}} \left[ \left( \frac{(1 + \sqrt{x})(1 + \sqrt{1 - x})}{2} \right)^{1/2} + x^{1/4} + ((1 - x)x)^{1/4} + (1 - x)^{1/4} \right]^{1/2} .
\]

\( ^5 \) Because of the symmetry \( \eta \rightarrow 1/\eta \) or \( \rho_{\text{circle}} \rightarrow 1/2\rho_{\text{circle}} \) for any conformal property one could also define \( \eta = 1/2\rho_{\text{circle}}^2 \) as sometimes done in the literature. However, corrections to the scaling are not symmetric in \( \eta \rightarrow 1/\eta \) and this is often a source of confusion. A lot of care should be used when referring to one or another notation.
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In [30], it has been proved that in any CFT the function $F_n(x)$ admits the small $x$ expansion

$$F_n(x) = 1 + \left(\frac{x}{4n^2}\right)^\alpha s_2(n) + \left(\frac{x}{4n^2}\right)^{2\alpha} s_4(n) + \cdots,$$

where $\alpha$ is the lowest scaling dimension of the theory. The functions $s_j(n)$ are calculable from a modification of the short-distance expansion [30], and in particular it has been found that [30]

$$s_2(n) = \mathcal{N} \frac{n}{2} \sum_{j=1}^{n-1} \frac{1}{|\sin(\pi(j/n))|} 2^{\alpha},$$

where the integer $\mathcal{N}$ counts the number of inequivalent correlation functions giving the same contribution. This expansion has been tested against the exact results for the free compactified boson (Ising model) with $\alpha = \min[\eta, 1/\eta]$ ($\alpha = 1/4$) and $\mathcal{N} = 2$ ($\mathcal{N} = 1$).

All the results we have reported so far are valid for an infinite system. Numerical simulations are instead performed for finite, but large, system sizes. According to CFT [8], we obtain the correct result for a chain of finite length $L$ by replacing all distances $u_{ij}$ with the chord distance $L/\pi \sin(\pi u_{ij}/L)$ (but different finite-size forms exist for excited states [33]). In particular the single interval entanglement is [6]

$$\text{Tr } \rho_A^n \simeq c_n \left[ \frac{L}{\pi a} \sin \left( \frac{\pi \ell}{L} \right) \right]^{-c(n-1/n)/6},$$

and for two intervals, in the case where the two subsystems $A_1$ and $A_2$ have the same length $\ell$ and are placed at distance $r$, the four-point ratio $x$ is

$$x = \left( \frac{\sin \pi \ell/L}{\sin \pi (\ell + r)/L} \right)^2.$$

1.2. Organization of the paper

In this paper we provide accurate numerical tests for the functions $F_n(x)$ in truly interacting lattice models described by a CFT with $c = 1$. In section 2 we derive the CFT prediction for the function $F_2(x)$ of a free boson compactified on an orbifold describing, among other things, the self-dual line of the AT model when $r_{orb} \in [\sqrt{2/3}, \sqrt{2}]$. In order to check this result, we needed to develop a classical Monte Carlo algorithm in section 3 based on the ideas introduced in [18]. This algorithm is used in section 4 to determine $F_2(x)$ for several points on the self-dual line. We also consider the XXZ spin chain in zero magnetic field to test the correctness of equation (7). In order to extend the results of [17] to longer chains, we have used a tree tensor network algorithm that has allowed us to study chains of length up to $L = 128$ with periodic boundary conditions. In this way, we have been able to perform a detailed finite-size analysis that was difficult solely with the data from exact diagonalization reported in [17]. The analysis also shows that only through the knowledge of the unusual corrections to the leading scaling behavior [34]–[38], [26] are we able to perform a quantitative test of equation (7). The tree tensor network algorithm is described in section 5, while the numerical results are presented in section 6. The various sections are independent of each other, so that readers interested only in some of the results should have easy access to them without reading the whole paper.

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2. $n = 2$ Rényi entanglement entropy for two intervals in the Ashkin–Teller model

In a quantum field theory $\text{Tr} \rho_A^n$ for integer $n$ is proportional to the partition function on an $n$-sheeted Riemann surface with branch cuts along the subsystem $A$, i.e. $\text{Tr} \rho_A^n = Z_n(A)/Z_1^n$ where $Z_n(A)$ is the partition function of the field theory on a conifold where $n$ copies of the manifold $\mathcal{R} = \text{system} \times R^1$ are coupled along branch cuts along each connected piece of $A$ at a time-slice $t = 0$ [8, 39]. Specializing to CFT, for a single interval on the infinite line, this equivalence leads to equations (2) [6], whose analytic continuation to non-integer $n$ is straightforward. When the subsystem $A$ consists of $N$ disjoint intervals (always in an infinite system), the $n$-sheeted Riemann surface $\mathcal{R}_{n,N}$ has genus $(n - 1)(N - 1)$ and cannot be mapped to the complex plane so that the CFT calculations become more complicated.

However, for two intervals ($N = 2$), when for a given theory the partition function on a generic Riemann surface of genus $g$ with arbitrary period matrix is known, $\text{Tr} \rho_A^n$ can be easily deduced exploiting the results of [19, 30]. In fact, a by-product of the calculation for the free boson [19] is that the $(n - 1) \times (n - 1)$ period matrix is always given by equation (8). Although derived for a free boson, the period matrix is a pure geometrical object and it is only related to the structure of the world-sheet $\mathcal{R}_{n,2}$, and so it is the same for any theory. This property has been used in [30] to obtain $F_n(x)$ for the Ising universality class for any $n$, in agreement with previously known numerical results [26]. When also $n = 2$, the surface $\mathcal{R}_{2,2}$ is topologically equivalent to a torus for which the partition function is known for most of the CFT. The torus modular parameter $\tau$ is related to the four-point ratio by equation (6). Thus, the function $F_2(x)$ is proportional to the torus partition function where $\tau$ is given by equation (6) and with the proportionality constant fixed by requiring $F_2(0) = 1$. This way of calculating $S_A^{(2)}$ is much easier than the general one for $S_A^{(n)}$ [40, 19] and indeed it has been used to obtain the first results both for the free compactified boson [17] and for the Ising model [24].

For a conformal free bosonic theory with action

$$S = \frac{1}{2\pi} \int d\zeta d\bar{\zeta} \partial \phi \bar{\partial} \bar{\phi},$$

(16)
the torus partition functions are known exactly for both circle and orbifold compactification [41, 42, 12].

We now recall some well-known facts in order to fix the notations and derive the function $F_2(x)$ for the Ashkin–Teller model. The bosonic field $\phi$ is said to be compactified on a circle of radius $r_{\text{circle}}$ when $\phi = \phi + 2\pi r_{\text{circle}}$. The torus partition function (and the one on the $n$-sheeted Riemann surface) should be derived with this constraint. It is a standard CFT exercise to calculate the resulting torus partition function [41, 12]

$$Z_{\text{circle}}(\eta) = \frac{\theta_3(\eta \tau) \theta_3(\tau / \eta)}{[\eta_0(\tau)]^2},$$

(17)
where $\eta_0(\tau)$ is the Dedekind eta function and $\eta = 2 \tau_{\text{circle}}^2$. Using equation (6) and some properties of the elliptic functions, equation (5) for $F_2(x)$ follows [17]. When specialized at $\eta = 1/2$ (or $\eta = 2$), $F_2(x)$ has the simple form

$$F_2^{XX}(x) = \sqrt{(1 + x^{1/2})(1 + (1 - x)^{1/2})/2},$$

(18)
that describes the \( XX \) spin chain (that is equivalent to free fermions via the non-local Jordan–Wigner transformation).

The concept of orbifold emerges naturally in the context of theories whose Hilbert space admits some discrete symmetries. Let us assume that \( G \) is a discrete symmetry. For the free bosonic theory, the simplest example is the one we are interested in, i.e. the \( \mathbb{Z}_2 \) symmetry. It acts on the point of the circle \( S^1 \) in the following way:

\[
g : \phi \rightarrow -\phi.
\]

For the partition function of a theory on the torus, we introduce the notation \[12\]

\[
\pm \begin{array}{c}
\vspace{1cm}
\end{array}
\]

(20)

where the \( \pm \) denotes the boundary conditions on the two directions on the torus. The full partition function, given a finite discrete group \( G \), is

\[
Z_{T/G} = \frac{1}{|G|} \sum_{g, h \in G} g \begin{array}{c}
\vspace{1cm}
\end{array} h
\]

(21)

where \( |G| \) denotes the number of elements in the group. The generalization to higher genus Riemann surfaces is straightforward (but it is not so easy to obtain results, see e.g. \[13, 43\]).

Now we specialize equation (21) to the case of the \( \mathbb{Z}_2 \) symmetry. Since the action (16) is invariant under \( g : \phi \rightarrow -\phi \), we have the torus partition function for the free boson on the orbifold \[41, 42, 12\]

\[
Z_{\text{orb}} = \frac{1}{2} \left( + \begin{array}{c}
\vspace{1cm}
\end{array} + \begin{array}{c}
\vspace{1cm}
\end{array} + \begin{array}{c}
\vspace{1cm}
\end{array} + \begin{array}{c}
\vspace{1cm}
\end{array} + \begin{array}{c}
\vspace{1cm}
\end{array} \right).
\]

(22)

Standard CFT calculations lead to the result \[12\]

\[
Z_{\text{orb}}(\eta) = \frac{1}{2} \left( Z_{\text{circle}}(\eta) + \left| \frac{\theta_3\theta_1}{\eta_D\eta_D} \right| + \left| \frac{\theta_3\theta_3}{\eta_D\eta_D} \right| + \left| \frac{\theta_2\theta_1}{\eta_D\eta_D} \right| \right),
\]

(23)

where all the \( \tau \) arguments in \( \theta \) and \( \eta_D \) are understood. At the special point \( \eta = 1/2 \) (or \( \eta = 2 \)) we get

\[
Z_{\text{orb}}(\eta = 1/2) = \frac{1}{2} \left( \frac{\left| \theta_3 \right|^2 + \left| \theta_1 \right|^2 + \left| \theta_2 \right|^2}{2|\eta_D|^2} + \frac{\left| \theta_3 \theta_1 \right|}{\eta_D\eta_D} + \frac{\left| \theta_3 \theta_3 \right|}{\eta_D\eta_D} + \frac{\left| \theta_2 \theta_1 \right|}{\eta_D\eta_D} \right) = Z^2_{\text{Ising}}.
\]

(24)

Thus, from the orbifold partition function, using the last identity and normalizing such that \( F_2^{\text{AT}}(0) = 1 \), we can write the function \( F_2^{\text{AT}}(x) \) as

\[
F_2^{\text{AT}}(x) = \frac{1}{2}(F_2(x) - F_2^{XX}(x)) + (F_2^{\text{Is}}(x))^2,
\]

(25)

where \( F_2(x) \) is given in equation (5), \( F_2^{XX}(x) \) is the same at \( \eta = 1/2 \) (cf equation (18)) and \( F_2^{\text{Is}}(x) \) is the result for the Ising model (cf equation (11)). As a consequence of the \( \eta \leftrightarrow 1/\eta \) symmetry of \( F_2(x) \), also \( F_2^{\text{AT}}(x) \) displays the same invariance. For small \( x \), recalling that \( F_2(x) - 1 \sim x^{\min[\eta, \eta^{-1}]} \), \( F_2^{XX} - 1 \sim x^{1/2} \) and \( F_2^{\text{Is}} - 1 \sim x^{1/4} \), we have

\[
F_2^{\text{AT}}(x) - 1 \sim \begin{cases} 
x^{1/4} & \text{for } \eta \geq 1/4, \\
 x^{\min[\eta, \eta^{-1}]} & \text{for } \eta \leq 1/4.
\end{cases}
\]

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Figure 2. $F_2(x)$ for the Ashkin–Teller model on the self-dual line for some values of $\eta$. Inset: $F_2(x) - 1$ in log-log scale to highlight the small $x$ behavior. The black dashed line is $\sim x^{1/4}$.

The critical Ashkin–Teller model lies in the interval $\sqrt{2}/3 < r_{\text{orb}} < \sqrt{2}$ and so $4/3 < \eta = 2r_{\text{orb}}^2 < 4$. Thus we have $F_{2\text{AT}}^2(x) - 1 \sim x^{1/4}$ along the whole self-dual line. $F_{2\text{AT}}^2(x)$ for various values of $\eta$ in the allowed range is reported in figure 2, where the behavior for small $x$ is highlighted in the inset to show the constant $1/4$ exponent.

3. The classical Ashkin–Teller model and the Monte Carlo simulation

The two-dimensional Ashkin–Teller (AT) model on a square lattice is defined by the Hamiltonian

$$H = J \sum_{\langle ij \rangle} \sigma_i \sigma_j + J' \sum_{\langle ij \rangle} \tau_i \tau_j + K \sum_{\langle ij \rangle} \sigma_i \sigma_j \tau_i \tau_j,$$

(27)

where $\sigma_i$ and $\tau_i$ are classical Ising variables (i.e. can assume only the values $\pm 1$). Also the product $\sigma \tau$ can be considered as an Ising variable. The model has a rich phase diagram whose features are reported in full detail in Baxter’s book [45]. We review in the following only the main features of this phase diagram. Under any permutation of the variables $\sigma, \tau, \sigma \tau$ the AT model is mapped onto itself. At the level of the coupling constants, this implies that the model is invariant under any permutation of $J, J', K$. For $K = 0$, the AT model corresponds to two decoupled Ising models in $\sigma$ and $\tau$ variables. For $K \to \infty$ it reduces to a single Ising model with coupling constant $J + J'$. For $J = J' = K$ it corresponds to the four-state Potts model. It is useful to restrict to the symmetric Ashkin–Teller model where $J = J'$

$$H = J \sum_{\langle ij \rangle} (\sigma_i \sigma_j + \tau_i \tau_j) + K \sum_{\langle ij \rangle} \sigma_i \sigma_j \tau_i \tau_j.$$

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Figure 3. Phase diagram of the 2D symmetric Ashkin–Teller model defined by the Hamiltonian (28). The red ABC line is the self-dual line. The point B at $K = 0$ corresponds to two uncoupled Ising models. The point C is the critical four-state Potts model at $K = J = (\log 3)/4$. At $J = 0$ there are two critical Ising points at $K = \pm (\log(1+\sqrt{2}))/2$, one (Is) ferromagnetic and the other (AFIs) antiferromagnetic. For $K \to \infty$ there is another critical Ising point at $J = (\log(1+\sqrt{2}))/2$. All continuous lines are critical. The blue lines C–Is and the one starting at AFIs are in the Ising universality class. The red line is critical with continuously varying critical exponents. The region denoted by I corresponds to a ferromagnetic phase for all the variables. In the region II, $\sigma$, $\tau$, and $\sigma \tau$ are paramagnetic. In the region III only $\sigma \tau$ is ferromagnetic and in region IV $\sigma \tau$ exhibits antiferromagnetic order while $\sigma$ and $\tau$ are paramagnetic.

The full phase diagram is reported in figure 3 (in units of the inverse temperature $\beta = 1$). The model corresponds to two decoupled critical Ising models at $K = 0$ and $2J = \log(1+\sqrt{2})$. For $J = 0$ it is equivalent to a critical Ising model in the variable $\sigma \tau$ with critical points at $2K_{\pm} = \pm \log(1+\sqrt{2})$. For $K \to \infty$ there are two critical Ising points at $2J = \pm \log(1+\sqrt{2})$. On the diagonal $J = K$ the system corresponds to a four-state Potts model which is critical at $K = (\log 3)/4$. The different kinds of order appearing in the phase diagram are explained in the caption to figure 3. All the continuous lines in figure 3 are critical lines. The blue lines C–Is are in the Ising universality class. The line starting from AFIs belongs to the antiferromagnetic Ising universality class. On the red line ABC the system is critical and the critical exponents vary continuously [46, 45].

The AT model on a planar graph can be mapped to another AT model on the dual graph. When specialized to the square lattice, the phase diagram is equivalent to its dual on the self-dual line:

$$e^{-2K} = \sinh(2J).$$

On this line, the symmetric AT model maps onto a homogeneous six-vertex model which is exactly solvable [45]. It follows that on the self-dual line the model is critical for

\cite{doi:10.1088/1742-5468/2011/06/P06012}
$K \leq (\log 3)/4$ and its critical behavior is described by a CFT with $c = 1$. Along the self-dual line the critical exponents vary continuously and are exactly known. For later convenience it is useful to parametrize the self-dual line by a new parameter $\Delta$:

$$e^{4J} = \frac{\sqrt{2 - 2\Delta} + 1}{\sqrt{2 - 2\Delta} - 1}, \quad e^{4K} = 1 - 2\Delta,$$

with $-1 < \Delta < 1/2$. In terms of $\Delta$, the orbifold compactification radius is [42]

$$\eta = 2\nu^2 = \frac{4 \arccos(-\Delta)}{\pi} = \frac{2}{K_L},$$

where $K_L$ is the equivalent of the Luttinger liquid parameter for the AT model.

### 3.1. Cluster representation and Monte Carlo simulation

A Swendsen–Wang-type cluster algorithm for the AT model has been proposed in [47] and then re-derived in a simpler way by Salas and Sokal [48]. Here we partly follow the derivation of Salas and Sokal and we restrict ourselves to the symmetric AT Hamiltonian (28) and assume $J \geq |K|$. Using the identities for Ising-type variables

$$\delta_{i,j} = 2\delta_{\sigma_i, \sigma_j} - 1, \quad \tau_{i,j} = 2\tau_{\tau_i, \tau_j} - 1,$$

we can rewrite equation (28) as

$$-H = J \sum_{\langle ij \rangle} (2\delta_{\sigma_i, \sigma_j} + 2\delta_{\tau_i, \tau_j} - 2) + K \sum_{\langle ij \rangle} (2\delta_{\sigma_i, \sigma_j} - 1)(2\delta_{\tau_i, \tau_j} - 1).$$

For convenience we shift the interaction (28) by $-4J$. In order to write the Boltzmann weight associated to a specific configuration we use $\exp(w\delta_{\sigma_i, \sigma_j}) = (\exp(w) - 1)\delta_{\sigma_i, \sigma_j} + 1$ and the analogous identity for the $\tau$ variables. The Boltzmann weight of a given link $\langle ij \rangle$ is then

$$W_{\langle ij \rangle}(\sigma_i, \sigma_j, \tau_i, \tau_j) = e^{-4J}[e^{-2(J+K)} - e^{-4J}]\delta_{\sigma_i, \sigma_j} + \delta_{\tau_i, \tau_j} + [1 - 2e^{-2(J+K)} + e^{-4J}]\delta_{\sigma_i, \sigma_j}\delta_{\tau_i, \tau_j}.$$ (34)

The key idea for the Swendsen–Wang algorithm is to introduce two new auxiliary Ising-type variables $m_{ij}$ and $n_{ij}$ living on the link $\langle ij \rangle$. We redefine the Boltzmann weight on the link $\langle ij \rangle$ as [48]

$$W_{\langle ij \rangle}(\sigma_i, \sigma_j, \tau_i, \tau_j, m_{ij}, n_{ij}) = e^{-4J}\delta_{m_{ij},0}\delta_{n_{ij},0} + e^{-2(J+K)} - e^{-4J}]\delta_{\sigma_i, \sigma_j}\delta_{m_{ij},1}\delta_{n_{ij},0} + \delta_{\tau_i, \tau_j}\delta_{m_{ij},0}\delta_{n_{ij},1} + [1 - 2e^{-2(J+K)} + e^{-4J}]\delta_{\sigma_i, \sigma_j}\delta_{\tau_i, \tau_j}\delta_{m_{ij},1}\delta_{n_{ij},1}.$$ (35)

Summing over $m_{ij}$ and $n_{ij}$ we obtain the weight in equation (34). Equation (35) has a graphical interpretation in terms of clusters. In fact we can divide the links of the lattice into ‘activated’ (if $m_{ij} = 1$) or ‘inactive’ (if $m_{ij} = 0$). The same considerations hold for the $n_{ij}$ variables. Therefore, each link of the lattice can be activated by setting $m_{ij} = 1$ or $n_{ij} = 1$. The active links connect different lattice sites forming clusters. There are clusters referring to the $\sigma$ variables (called $\sigma$-clusters) and to the $\tau$ variables ($\tau$-clusters). Isolated
lattice sites are clusters as well. Obviously, the lattice sites belonging to the $\sigma$-clusters ($\tau$-clusters) have the same value of $\sigma$ ($\tau$). The partition function of the extended model defined by the weight (35) can be written as

$$Z = \sum_{\sigma,\tau=\pm 1} \sum_{m,n=\pm 1} \prod_{\langle ij \rangle} \mathcal{W}_{\langle ij \rangle}(\sigma_i, \sigma_j, \tau_i, \tau_j, m_{ij}, n_{ij}).$$  

We now proceed to the following definitions. We divide all the links into three classes: we define $l_0$ as the total number of inactivated links and $l_1$ as the total number of links connecting sites which belong only to one type of cluster, either a $\sigma$-cluster or a $\tau$-cluster. We define $l_2$ as the total number of links on which $m$ and $n$ are both equal to 1. Furthermore we introduce the quantities

$$B_0 \equiv e^{-4J},$$  

$$B_1 \equiv [e^{-2(J+K)} - e^{-4J}],$$  

$$B_2 \equiv [1 - 2e^{-2(J+K)} + e^{-4J}].$$  

The following step is to perform the summation over $\sigma, \tau$ in equation (35). This is readily done, obtaining the final expression for the partition function

$$Z = \sum_{C(\tau,\sigma)} B_0^0 B_1^1 B_2^2 2^{C^\sigma + C^\tau},$$  

where we denoted by $C^\sigma$ the number of $\sigma$-clusters and by $C^\tau$ the total number of $\tau$-clusters. In the counting of $\tau$-clusters ($\sigma$-clusters) we included all the lattice sites connected by a link on which $m_{ij} = 1$ ($n_{ij} = 1$). Isolated sites (with respect to $m$ or $n$ or both) count as single clusters. The links where $m_{ij} = 1$ and $n_{ij} = 1$ contribute to both types of clusters. An example of a cluster configuration for a $12 \times 12$ lattice is reported in figure 4.

Figure 4. A typical cluster configuration on a $12 \times 12$ lattice. The green lines are $\sigma$-clusters and the red dashed lines are $\tau$-clusters. The links in blue are double links. Periodic boundary conditions on both directions are used.
3.2. Swendsen–Wang algorithm (the direct and embedded algorithms)

We are now in a position to write the Swendsen–Wang algorithm for the symmetric AT model. The Monte Carlo procedure can be divided into two steps. In the first one, given a configuration for \((\sigma, \tau)\) variables, we construct a configuration of the \((m, n)\) variables. In the second step we update the \((\sigma, \tau)\) variables at given \((m, n)\). The details of step one are

- if \(\sigma_i = \sigma_j\) and \(\tau_i = \tau_j\), we choose \((m_{ij}, n_{ij})\) with the following probabilities:
  * \((m_{ij}, n_{ij}) = (1, 1)\) with \(p_1 = 1 - 2e^{-2(J+K)} + e^{-4J}\),
  * \((m_{ij}, n_{ij}) = (1, 0)\) with \(p_2 = e^{-2(J+K)} + e^{-4J}\),
  * \((m_{ij}, n_{ij}) = (0, 1)\) with \(p_2 = e^{-2(J+K)} + e^{-4J}\),
  * \((m_{ij}, n_{ij}) = (0, 0)\) with \(p_3 = 1 - p_1 - 2p_2\);
- if \(\sigma_i = \sigma_j\) and \(\tau_i = -\tau_j\), the probabilities are
  * \((m_{ij}, n_{ij}) = (1, 0)\) with \(p_1 = 1 - e^{-2(J-K)}\),
  * \((m_{ij}, n_{ij}) = (0, 0)\) with \(p_2 = 1 - p_1\);
- if \(\sigma_i = -\sigma_j\) and \(\tau_i = \tau_j\), the probabilities are
  * \((m_{ij}, n_{ij}) = (1, 0)\) with \(p_1 = 1 - e^{-2(J-K)}\),
  * \((m_{ij}, n_{ij}) = (0, 0)\) with \(p_2 = 1 - p_1\);
- if \(\sigma_i = -\sigma_j\) and \(\tau_i = -\tau_j\) we choose \((m_{ij}, n_{ij}) = (0, 0)\) with probability 1.

In step two, given the configuration of \((m, n)\) generated using the rules above we build the connected \(\sigma\)-clusters and \(\tau\)-clusters. The values of \(\sigma\) (\(\tau\)) spins are required to be equal within each \(\sigma\)-cluster (\(\tau\)-cluster). We choose the spin value in each cluster randomly and independently of the value assumed on the other clusters. This completes the update scheme. (Note a typo in [48]: the minus sign in steps 2 and 3 of the update is missing.)

In [48] also the so called embedded version of the cluster algorithm is introduced. Its implementation is slightly easier compared to the direct algorithm. In the embedded algorithm, instead of treating both \(\sigma\) and \(\tau\) at the same time, one deals with only one variable per time. Let us consider the Boltzmann weight of a link \((ij)\) at fixed configuration of \(\tau\)

\[
\mathcal{W}_{(ij)}(\sigma_i, \sigma_j, \tau_i, \tau_j) = e^{-2(J+K\tau_i\tau_j)} + (1 - e^{-2(J+K\tau_i\tau_j)})\delta_{\sigma_i, \sigma_j}.
\]

The model defined by this weight can be simulated with a standard Swendsen–Wang algorithm for the Ising model using the effective coupling constant

\[
J_{ij}^{\text{eff}} = J + K\tau_i\tau_j.
\]

This is no longer translation invariant, but this does not affect the effectiveness of the cluster algorithm for the Ising model as long as \(J_{ij}^{\text{eff}} \geq 0\). The same reasoning applies to the case of fixed \(\sigma\). Thus, the embedded algorithm is made of two steps.

- For a given configuration of \(\tau\) variables, we apply a standard Swendsen–Wang algorithm to \(\sigma\) spins. The probability arising in the update step is \(p_{ij} = 1 - e^{-2(J+K\tau_i\tau_j)}\).
For a given configuration of $\sigma$ variables, we update $\tau$ with the same algorithm and probability $p_{ij} = 1 - e^{-2(J+K)\sigma_i\sigma_j}$.

Direct and embedded algorithms are both extremely effective procedures to sample the AT configurations. However, very importantly for the following, equation (40) for the partition function does not hold anymore for an $n$-sheeted Riemann surface and we do not know whether it is possible to write the embedded algorithm for this case.

3.3. Rényi entanglement entropies via Monte Carlo simulation of a classical system.

In this section we summarize the method introduced by Caraglio and Gliozzi [18] to obtain the Rényi entropies via simulations of classical systems and we generalize it to the AT model. The partition function $Z = \text{Tr} e^{-\beta H}$ of a $d$-dimensional quantum system at inverse temperature $\beta$ can be written as a Euclidean path integral in $d + 1$ dimensions [8]. Thus for the $n$th power of the partition function one has

$$Z^n = \int \prod_{k=1}^{n} D[\phi_k] e^{-\sum_{k=1}^{n} S(\phi_k)}, \quad (43)$$

where $\phi_k \equiv \phi_k(\vec{x}, \tau)$ is a field living on the $k$th replica of the system and $S(\phi_k)$ is the Euclidean action ($\tau$ is the imaginary time). The actual form of the action is not important, but for the sake of simplicity we restrict ourselves to the case of nearest-neighbor interactions

$$S(\phi_k) = \sum_{\langle ij \rangle} F(\phi_k(i), \phi_k(j)), \quad (44)$$

and the function $F$ is arbitrary. We recall that $\text{Tr} \rho_A^n$ can be obtained by considering the Euclidean partition function over an $n$-sheeted Riemann surface with branch cuts along the subsystem $A$ [8]. (This equivalence is also the basis of all quantum Monte Carlo methods to simulate the block entanglement in any dimension [49].) Caraglio and Gliozzi constructed this $n$-sheeted Riemann surface for the lattice model in the following way. Let us consider a square lattice (for simplicity) and take the two points of its dual lattice surrounding $A$ (that in $1 + 1$ dimension is just an interval with two endpoints). The straight line joining them defines the cut that we call $\lambda$. The length of $\lambda$ is equal to the length of $A$. Let us consider $n$ independent copies of this lattice with a cut. The $n$-sheeted Riemann lattice is defined by assuming that all the links of the $k$th replica intersecting the cut connect with the next replica $k + 1(\text{mod } n)$. To get the partition function over the $n$-sheeted Riemann surface we define the corresponding coupled action

$$S^n(\phi_k) = \sum_{k=1}^{n} \sum_{\langle ij \rangle \notin \lambda} F(\phi_k(i), \phi_k(j)) + \sum_{\langle ij \rangle \in \lambda} F(\phi_k(i), \phi_{k+1(\text{mod } n)}(j)). \quad (45)$$

This definition can be used in any dimension, even though we will use here only $d = 2$. Finally, calling $Z_n(A)$ the partition function over the action (45), $\text{Tr} \rho_A^n$ is given by

$$\text{Tr} \rho_A^n = Z_n(A) \frac{Z^n}{Z^n}. \quad (46)$$

\[ \text{doi:10.1088/1742-5468/2011/06/P06012} \]
Following [18] we introduce the observable
\[ O \equiv e^{-S^n(\phi_1, \phi_2, \ldots, \phi_n; \lambda)} + \sum_{k=1}^n S(\phi_k; \lambda) , \tag{47} \]
where \( S^n \) and \( S \) are the Euclidean actions of the model defined on the \( n \)-sheeted lattice and on the \( n \) independent lattices respectively. The sum is restricted to links crossing the cut, as the presence of \( \lambda \) in the arguments stresses. It then follows that
\[ \langle O \rangle_n \equiv \frac{Z_n(A)}{Z^n} = \text{Tr} \rho^n_A , \tag{48} \]
where \( \langle \cdot \rangle_n \) stands for the average taken on the uncoupled action \( \sum_{k=1}^n S(\phi_k) \).

We can now discuss our improvement to the procedure highlighted so far. The practical implementation of equation (47) to calculate \( \text{Tr} \rho^n_A \) is plagued by severe limitations: analyzing the Monte Carlo evolution of the observable, one notices that it shows a huge variance because it is defined by an exponential. Direct application of equation (47) is possible then only for small lengths of the subsystem \( A \). In order to overcome this problem, let us consider the quantity \( Z_n(A)/Z^n \) and imagine dividing the subsystem into \( L \) parts to have \( A = A_1 \cup A_2 \cdots \cup A_L \), with the lengths of the various parts being arbitrary. Moreover we define a set of subsystems \( \hat{A}_i \equiv \cup_{k=1}^i A_i \). Then it holds that
\[ \frac{Z_n(A)}{Z^n} = \prod_{i=0}^L \frac{Z_n(\hat{A}_{i+1})}{Z_n(\hat{A}_i)} . \tag{49} \]
Equation (49) is very useful because each term in the product can be simulated effectively using a modified version of (47) if we choose the length of \( A_i \) to be small enough. In fact, by definition, we have
\[ \langle O(\hat{A}_i) \rangle_{\mathcal{R}_n(\hat{A}_i)} \equiv \frac{Z_n(\hat{A}_{i+1})}{Z_n(\hat{A}_i)} , \tag{50} \]
where \( O(\hat{A}_i) \) is the modified observable
\[ O(\hat{A}_i) \equiv \exp(-S^n(\hat{A}_{i+1}) + S^n(\hat{A}_i)) . \tag{51} \]
We stress that in equation (50) the expectation value in the l.h.s. must be taken on the coupled action on the Riemann surface with cut \( \hat{A}_i \). The disadvantage of equation (49) is that, to simulate large subsystems, one has to perform \( L \) independent simulations and then build the observable taking the product of the results. If the dimension of each piece \( A_i \) is small this task requires a large computational effort. Another important aspect is the estimation of the Monte Carlo error: if each term in (49) is obtained independently, the error in the product is
\[ \frac{\sigma(O)}{O} = \sqrt{\sum_{i=0}^L \frac{\sigma^2(O(\hat{A}_i))}{O(\hat{A}_i)^2}} . \tag{52} \]
If the lengths of the intervals \( A_i \) are all equal, then the single terms of the summation in equation (52) do not change much and the total error should scale as \( \sqrt{L} \).

Caraglio and Gliozzi [18] used another strategy to circumvent the problem with the observable in equation (47). The trick was to consider the Fortuin–Kasteleyn cluster

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expansion of the partition function of the Ising model. The analog for the AT model was reported in section 2:

\[ Z = \sum_{C(\sigma, \tau)} B_0 B_1 B_2 2^{C_\sigma + C_\tau}, \]  

(53)

where \( C_\sigma, C_\tau \) are the \( \sigma/\tau \)-cluster configurations. Going from \( n \) independent sheets to the \( n \)-sheeted lattice, the type of links and their total number do not change, but the number of clusters does change, and so we get the cluster expression of observable (47) for the AT model

\[ \mathcal{O}(\hat{A}_i) = 2^{C_\sigma(\hat{A}_{i+1}) + C_\tau(\hat{A}_{i+1}) - C_\sigma(\hat{A}_i) - C_\tau(\hat{A}_i)}, \]  

(54)

where \( C_\sigma(\hat{A}_i) \) \( (C_\tau(\hat{A}_i)) \) denotes the total number of \( \sigma \)-clusters \( (\tau \)-clusters) on the Riemann surface with cut \( \hat{A}_i \). Since the clusters are non-local objects, they represent ‘improved’ observables and the variance for the Monte Carlo history of equation (54) is much smaller than in the naive implementation.

### 4. The entanglement entropy in the Ashkin–Teller model

#### 4.1. The single interval

We first present the results for the Ashkin–Teller model for a single interval. Although these results do not provide any new information about the model, they are fundamental checks of the effectiveness of the Monte Carlo algorithms. We performed simulations using both algorithms described in section 2: the direct cluster algorithm and the embedded one. When using the direct algorithm, measures are performed using the observable (54), while for the embedded algorithm we used the observable in equation (47). In figure 5 we report the results of the simulations of \( \text{Tr} \rho_A^2 \) for the SUSY model \( (r_{\text{orb}} = \sqrt{3}/2 \) in figure 1) and for the \( Z_4 \) parafermions \( (r_{\text{orb}} = \sqrt{3}/2) \), both for \( L = 120 \). The orange and green points are obtained using the embedded algorithm. To check the implementation of the cluster observable, we report at \( \ell = 10 \) the data obtained using the direct algorithm and equation (54). The perfect agreement between the two results confirms the correctness of both implementations. Note that \( \text{Tr} \rho_A^2 \) is a monotonic function of \( \ell \), in contrast with the parity effects found for the \( XXZ \) spin chain [34,35] that also corresponds to a vertex model [45]. In the inset we show the behavior of the statistical error of the observable (47) in the SUSY case as a function of the subsystem length \( \ell \). It agrees with the prediction in equation (52) and its absolute value is extremely small, smaller than the size of the points in the main plot of figure 5. Analogous results have been obtained for all the critical points on the self-dual line using both algorithms.

The results for \( \text{Tr} \rho_A^2 \) in a finite system are asymptotically described by the CFT prediction (14) with \( n = 2 \) and \( c = 1 \). It is then natural to compute the ratio

\[ c_2(L_c) = \frac{\text{Tr} \rho_A^2}{((L/\pi) \sin((\pi/L)\ell))^{-1/4}}, \]  

(55)

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Figure 5. $\text{Tr} \rho_A^2$ for a single interval of length $\ell$ in a finite system of length $L = 120$. The data have been obtained by Monte Carlo simulations using the embedded algorithm. The orange points correspond to the SUSY model and the green ones to the $Z_4$ parafermions. The black crosses at $\ell = 10$ are data obtained using the direct algorithm. Inset: behavior of the statistical error of $\text{Tr} \rho_A^2$ versus $\ell$ for the SUSY model. The blue dashed line is the expected form $A + B\ell^{1/2}$.

that is expected to be asymptotically a function of the chord length $L_c = [(L/\pi)\sin((\pi/L)\ell)]$. This allows us to extract the non-universal quantity $c_2$ and to check the form of the corrections to the scaling. In figure 6 we report the results for $c_2(L_c)$ for the SUSY point, for the two uncoupled Ising models, and for the four-states Potts model. It is evident that for large $L_c$, $c_2(L_c)$ approaches a constant value around 0.5. This is a first confirmation of the CFT predictions on the self-dual line.

The previous results also provide a test for the theory of the corrections to the scaling to $S_A^{(n)}$. It has been shown [34,35] that for gapless models described by a Luttinger liquid theory, the corrections to the scaling have the form $\ell^{-2K_L/n}$ (or $L_c^{-2K_L/n}$ for finite systems), where $K_L$ is the Luttinger parameter, related to the circle compactification radius $K_L = 1/2\eta$. On the basis of general CFT arguments [36], it has been argued that this scenario is valid for any CFT and so also for the AT model with $K_L$ replaced by the dimension of a proper operator. It is then natural to expect that for the AT model this dimension is $K_L$ in equation (31), also on the basis of the results for the Ising model [34,50]. The dashed lines in figure 6 are fits of $c_2(L_c)$ with the function $c_2 + AL_c^{-K_L}$. The agreement is always very good, except for the four-state Potts model, for which the exponent of the leading correction $K_L$ assumes the smallest value and so subleading corrections enter (as elsewhere in similar circumstances, see e.g. [35]). In fact, the fit with the function $c_2 + AL_c^{-K_L} + BL_c^{-2K_L}$ is in perfect agreement with the data (but the presence of another fit parameter makes this result not so robust). This analysis confirms that $K_L$ is the right exponent governing the corrections to the scaling.

In the inset to figure 6 we also report the values of $c_n$ for $n = 3, 4$ as a function of $L_c$. $c_n$ becomes smaller as $n$ increases, as for the XXZ [34], XX [51], and Ising [50,52]

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4.2. The entanglement entropy of two disjoint intervals

In this section we investigate the entanglement entropy of two disjoint intervals and check the correctness of our prediction (25) for the AT model on the self-dual line. As for all other cases studied so far numerically (i.e. Heisenberg [17], Ising [24, 26], and XY [26] chains), strong scaling corrections affect the determination of the scaling function $F_n(x)$. The CFT predictions have been confirmed only using the general theory of corrections to the scaling [34]–[37].

In order to determine the function $F_n(x)$, we consider the ratio

$$F_n^{\text{lat}}(x) = \frac{\text{Tr} \rho_A^{A_1 \cup A_2} (1 - x)^{c(n-1)/6}}{\text{Tr} \rho_A^{A_1} \text{Tr} \rho_A^{A_2}}$$

and, on the basis of the general CFT arguments [36], we expect that the leading correction to scaling can be effectively taken into account by the scaling ansatz

$$F_n^{\text{lat}}(x) = F_n^{\text{CFT}}(x) + \ell^{-2\omega/n} f_n(x) + \cdots.$$  

For the Ising model it has been found that $\omega = 1/2$ [24, 26]. Since for $\eta = 2$ the AT Hamiltonian reduces to two uncoupled Ising models, one naively expects $\omega = K_L/2$ along the whole self-dual critical line of the AT model.

Hereafter we only consider $\text{Tr} \rho_A^{A}$. We start our analysis from the SUSY point that (assuming $\omega = K_L/2$) should have the smaller corrections to scaling. In figure 7 we show
Monte Carlo data at $\ell = 10, 20$ ($L = 120$) for $F_2^{\text{lat}}(x)$ plotted against the four-point ratio $x$ defined as in equation (15). We report with the blue dashed line the asymptotic CFT result (cf equation (25)). As in all other cases considered in the literature [24, 26], the curves for $F_2(x)$ at $\ell = 10, 20$ are not symmetric functions of $x \to 1 - x$, as the asymptotic CFT prediction must always be [17]. This is due to the non-symmetrical finite-size corrections $f_2(x)$ in equation (57). We extrapolate the result at $\ell \to \infty$ using the ansatz (57) and $\omega = 2/3$. The extrapolations are reported as red points in figure 7. There is a very good agreement between the extrapolations and the theoretical curve. Since the correction exponent $\omega = 2/3$ is rather large, and so the corrections small, even small subsystems such as $\ell = 10, 20$ are sufficient to obtain a good extrapolation. In the inset to figure 7 we report the Monte Carlo data for $F_2^{\text{lat}}(x)$ against $1/\ell^{2/3}$. The linear behavior in this inset confirms the validity of the ansatz (57) and the reported straight lines are the fits giving the extrapolations reported in the main figure.

We also investigate other points on the self-dual line, namely the four-states Potts model ($\eta = 4$), the parafermion $Z_4$ ($\eta = 3$), and the uncoupled Ising ($\eta = 2$). In figure 8 we report $F_2^{\text{lat}}(x) - F_2^{\text{CFT}}(x)$ at fixed $x = 1/2$ versus $\eta^{-1}$ for all the mentioned models. We report $x = 1/2$ because it is the value of $x$ providing the most stable estimate, but other values have also been studied. Indeed, on one hand, the computational cost of the simulations decreases going toward $x = 1$ (the reason being evident from the definition of $x$ for which smaller lattice sizes are needed). On the other hand, the scaling corrections become more severe in the region $x \sim 1$, as is clear from the results for the SUSY model in figure 7. Thus $x = 1/2$ represents the best compromise between these two drawbacks. The dashed curves in the left panel of figure 9 are fits of the data with equation (57).
Figure 8. $F^\text{lat}_2(1/2)$ as a function of $\eta^{-1}$ for different models (Ising, SUSY, $Z_4$ parafermions, and four-states Potts model). The blue dashed line is the CFT prediction. The (colored) points close to the curve are extrapolations obtained with the finite-size scaling ansatz (57). The black crosses are the Monte Carlo data used for the fits. The block lengths used range from $\ell = 5$ to 80.

Figure 9. $F^\text{CFT}_2(1/2) - F^\text{lat}_2(1/2)$ versus $1/\ell$. The dashed lines are fits to the finite-size scaling ansatz (57) fixing the value of $F^\text{CFT}_2(1/2)$. Left: the same plot in log–log scale. Obtained by fixing the value of $F^\text{CFT}_2(x)$ to its predicted value (cf equation (25)). There is a very good agreement with the full theoretical picture, confirming in particular the correctness of the exponent governing the leading correction to the scaling. For the $Z_4$ parafermions and for the four-state Potts model, we needed very large values of $\ell$ in order to show the correct asymptotic behavior (the range of $\ell$ reported in the plot is in fact $5 \leq \ell \leq 80$). This is made clearer in the right panel of figure 9 where the same data are shown in log–log scale. In figure 8 we reports the fits obtained by fixing only the exponent of the corrections $\omega = K_L/2$ and leaving $F^\text{CFT}_2(1/2)$ free. For all considered values of
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**Figure 10.** Monte Carlo data for $f_2(x)$ obtained as $f_2(x) = (F_2^{\text{lat}}(x) - F_2^{\text{CFT}}(x))\ell K_{L/2}$ as a function of $x$. We show data for $\ell = 10$ and various models (SUSY, $Z_4$ parafermions, Ising model and the model corresponding to $\eta^{-1} = 0.74$). The blue dashed lines are asymptotic fits to $Ax^{1/4}$. The extrapolation of $F_2^{\text{lat}}(1/2)$ to $\ell \to \infty$ is compatible (within error bars) with the expected result $F_2^{\text{CFT}}(1/2)$.

We finally study the correction amplitude $f_2(x)$ in equation (57). This function is the main reason for the asymmetry in $x \to 1 - x$ for $F_2^{\text{lat}}(x)$ and knowing its gross features could greatly simplify future analyses. For the Ising model, it has been found that $f_2(x) \sim x^{1/4}$ for small $x$, that is the same behavior as $F_2(x) - 1$. Since along the whole self-dual line $F_2(x) - 1 \sim x^{1/4}$, we would expect

$$f_2(x) \sim x^{1/4}.$$  

(58)

For the Ising model (i.e. $\eta = 2$), this scenario has already been verified with high precision [24].

In figure 10 we report $f_2(x)$ obtained as $f_2(x) = (F_2^{\text{CFT}}(x) - F_2^{\text{lat}})\ell K_{L/2}$ as a function of $x$ (in logarithmic scale to highlight the small $x$ behavior). All the data correspond to $\ell = 10$ and various values of $L$. For the two largest values of $\eta$ ($Z_4$ parafermionic theory at $\eta = 3$ and Ising model at $\eta = 2$), we observe an excellent agreement with our conjecture $f_2(x) \sim x^{1/4}$. However, decreasing the value of $\eta$, i.e. for the SUSY model at $\eta = 3/2$ and for the model at $\eta^{-1} = 0.74$, the behavior of $f_2(x)$ is not as linear as before, especially for high values of $x$. Nonetheless, for $x < 0.4$ the data confirm the behavior $x^{1/4}$. Furthermore, it seems that for any $\eta \neq 2$, subleading terms in the expansion for small $x$ appear and they are vanishing only for the Ising model.

5. The tree tensor network

This section is divided into two parts. Firstly we explain in a self-contained way how to extract the spectrum of the reduced density matrix of some specific bipartitions of a pure state encoded in a tree tensor network (TTN). We only recall the basic definitions
introduced in [53] and refer the reader to the literature for complementary works on the subject [54]–[66]. Secondly we quickly recall how to use a TTN to calculate the ground state of the anisotropic Heisenberg spin chain.

5.1. Tree tensor network and reduced density matrices

We consider a one-dimensional lattice $\mathcal{L}$ made of $N$ sites, where each site is described by a local Hilbert space $\mathbf{V}$ of finite dimension $d$. In this work the state is the ground state $|\Psi_{\text{GS}}\rangle$ of some local Hamiltonian $H$ defined on $\mathcal{L}$, but in general it could be an arbitrary pure state $|\Psi\rangle \in \mathbf{V} \otimes^N$ defined on the lattice $\mathcal{L}$.

A generic state $|\Psi\rangle \in \mathbf{V} \otimes^N$ can always be expanded as

$$|\Psi\rangle = \sum_{i_1=1}^d \sum_{i_2=1}^d \cdots \sum_{i_N=1}^d T_{i_1 i_2 \cdots i_N} |i_1\rangle |i_2\rangle \cdots |i_N\rangle,$$

(59)

where the $d^N$ coefficients $T_{i_1 i_2 \cdots i_N}$ are complex numbers and the vectors $\{|1_s\rangle, |2_s\rangle, \ldots, |d_s\rangle\}$ denote a local basis on the site $s \in \mathcal{L}$. We refer to the index $i_s$ that labels a local basis for site $s$ ($i_s = 1, \ldots, d$) as a physical index.

In the case we are interested in, the tensor of coefficients $T_{i_1 i_2 \cdots i_N}$ in equation (59) is the result of the contraction of a TTN. As shown in figure 11 for lattices of $N = 4$ and 8 sites, a TTN decomposition of $T_{i_1 i_2 \cdots i_N}$ consists of a collection of tensors $w$ that have both bond indices and physical indices. The tensors are interconnected by the bond indices according to a tree pattern. The $N$ physical indices correspond to the leaves of the tree. Upon summing over all the bond indices, the TTN produces the $d^N$ complex coefficients $T_{i_1 i_2 \cdots i_N}$ of equation (59).

The tensors in the TTN will be constrained to be isometric, in the following sense. As shown in figure 12 for the $N = 4$ lattice of figure 11, each tensor $w$ in a TTN has at most one upper leg/index $\alpha$ and two lower indices/legs $\beta_1, \beta_2$, so that its entries read $(w)^{\alpha}_{\beta_1 \beta_2}$ (everything can be generalized to tensors with more upper and lower legs [53]).
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Figure 12. (i) Diagrammatic representation of the two types of isometric tensors in the TTN for an $N = 4$ lattice in figure 11. (ii) Graphical representation of the constraints in equations (61) and (62) fulfilled by the isometric tensors.

Then we impose that

$$\sum_{\beta_1, \beta_2} (w)_{\alpha_1, \beta_2}^{\alpha} (w^+)_{\beta_1, \beta_2}^{\beta_1, \beta_2} = \delta_{\alpha \alpha'}.$$  (60)

For clarity, throughout this paper we use diagrams to represent tensor networks as well as tensor manipulations. For instance, the constraints for the tensors $w_1$ and $w_2$ of the TTN of figure 11 for a $N = 4$ lattice, namely

$$\sum_{\beta_1, \beta_2} (w_1)_{\beta_1, \beta_2}^{\alpha_1, \beta_2} (w_1^+)_{\alpha_1, \beta_2}^{\alpha} = \delta_{\alpha \alpha'},$$  (61)

$$\sum_{\beta_1, \beta_2} (w_2)_{\beta_1, \beta_2}^{\alpha_1, \beta_2} (w_2^+)_{\alpha_1, \beta_2}^{\beta_1, \beta_2} = 1,$$  (62)

are represented as the diagrams in figure 12(ii). We refer to a tensor $w$ that fulfils equation (60) as an isometry.

An intuitive interpretation of the use of a TTN to represent a state $|\Psi\rangle$ can be obtained in terms of a coarse-graining transformation for the lattice $\mathcal{L}$. Notice that the isometries $w$ in figure 11 are organized in layers. The bond indices between two layers can be interpreted as defining the sites of an effective lattice. In other words, the TTN defines a sequence of increasingly coarser lattices $\{\mathcal{L}_0, \mathcal{L}_1, \ldots, \mathcal{L}_{T-1}\}$, where $\mathcal{L}_0 \equiv \mathcal{L}$ and each site of lattice $\mathcal{L}_\tau$ is defined in terms of several sites of $\mathcal{L}_{\tau-1}$ by means of an isometry $w_\tau$, see figure 13. In this picture, a site of the lattice $\mathcal{L}_\tau$ effectively corresponds to some number $n_\tau$ of sites of the original lattice $\mathcal{L}_0$. For instance, each of the two sites of $\mathcal{L}_2$ in figure 13 corresponds to eight sites of $\mathcal{L}_0$. Similarly, each site of lattice $\mathcal{L}_1$ corresponds to four sites of $\mathcal{L}_0$.

The use of isometric tensors, and the fact that each bond unambiguously defines two parts $(A : B)$ of the chain which are connected only through that bond, as displayed in figure 14, implies that the rank of that bond in the TTN is given by the Schmidt rank

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Figure 13. The isometric TTN of figure 11 for an $N=8$ lattice $\mathcal{L}_0$ with periodic boundary conditions (the blue external circle) is associated with a coarse-graining transformation that generates a sequence of increasingly coarse-grained lattices $\mathcal{L}_1$, $\mathcal{L}_2$ and $\mathcal{L}_3$ (the inner circles). Notice that in this example we have added an extra index to the top isometry $w_3$, corresponding to the single site of an extra top lattice $\mathcal{L}_3$, which we can use to encode in the TTN a whole subspace of $V^\otimes N$ instead of a single state $|\Psi\rangle$.

$\chi(A:B)$ of the partition $(A:B)$ [59]. Thus the reduced density matrix $\rho_A$ for a set $A$ of sites of $\mathcal{L}$ is

$$\rho_A = \text{tr}_B |\Psi\rangle\langle\Psi| = \sum_\alpha p_\alpha |\Psi_\alpha^A\rangle\langle\Psi_\alpha^A|,$$

where $p_\alpha$ are the eigenvalues of $\rho_A$. It follows then the Rényi entanglement entropies $S_A^{(n)}$ are

$$S_A^{(n)} = \frac{1}{1-n} \log \text{Tr} \rho_A^n = \frac{1}{1-n} \log \sum_\alpha p_\alpha^n,$$

and for $n=1$

$$S_A^{(1)} = -\text{tr}(\rho_A \log \rho_A) = -\sum_\alpha p_\alpha \log p_\alpha.$$

In the following we denote the ranks of the tensor $w_\tau$, $\alpha, \beta_1, \beta_2$, as $\chi^\tau, \chi^{\tau-1}, \chi^{\tau-1}$. In general, they fulfil

$$\chi^\tau < (\chi^{\tau-1})^2,$$

meaning that $w_\tau$ projects states in $V^{\tau-1} \otimes V^{\tau-1}$ into the smaller Hilbert space $V^\tau$. 

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For a critical chain, the logarithmic scaling of the entanglement entropy (cf equations (2)) implies that the rank of the isometries should at least grow proportionally to the length of the block represented by the effective spins

$$\chi^\tau \propto n_\tau,$$

which means that while moving to a higher layer of the tensor network the rank of the isometries increases. This also implies that the leading cost of the computation is concentrated in contracting the first few layers of the TTN. If $N = 2^T$ and we describe a pure state (so that the rank of the $\alpha_\tau$ is one) the maximal rank of the tensors in the TTN is

$$\chi = \max_\tau \chi^\tau = \chi^{T-1}. \tag{68}$$

In [53] the following has been shown. (i) A TTN description of the ground state of a chain of length $N$ with periodic boundary conditions can be obtained numerically with a cost of order $O(\log N \chi^4)$. (ii) From the TTN it is also straightforward to compute the spectrum $\{p_\alpha\}$ of the reduced density matrix $\rho_A$ (cf equation (63)) when $A$ is a block of contiguous sites corresponding to an effective site of any of the coarse-grained lattices $L_1, \ldots, L_{T-1}$. Figure 15 illustrates the tensor network corresponding to $\rho_A$ for the case.
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Figure 15. Computation of the spectrum $\{p_\alpha\}$ of the reduced density matrix $\rho_A$ for a block $A$ that corresponds to one of the coarse-grained sites. (i) Tensor network corresponding to $\rho_A$ where $A$ is half of the lattice. (ii) Tensor network left after several isometries are annihilated with their Hermitian conjugates. (iii) Since the spectrum of $\rho_A$ is not changed by the isometries acting on $A$, we can eliminate them and we are left with a network consisting of only two tensors, which can now be contracted together. The cost of this computation is proportional to $O(\chi^3\chi^2) \leq O(\chi^5)$.

when $A$ is one half of the chain. Many pairs of isometries are annihilated. In addition, the isometries contained within region $A$ can be removed since they do not affect the spectrum of $\rho_A$. From the spectrum $\{p_\alpha\}$, we can now obtain the Rényi entropies $S_A^{(n)}$. The leading cost of computing the spectrum of the reduced density matrix $\rho_A$ for this class of bipartitions is due to the contractions of the first layers of the TTN. When the bipartition is such that $A$ is a quarter of the chain, this implies a cost proportional to $O(\chi^3\chi^2) \leq \chi'\chi^4$, where $\chi' = \chi^{T-2}$.

It is also possible to compute the reduced density matrix $\rho_A$ when $A$ is composed of two disjoint subintervals $A_1$ and $A_2$, where now each of the two intervals is a block of contiguous sites corresponding to an effective site of the coarse-grained lattice. The cost of this computation is again dominated by contracting the upper part of the tensor network, and the most expensive case is obtained by considering $A$ as the collection of two $N/4$ spins blocks, separated by $N/4$ spins. The tensor network corresponding to this $\rho_A$ is shown in figure 16. Also in this case many pairs of isometries are annihilated. The isometries contained within the composed region $A$ can also be removed since they do not affect the spectrum of $\rho_A$. The cost of contracting this tensor network is proportional to $\max[O(\chi^2\chi'^4), O(\chi^3\chi'^2)] \leq O(\chi^6)$.

5.2. The TTN and the anisotropic Heisenberg spin chain

In section 5.1 we have shown how to extract the spectrum of the reduced density matrix for a single and a double spin block from a TTN state. In this paper we are interested...
Figure 16. Computation of the spectrum \{p_\alpha\} of the reduced density matrix \rho_A when A corresponds to two coarse-grained sites separated by one coarse-grained site from both sides. (i) The tensor network corresponding to \rho_A where A is a quarter of the lattice. (ii) The tensor network left after several isometries are annihilated with their Hermitian conjugates. (iii) Since the spectrum of \rho_A is not changed by the isometries acting on A, we can eliminate them and we are left with a network consisting of only a few tensors, which can now be contracted together. The cost of contracting this tensor network is proportional to \max[O(\chi^2\chi^4), O(\chi^3\chi^2)] < O(\chi^6).

in reduced density matrices calculated on the ground state of the anisotropic Heisenberg spin chain (XXZ model) in zero magnetic field, defined by the Hamiltonian

\[ H = \sum_{j=1}^{L} [\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z], \tag{69} \]

where \( \sigma_j^\alpha \) are the Pauli matrices at the site \( j \). Periodic boundary conditions are assumed. We are interested in gapless conformal phases of the model, that is \(-1 < \Delta \leq 1\). This phase is described by a free bosonic CFT compactified on a circle with radius that depends on the parameter \( \Delta \):

\[ \eta = 2r_{\text{circle}}^2 = \frac{1}{2K_L} = \frac{\arccos(-\Delta)}{\pi}, \tag{70} \]

where \( K_L \) is the Luttinger liquid parameter.\(^6\) The sign convention in the Hamiltonian (69) is such that the model is (anti)ferromagnetic for \( \Delta < 0 \) (\( \Delta > 0 \)). The Hamiltonian (69) is diagonalizable by means of the Bethe ansatz. However, it is still a major problem to obtain the spectrum of the reduced density matrix from the Bethe ansatz and only

\(^6\) Notice the similarities and differences between equation (70) and its analog for the AT model (31). The relation between \( \eta \) and \( r^2 \) and the relation between \( K_L \) and \( \Delta \) are the same for both the XXZ spin chain and the AT model, but the relation between \( \eta \) and \( \Delta \) (or \( K_L \) and \( r \)) is different.

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results for small subsystems are known \[^{[44,67]}\]. For this reason we exploit variational TTN techniques to obtain the ground state.

Here we follow the variational procedure described in detail in \[^{[53]}\], where the generic technique (consisting of assuming a tensor network description of the ground state and minimizing the energy variationally, improving the tensors one by one, as described, i.e., in \[^{[4]}\]) has been specialized and optimized for the case of a TTN. We exploit translation invariance by using the same tensor at each layer of the TTN. One could also improve the efficiency further by exploiting the \(U(1)\) symmetry of the Hamiltonian \[^{(69)}\], i.e. the rotations around the \(z\) axis. However, we did not make use of this symmetry here.

6. The block entanglement of the anisotropic Heisenberg spin chain

In this section we report the TTN results for the Rènyi entropies in the \(XXZ\) spin chain for a single and a double interval. As a main advantage compared to the classical Monte Carlo simulations performed for the AT model, with a single TTN simulation we obtain the spectrum of the reduced density matrix and hence any Rènyi entropy, including von Neumann \(S_A^{(1)}\). Conversely, with the Monte Carlo methods only Rènyi entropies \(S_A^{(n)}\) of integer order \(n \geq 2\) can be obtained and each of them requires an independent simulation.

6.1. The single interval

We first present the TTN results for the single interval. These have already been obtained with many numerical variational techniques \[^{[34,68,69,38]}\] and are reported here only to test the accuracy of the TTN and to fix units/scales, etc. Using variational TTN, we find the ground state of the \(XXZ\) Hamiltonian \[^{(69)}\] and from this we extract the spectrum of the reduced density matrix of the single block, as explained in section 5. We then numerically obtain \(\text{Tr}\rho_A^n\). The maximum size of the chain that we consider is \(L = 128\). The subsystem lengths considered are \(\ell = 2, 4, 8, 16, 32\). Notice that with the TTN method, using a binary tree as we are doing, we can effectively access only subsystem sizes of the form \(2^m\) with \(m\) an arbitrary integer, as should be clear from section 5. In particular, this limits the calculation to even values of \(\ell\) and we cannot study the parity effects reported \[^{[34,35]}\].

We considered different values of the anisotropy parameter \(\Delta\), namely \(\Delta = -0.3, -0.1, 0.0, 0.1, 0.2, 0.4, 0.6, 0.8, 1\). The TTN becomes less effective for values of \(\Delta \leq -0.5\). This can be easily traced back to the smallness of the finite-size gap that in the minimization process causes the algorithm to be stuck in meta-stable states when the system size is large enough. This drawback could be cured by using larger values of \(\chi\) (and so larger computational cost), but, as we shall see, the considered values of \(\Delta\) suffice to draw a very general picture of the entanglement. For the isotropic Heisenberg antiferromagnet at \(\Delta = 1\) we ignore the presence of logarithmic corrections to the scaling \[^{[68,36]}\], that have a minimal effect for all our aims.

As for the AT model, we study the quantity \(c_2(L_\zeta)\) defined by the ratio in equation \[^{(55)}\]. The results are shown in figure 17 for all the considered values of \(\Delta\). The scaling corrections are evident, especially for larger values of \(\Delta\), as expected \[^{[34]}\]. These corrections for \(\text{Tr}\rho_A^n\) are indeed of the form \(L_\zeta^{-2K_\ell}/n\) \[^{[34]}\] \((K_\ell\) is defined in equation \[^{(70)}\]). The dashed lines reported in figure 17 are fits to this form for \(n = 2\), showing the agreement

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Figure 17. TTN data for the non-universal constant $c_2(L_c)$ as a function of the chord length $L_c$ for different values of $\Delta$. The dashed curves are fits to the function $A + BL_c^{-K_2}$. The reported data have been obtained with $L = 128$ for $\Delta = 0, 0.1, 0.6$ and $L = 64$ for the other values.

between the TTN data and the fits. We checked that all the TTN data agree with those obtained in [34] using density matrix renormalization group. The agreement is perfect and for this reason we refer to the above paper for a detailed study of Tr $\rho_n^A$ for $n > 2$.

6.2. Double interval: the $n = 2$ case

We now consider a subsystem made of two parts $A_1$ and $A_2$ of equal length $\ell$. We start by studying the quantity $\text{Tr} \rho_{A_1\cup A_2}^2$ for finite chains and extract the universal function $F_{CFT}^2(x)$ by proper extrapolation. Since we only consider even $\ell$, corrections to the scaling are expected to be monotonic in $\ell$ also for $F_2(x)$, oppositely to the case of arbitrary $\ell$ parity [17,26]. The CFT prediction for the function $F_2(x)$ for the XXZ chain is equation (5) with $\eta$ given by equation (70).

In figure 18 we report TTN data for $F_{2\text{lat}}^2(x)$ (obtained with the ratio defined in equation (56)) as function of the cross ratio $x$ for $\Delta = -0.3, -0.1, 0.1, 0.6$ and subsystem sizes $\ell = 4, 8, 16, 32$. The different values of $\Delta$ are denoted with different colors, while the different symbols stand for the various $\ell$. On the same figure we also show the asymptotic $F_{CFT}^2(x)$ as dashed lines. It is evident that strong scaling corrections affect the data, as expected. Colored arrows denote the directions of (asymptotically) increasing subsystem sizes. Very surprisingly, while for $\Delta = -0.3, -0.1, 0.1$ the asymptotic CFT result is approached from below, for $\Delta = 0.6$ it is approached from above. Moreover, for $\Delta = 0.6$ the behavior of the data is not monotonic. This contrasts with the results obtained for the AT model in the previous sections and the ones obtained for the $XX$ and Ising spin chains [26].

In order to shed some light on this unexpected phenomenon, it is worth looking at $F_{2\text{lat}}^2(x)$ as a function of $\ell$ for fixed values of $x$. In figure 19 we report one of these plots.
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Figure 18. TTN data for $F_{2}^{\text{lat}}(x)$ as a function of $x$ for various sizes of the chain $L = 16, 32, 64, 128$, subsystem lengths $\ell = 4, 8, 16, 32$, and $\Delta = -0.3, -0.1, 0.1, 0.6$. Different values of $\Delta$ are distinguished by different colors, while different symbols denote different values of $\ell$. The arrows denote the (asymptotically) increasing subsystem sizes $\ell$.

Figure 19. TTN data for $F_{2}^{\text{lat}}(1/2) - F_{2}^{\text{CFT}}(1/2)$ as a function of $1/\ell$ for various $\Delta$. The dashed lines are fits to the function with the generalized finite-$\ell$ ansatz (71).

for $x = 1/2$. Analogous figures are obtained for other values of $x$. The corrections to the scaling are non-monotonic in the range $0.2 \leq \Delta \leq 0.7$. This phenomenon can be understood if further corrections to the scaling are taken into account. There are two corrections that can be responsible for this behavior. On the one hand, corrections of the form $\ell^{-mK_{L}}$ (from $\ell^{-2mK_{L}/n}$ at $n = 2$) for any integer $m$ are known to be present [35], and on the other hand the usual analytic corrections such as $\ell^{-1}$ are generically expected to exist for any quantity from general scaling arguments. Thus the most general finite-$\ell$
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Figure 20. TTN data for $F^\mathrm{lat}_3(x)$ as a function of $x$ for various sizes of the chain, $\Delta = -0.3, 0.1, 0.6, 1$, and subsystem lengths $\ell = 4, 8, 16, 32$. We denote with different symbols the values of $\ell$ and with different colors the various $\Delta$. The dashed curves are the theoretical results given by equation (7). The arrows denote the (asymptotically) increasing subsystem sizes $\ell$.

ansatz has the form

$$F^\mathrm{lat}_2(x) = F^\mathrm{CFT}_2(x) + \frac{f_2(x)}{\ell K_L} + \frac{f_A(x)}{\ell^2 K_L} + \frac{f_B(x)}{\ell^2 K_L} \ldots,$$

where the first correction is the unusual one employed also for the Ashkin–Teller model, and the other two are the ones just discussed. The effect of subleading corrections is enhanced by the fact the amplitude functions $f_2(x)$ and $f_A(x)$ or $f_B(x)$ have opposite signs, determining the non-monotonic behavior. Unfortunately, for values of $\Delta$ for which the effect of subleading corrections is more pronounced (i.e. $0.1 \leq \Delta \leq 0.6$), we have $K_L < 1 < 2K_L$, making it difficult to disentangle corrections with close exponents. Thus, in order to present analyses of a good quality, we ignore the last correction (i.e. we fix $f_B(x) = 0$). To check the proposed scenario, we performed the fit of the data in figure 19 with the ansatz (71) and $f_B(x) = 0$. The results of the fits are reported in the same figure, showing perfect agreement with the data for all the values of $\Delta$. We repeated the same analysis for other values of $x$, finding the same quality of fits as for $x = 1/2$. However, we cannot exclude that corrections of the form $\ell^{-2K_L}$ have an important role.

6.3. Double interval: the $n=3$ case

Now we report the same analysis performed for $\Tr \rho_A^3$ for the third moment of $\rho_A$, i.e. $\Tr \rho_A^3$. Again we consider finite-size $XXZ$ spin chains and extract the universal function $F^\mathrm{CFT}_3(x)$ by finite-size analysis. The expected CFT result is given for general $n$ by equation (7). In figure 20 we show TTN data for $F^\mathrm{lat}_3(x)$ (obtained from equation (56)) at $\Delta = -0.3, 0.1, 0.6, 1$ and subsystem sizes up to $\ell = 32$. We also show the theoretical curves given by equation (7). As for $n = 2$, the asymptotic universal curve is approached.
from below for $\Delta \leq 0.6$, and from above for $\Delta \geq 0.6$. Furthermore, the behavior of the numerical data for $\Delta > 0.6$ is non-monotonic. This suggests that the ansatz in equation (57) is not sufficient to describe accurately the TTN data and further corrections to the scaling should be included as for $\text{Tr} \rho^2_A$.

For $n = 3$, the leading corrections to the scaling are described by the ansatz (57), i.e. the leading exponent is $2K_L/3$. Thus, for the cases when subleading corrections are more important (i.e. for $\Delta \geq 0.6$), the ordering of the exponents is $2K_L/3 < 4K_L/3 < 1$ and so it is reasonable to ignore the analytic correction. Thus we fit the TTN data with the function

$$F_{3}^{\text{lat}}(x) - F_{3}^{\text{CFT}}(x) = f_3(x)\ell^{-2K_L/3} + f_B(x)\ell^{-4K_L/3}.$$  \hspace{1cm} (72)

In figure 21 we report TTN data for $F_{3}^{\text{lat}}(x) - F_{3}^{\text{CFT}}(x)$ for $x = 1/2$ and several values of $\Delta$. The dashed lines are fits with the finite-size ansatz (72) that perfectly reproduce the data.

### 6.4. Double interval: the von Neumann entropy

The TTN gives access to the full spectrum of the reduced density matrix of $A_1 \cup A_2$ and so to the entanglement entropy $S_A^{(1)}$ as well. In figure 22 we report the function $F_{\text{VN}}^{\text{lat}}(x)$ defined as

$$F_{\text{VN}}^{\text{lat}}(x) = -S_{A_1 \cup A_2}^{(1)} + S_{A_1}^{(1)} + S_{A_2}^{(1)} - \frac{1}{3} \log(1 - x),$$  \hspace{1cm} (73)

for $\Delta$ in the interval $[-0.3,1]$ for various $L$ up to 128 and subsystem sizes $\ell = 2, 4, 8, 16, 32, 64$. We indicate with different symbols different values of $\Delta$, while the colors are for various sizes $\ell$. As known from many other investigations on single and double intervals (quantum Ising spin chain, $XY$ model, $XXZ$), the von Neumann entropy does...
Figure 22. TTN data for the von Neumann entropy for various values of $\Delta$ in the interval $[-0.3, 1]$. We show with different symbols the values of $\Delta$ while different colors stand for different $\ell$ and lattice sizes.

not show oscillations with the parity of the subsystem and the corrections are much smaller, actually negligible for any practical purpose. Figure 22 confirms this observation for the two interval entanglement entropy for the XXZ spin chain in a wide range of $\Delta$. Indeed, at fixed value of $\Delta$ perfect data collapse is observed even for very small values of $\ell$.

Unfortunately, as already stated in the introduction, the CFT prediction for $F_{VN}(x)$ is unknown for general $x$ because the analytic continuation of $F_n(x)$ to non-integer $n$ is not achievable. However, an expression for the leading term of the small $x$ expansion of $F_{VN}(x)$ has recently been extracted [30] from equation (13):

$$F_{VN}(x) = \left(\frac{x}{4}\right)^\alpha \sqrt{\frac{\pi}{2}} \frac{\Gamma(\alpha + 1)}{2\Gamma(\alpha + 3/2)},$$

(74)

where $\alpha = \min[\eta, 1/\eta]$ and $\Gamma$ is the Euler function (not to be confused with the $\Gamma$ matrix in equation (8)). In order to check the correctness of this formula, in figure 23 we report the same data for $F_{VN}(x)$ in a log–log scale to highlight the power-law behavior for small $x$. We also report the small $x$ behavior expected from equation (74). For $\Delta = -0.3$ the agreement is good, but it gets worse on increasing $\Delta$. The natural explanation is that the considered values of $x$ are not small enough for the asymptotic equation (74) to be valid. We should then include further terms in the small $x$ expansion. As explained in [30], further coefficients in the expansion for small $x$ are difficult to obtain in general. However, there is a term that is very easy to obtain and that (luckily enough) is responsible for the previous disagreement. Indeed, as shown in [30] (cf equations (70) and (71) there), the function $F_n(x)$ has always (i.e. independently of $\eta$) a simple $O(x)$ contribution coming from the denominator in equation (7), i.e. $|\Theta(0|\Gamma)|^2 = 1 + x(x - 1/n)/6$, that can be easily analytically continued, giving

$$F_{VN}(x) = \left(\frac{x}{4}\right)^\alpha \sqrt{\frac{\pi}{2}} \frac{\Gamma(\alpha + 1)}{2\Gamma(\alpha + 3/2)} - \frac{x}{3} + O(x^{2\alpha}).$$

(75)
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Figure 23. TTN data for the von Neumann entropy for $\Delta = -0.3, 0.1, 0.6, 0.8$ (the data for different $\Delta$ are denoted with different symbols) in log–log scale. We use different colors to indicate the different block sizes $\ell$ and lattice sizes $L$. The continuous lines show the small $x$ behavior obtained from (74). The dashed lines show the small $x$ behavior where the $O(x)$ term has been added as in equation (75).

Notice that the added term becomes more important when $\alpha$ is close to 1, i.e. in the XXZ spin chain when $\Delta$ approaches 1. In figure 23 we also report the prediction (75) as a dashed line, that is asymptotically in perfect agreement with the numerical data for all values of $\Delta$.

7. Conclusions

In this paper we provided a number of results for the asymptotic scaling of the Rényi entanglement entropies in strongly interacting lattice models described by CFTs with $c = 1$. Schematically our results can be summarized as follows.

- We provided the analytic CFT result for the scaling function $F_2(x)$ for $S_A^{(2)}$ in the case of a free boson compactified on an orbifold describing, among the other things, the scaling limit of the Ashkin–Teller model on the self-dual line. The final result is given in equation (25).

- We developed a cluster Monte Carlo algorithm for the two-dimensional Ashkin–Teller model (generalizing the procedure of Caraglio and Gliozzi [18] for the Ising model) that gives the scaling functions of the Rényi entanglement entropy (for integer $n$) of the corresponding one-dimensional quantum model. With this algorithm, we calculated numerically the scaling function $F_2(x)$ of the AT model along the self-dual line and we confirmed the validity of the CFT prediction. In order to obtain a quantitative agreement, the corrections to scaling induced by the finite length of the blocks were properly taken into account.
We considered the $XXZ$ spin chains by means of a tree tensor network (TTN) algorithm. The low-energy excitations of the model are described by a free boson compactified on a circle for which CFT predictions are already available both for $n = 2$ [17] and for general integer $n$ [19]. Taking into account the corrections to the scaling, we confirmed these predictions (that resisted until now to quantitative tests) for $n = 2, 3$. Furthermore, we provided numerical determinations of the scaling function of the von Neumann entropy (cf figure 22) for which CFT predictions do not exist yet for general $x$. For small $x$ we confirmed the recent prediction of [30] (cf figure 23).

The methods we employed (classical Monte Carlo with cluster observables and TTN) are very general techniques that can be easily adapted to other models of physical interest. On the CFT side, it must be mentioned that a closed form for the functions $F_n(x)$ at integer $n$ for a free boson compactified on an orbifold is not yet available, but work in this direction is in progress [70].

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