Permutation operators, entanglement entropy, and the XXZ spin chain in the limit $\Delta \to -1^+$

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In this paper we develop a new approach to the investigation of the bi-partite entanglement entropy in integrable quantum spin chains. Our method employs the well-known replica trick, thus taking a replica version of the spin chain model as starting point. At each site i of this new model we construct an operator $\mathcal{T}_i$ which acts as a cyclic permutation among the n replicas of the model. Infinite products of $\mathcal{T}_i$ give rise to local operators, precursors of branch-point twist fields of quantum field theory. The entanglement entropy is then expressed in terms of correlation functions of such operators. Employing this approach we investigate the von Neumann and Rényi entropies of a particularly interesting quantum state occurring as a limit (in a compact convergence topology) of the antiferromagnetic XXZ quantum spin chain. We find that, for large sizes, the entropy scales logarithmically, but not conformally.

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1 Introduction

Entanglement is a fundamental property of quantum systems. Historically, there has been great interest in developing efficient theoretical measures of entanglement, one of which is known as the bi-partite entanglement entropy [1]. This entropy measures the amount of quantum entanglement, in some pure quantum state, between the degrees of freedom associated to two sets of independent observables whose union is complete on the Hilbert space.

To make this definition more precise, let us consider a one-dimensional quantum spin chain such as the one depicted in Fig. 1 and let $|\text{gs}\rangle$ be the ground state of that chain. We will

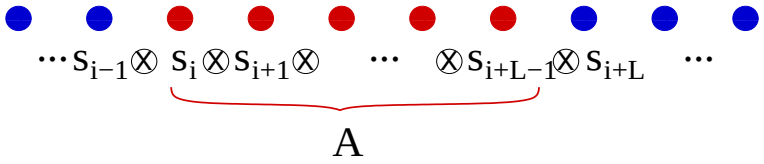

Figure 1: A region A of length L of a quantum spin chain

subdivide the chain in two regions, A and its complement $\bar{A}$. In the figure, region A is the block of L spins in red whereas $\bar{A}$ is the rest of the chain, in blue. Associated to this quantum spin chain there is a Hilbert space which can be expressed as a tensor product of local Hilbert spaces associated to its sites. This can be written as a tensor product of the two Hilbert spaces associated to the regions A and $\bar{A}$:

$$\mathcal{H} = \mathcal{A} \otimes \bar{\mathcal{A}}. \tag{1.1}$$

The bi-partite entanglement entropy is the von Neumann entropy of the reduced density matrix ρ_A associated to A, that is:

$$S_A = -\text{Tr}_{\mathcal{A}} \left(\rho_A \log \rho_A \right) \ , \quad \rho_A = \text{Tr}_{\bar{\mathcal{A}}} \left(|\text{gs}\rangle\langle\text{gs}| \right). \tag{1.2}$$

It is the entropy of the region A with respect to the rest of the chain, regarded as its environment. Another measure of entanglement that is widely studied in the literature is the Rényi entropy [2], given by

$$S_A^{\text{Rényi}}(n) = \frac{\log \left(\text{Tr}_{\mathcal{A}} \left(\rho_A^n \right) \right)}{1-n}, \tag{1.3}$$

whose $n \to 1$ limit gives the von Neumann entropy.

The bi-partite entanglement entropy of one-dimensional (integrable) quantum spin chains has been extensively studied in the literature from different points of view. One may for instance consider a quantum spin chain divided in two parts, both of which are infinitely long. If the spin chain has a finite gap, the entropy saturates to a constant value which depends on the parameters of the model under consideration and can in some cases be computed analytically [3, 4, 5]. The methods used are based on the algebraic Bethe ansatz or on the corner transfer matrix. Another interesting set-up are quantum spin chains which are infinitely long but where the block A is kept of finite length. In the critical regime, it has been found through a combination of numerical and analytical approaches (many of which can only be applied for integrable models) [7, 8, 9, 10, 11, 12] that the entropy of a block diverges logarithmically with the size of the block, as expected from conformal field theory (CFT) considerations [13, 14, 15, 16].

The regions A and $\bar{A}$ can take many different shapes and need not necessarily consist of connected blocks of spins. That is, we may also consider a situation in which both A and $\bar{A}$ are made out of the union of several disjoint blocks of spins. The entropy of disconnected

regions has been the object of numerical and analytical study recently in the context of CFT [17, 18, 19, 20, 21] and quantum spin chains and lattice models [22, 23].

The goal of this paper is two-fold. First, we introduce the quantum chain precursors of branch-point twist fields of quantum field theory (QFT), and explain their use for the computation of the bi-partite entanglement entropy. Branch-point twist fields were introduced in a series of recent works in order to compute the bi-partite entanglement entropy of 1+1-dimensional QFT [24, 25, 26, 27, 28]. Using the "replica trick," one writes the entropy (1.2) as

$$S_A = -\lim_{n\to 1} \frac{d}{dn} \mathrm{Tr}_{\mathcal{A}} \left(\rho_A^n\right). \tag{1.4}$$

The quantity $\mathrm{Tr}_{\mathcal{A}} \left(\rho_A^n\right)$, for integer n, can be interpreted as the partition function associated to n copies or replicas of the model, branched in a particular way. In the context of 1+1-dimensional QFT, we found [24] that the partition function is proportional to the two-point function of a pair of branch-point twist fields $\mathcal{T}$, $\tilde{\mathcal{T}}$:

$$\mathrm{Tr}_{\mathcal{A}} \left(\rho_A^n\right) \sim \langle \mathcal{T}(r)\tilde{\mathcal{T}}(0)\rangle. \tag{1.5}$$

These twist fields are characterized by their exchange relations with any local field φ_i of the i-th copy of the model*

$$\varphi_i(y)\mathcal{T}(x) = \Theta(x^1 > y^1)\, \mathcal{T}(x)\varphi_{i+1}(y) + \Theta(x^1 < y^1)\, \mathcal{T}(x)\varphi_i(y) \tag{1.6}$$

$$\varphi_i(y)\tilde{\mathcal{T}}(x) = \Theta(x^1 > y^1)\, \tilde{\mathcal{T}}(x)\varphi_{i-1}(y) + \Theta(x^1 < y^1)\, \tilde{\mathcal{T}}(x)\varphi_i(y) \tag{1.7}$$

for $i = 1, \ldots, n$ and where we identify the indices $n + i \equiv i$. Hence, branch-point twist fields are local twist fields in the replica model associated with generating elements of its $\mathbb{Z}_n$ symmetry. Locality plays a crucial role in evaluating their two-point function. Of course, in order to obtain the entanglement entropy, one performs a continuation to real n and the limit $n \to 1$ in the resulting expression.

In the context of quantum spin chains, it is possible to define cyclic permutation operators in terms of which the equivalent of the branch-point twist fields of QFT can be constructed. Correlation functions of such permutation operators yield the entanglement entropy of subsets of the chain. In this context, there is also a concept of locality associated to such permutation operators, although we will not make explicit use of it. We will rather show, through examples, that the use of cyclic permutation operators provides a clear *combinatoric* method for evaluating the entanglement entropy.

Second, we use this tool in order to compute the von Neumann and Rényi entanglement entropies of the state obtained in the limit $\Delta \to -1^+$ of the infinite-length anisotropic XXZ quantum spin chain (Δ being the anisotropy parameter). The limit $\Delta \to -1^+$ and some special entanglement features of the associated ground state have been previously considered in [6], where the concurrence was computed, albeit for the case of finite chains. In the case of infinite chains, there are subtleties involved in this limit. In order to properly address them, we provide a treatment of quantum states in infinite-length chains based on linear functionals on the space of finitely-supported operators. Using a completely natural compact convergence topology on linear functionals, we describe the limit $\Delta \to -1^+$ as a proper quantum state in this framework.

We interpret our results by writing the state as a "hybrid" between a factorisable ground state of the XXZ chain at $\Delta = -1$, and a state preserving the antiferromagnetic property of

*Here we employ the standard notation in Minkowski space-time: x^ν with $\nu = 0, 1$, with x^0 being the time coordinate and x^1 being the position coordinate.

XXZ ground states in the range $-1 < \Delta \leq 1$ (the z component of the total spin being zero). We propose the existence of a new length scale, below which the spins behave as if they were in a ground state of the XXZ chain at $\Delta = -1$, and above which this antiferromagnetic property holds. As $\Delta \to -1^+$, this scale tends to infinity, and the entanglement entropy of finite blocks only measures the entanglement due to the antiferromagnetic condition.

Recent results [5] show that the entanglement entropy between the semi-infinite halves of the infinite-length XYZ spin chain behaves, near to certain critical lines, in ways that are not explained by the usual CFT arguments. Although the cases that we study do not overlap with the cases studied there, we obtain similar conclusions. The von Neumann and Rényi entanglement entropies associated to finite blocks of sites in the $\Delta \to -1^+$ limit-state behave, as the blocks become large, in a way that agrees with scale invariance, but not with conformal invariance. We suggest that some results of [5] may be due to an interplay between the new length scale that we propose and the usual length scale associated to the mass gap. We hope that the relationship between our results and those of [5] will be made more precise in a future publication [29].

The paper is organized as follows: in Section 2 we introduce a new type of local operators which can be defined for a replica version of any quantum spin chain model. These are local cyclic replica permutation operators, and we provide an explicit expression for them in terms of elementary matrices. For completeness, we provide proofs of their main properties, including their action on quantum states and their exchange relations with respect to other local operators in the chain. We explain how the bi-partite entanglement entropy can be expressed in terms of correlation functions of such operators. In Section 3 we apply the results of Section 2 to the particular case of the spin-$\frac{1}{2}$ XXZ quantum spin chain and compute the von Neumann entropy associated to one or two spins in the infinite chain. In Section 4 we define the notion of quantum state in infinite-length spin chains. In Section 5 we find exact formulae for the von Neumann and Rényi entropies associated to the quantum state occurring in the limit $\Delta \to -1^+$. We study the asymptotic behavior of the entropy for large subsystem size and find that it scales logarithmically but not conformally. We finish this section with a discussion and some speculation about the nature of this quantum state. We conclude the paper in Section 6.

2 Replica permutation operators and entanglement entropy in quantum chains

A quantum chain is a quantum system physically composed of a number N of locally-interacting sites along a one-dimensional chain. Mathematically, two conditions are imposed. First, the Hilbert space is $\mathcal{H}_N := \otimes_{i=1}^N V_i$ where $V_i \cong \mathbb{C}^d$ represents the states of the individual site i, with the usual inner product (we may think of this as a spin chain of spin $(d-1)/2$)[†]. Second, the Hamiltonian $H = \sum_{i=1}^N h_i$, representing the interaction between the sites, is a sum over local energy operators h_i, usually without explicit N dependence. Each h_i factorises to the identity on all but a certain number (independent of N) of sites. This gives rise to a notion of "neighbourhood": a site j is in a neighbourhood of a site i if h_i does not factorise to the identity on site j. It is this notion of neighbourhood that tells us that the chain is actually one-dimensional, that provides a concept of distance (e.g. the minimal length of a sequence of sequentially intersecting neighbourhoods required to cover two given sites), that tells us about its most natural topology (e.g. a chain with boundaries, or a periodic chain), and that usually gives rise, in the large-N limit, to factorisation of correlation functions at large distances. This

[†]It is not important for many of the considerations that all sites have the same dimension; yet, for simplicity, in most of this paper we will specialise to $d = 2$.

notion of neighbourhood is also at the source of the emergence of a local QFT in the scaling limit, when a quantum critical point exists. The notion of neighourhood extracted from the energy density can often be made to agree with the usual notion of neighbourhoods on a chain (and we will assume this throughout).

In this perspective, it is natural to look for a quantum-chain precursors for our branch-point twist field defined in 1+1 dimensional QFT [24]. Recalling the exchange relations (1.6)-(1.7), it is clear that these will be certain permutation operators (elements of a linear representation of the permutation group), and like in the context of QFT, the entanglement entropy in quantum spin chains can be expressed in terms of correlation functions of these operators.

We consider n independent copies, or *replicas*, of a quantum chain. The Hilbert space can be described by $\mathcal{H}_N^{\otimes n} \cong \mathcal{H}_N^{(n)} := \otimes_{i=1}^N \otimes_{\alpha=1}^n V_{\alpha,i} = \otimes_{i=1}^N V_i^{(n)}$ where $V_{\alpha,i} \cong \mathbb{C}^d$ and the vector space at site i is $V_i^{(n)} := \otimes_{\alpha=1}^n V_{\alpha,i}$. It will be convenient to denote vectors belonging to $V_i^{(n)}$ by $|s_1 s_2 \dots s_n\rangle_i,\ s_\alpha \in \{1, 2, \dots, d\}$, where the "spin" $s_\alpha,\ \alpha = 1, \dots, n$ belong to copy α of the model at that particular site i.

The precise permutation operators that we need, denoted $\mathcal{T}_i$, are *local cyclic replica permutation operators*, acting non-trivially only on site i in the n-copy spin chain, with $i = 1, \dots, N$. They act as follows:

$$\mathcal{T}_i |s_1 s_2 \dots s_n\rangle_i = |s_2 s_3 \dots s_n s_1\rangle_i. \tag{2.8}$$

For $A \subset \{1, 2, \dots, N\}$ a set of sites on the chain, we will also use the notation

$$\mathcal{T}_A := \prod_{i \in A} \mathcal{T}_i. \tag{2.9}$$

Following similar ideas as in QFT, the trace of the n-th power of the reduced density matrix ρ_A associated to a state $|\psi\rangle \in \mathcal{H}_N$ is

$$\begin{aligned}
\mathrm{Tr}_{\mathcal{A}}\,(\rho_A^n) &= \mathrm{Tr}_{\mathcal{B}}\,(\rho_B^n) \\
&= \frac{1}{(\langle\psi|\psi\rangle)^n} \sum_{\substack{\{|\phi_\alpha^A\rangle \in \mathcal{A}\} \\ \{|\phi_\alpha^B\rangle \in \mathcal{B}\}}} \langle \phi_n^A \phi_n^B |\psi\rangle \langle\psi| \phi_n^A \phi_{n-1}^B\rangle \cdots \langle \phi_2^A \phi_2^B |\psi\rangle \langle\psi| \phi_2^A \phi_1^B\rangle \langle \phi_1^A \phi_1^B |\psi\rangle \langle\psi| \phi_1^A \phi_n^B\rangle \\
&= \frac{1}{\langle\Psi|\Psi\rangle} \langle\Psi| \prod_{i \in A} \mathcal{T}_i \sum_{\substack{\{|\phi_\alpha^A\rangle \in \mathcal{A}\} \\ \{|\phi_\alpha^B\rangle \in \mathcal{B}\}}} \prod_{\alpha=1}^n |\phi_\alpha^A \phi_\alpha^B\rangle\langle \phi_\alpha^A \phi_\alpha^B|\ |\Psi\rangle \\
&= \frac{\langle\Psi|\mathcal{T}_A|\Psi\rangle}{\langle\Psi|\Psi\rangle},
\end{aligned} \tag{2.10}$$

where $|\Psi\rangle = |\psi\rangle^{\otimes n}$, and the sums are over orthonormal bases. Hence, the bi-partite Rényi and von Neumann entanglement entropies of the block A can be evaluated as follows:

$$S_A^{\text{Rényi}}(n) = \frac{1}{1-n} \log\left(\frac{\langle\Psi|\mathcal{T}_A|\Psi\rangle}{\langle\Psi|\Psi\rangle}\right). \tag{2.11}$$

and

$$S_A = -\lim_{n \to 1} \frac{d}{dn}\left(\frac{\langle\Psi|\mathcal{T}_A|\Psi\rangle}{\langle\Psi|\Psi\rangle}\right). \tag{2.12}$$

(Naturally, any other cyclic element of the permutation group could have been used, by permutation invariance). As usual, an analytic continuation in n is understood in the latter expression. We will come back below to the full relationship between these permutation operators and QFT branch-point twist fields.

2.1 Expressions in terms of elementary matrices

We now study the relation between these permutation operators and elementary matrices. This will be useful because correlation functions of the latter have tractable expressions in the context of integrable quantum chains. For simplicity, let us consider the case of a spin-$\frac{1}{2}$ chains, where the spin variables $s_1, \ldots, s_n$ above can only take two values (that is, $d = 2$). The generalisation to higher spins is straightforward and explained below. The 2×2 elementary matrices $E^{\epsilon\epsilon'}$, for $\epsilon, \epsilon' \in \{1, 2\}$, have matrix elements given by

$$(E^{\epsilon\epsilon'})_{kk'} = \delta_{\epsilon,k}\delta_{\epsilon',k'}. \tag{2.13}$$

From these matrices, we form the operators

$$E^{\epsilon\epsilon'}_{\alpha,i}, \qquad \alpha = 1, \ldots, n \qquad \text{and} \qquad i = 1, \ldots, N, \tag{2.14}$$

which act on site i and copy α of the quantum chain as the matrices $E^{\epsilon\epsilon'}$, and everywhere else as the identity operator.

In the simplest non-trivial situation, the two-copy model ($n = 2$), the permutation operator $\mathcal{T}_i$ simply exchanges copies 1 and 2 at site i. It has a well-known expression in terms of elementary matrices given by

$$\mathcal{T}_i = E^{11}_{1,i}E^{11}_{2,i} + E^{12}_{1,i}E^{21}_{2,i} + E^{21}_{1,i}E^{12}_{2,i} + E^{22}_{1,i}E^{22}_{2,i}. \tag{2.15}$$

It is a rather easy (although tedious) exercise to generalize "by hand" this result to higher values of n, keeping spin-$\frac{1}{2}$. We show here just the results for $n = 3$ and $n = 4$,

$$\begin{aligned}\mathcal{T}_i \;=\; & E^{11}_{1,i}E^{11}_{2,i}E^{11}_{3,i} + E^{12}_{1,i}E^{21}_{2,i}E^{22}_{3,i} + E^{21}_{1,i}E^{12}_{2,i}E^{11}_{3,i} + E^{22}_{1,i}E^{22}_{2,i}E^{22}_{3,i} + \\ & E^{11}_{1,i}E^{21}_{2,i}E^{12}_{3,i} + E^{12}_{1}E^{11}_{2,i}E^{21}_{3,i} + E^{22}_{1,i}E^{12}_{2,i}E^{21}_{3,i} + E^{21}_{1,i}E^{22}_{2,i}E^{12}_{3,i},\end{aligned} \tag{2.16}$$

$$\begin{aligned}\mathcal{T}_i \;=\; & E^{11}_{1,i}E^{11}_{2,i}E^{11}_{3,i}E^{11}_{4,i} + E^{21}_{1,i}E^{12}_{2,i}E^{11}_{3,i}E^{11}_{4,i} + E^{11}_{1,i}E^{21}_{2,i}E^{12}_{3,i}E^{11}_{4,i} + E^{21}_{1,i}E^{22}_{2,i}E^{12}_{3,i}E^{11}_{4,i} + \\ & E^{11}_{1,i}E^{11}_{2,i}E^{21}_{3,i}E^{12}_{4,i} + E^{21}_{1,i}E^{22}_{2,i}E^{22}_{3,i}E^{12}_{4,i} + E^{21}_{1,i}E^{12}_{2,i}E^{21}_{3,i}E^{12}_{4,i} + E^{11}_{1,i}E^{21}_{2,i}E^{22}_{3,i}E^{12}_{4,i} + \\ & E^{12}_{1,i}E^{11}_{2,i}E^{11}_{3,i}E^{21}_{4,i} + E^{22}_{1,i}E^{12}_{2,i}E^{11}_{3,i}E^{21}_{4,i} + E^{12}_{1,i}E^{21}_{2,i}E^{12}_{3,i}E^{21}_{4,i} + E^{22}_{1,i}E^{22}_{2,i}E^{12}_{3,i}E^{21}_{4,i} + \\ & E^{12}_{1,i}E^{21}_{2,i}E^{22}_{3,i}E^{22}_{4,i} + E^{22}_{1,i}E^{12}_{2,i}E^{21}_{3,i}E^{22}_{4,i} + E^{12}_{1,i}E^{11}_{2,i}E^{21}_{3,i}E^{22}_{4,i} + E^{22}_{1,i}E^{22}_{2,i}E^{22}_{3,i}E^{22}_{4,i}.\end{aligned} \tag{2.17}$$

Once a few explicit cases have been worked out the general structure of the permutation operator for generic n quickly starts to emerge. There are several features that we could have predicted from the start. For example, all the formulae above are sums of exactly 2^n terms, which is also the number of distinct basis vectors $|s_1 s_2 \ldots s_n\rangle_i$ that can be constructed for a spin-$\frac{1}{2}$ model. The permutation operator is a sum of 2^n such terms since its action (2.8) is a one-to-one map between such basis vectors. In addition, all expressions are symmetric under the combined exchanges $E^{11} \leftrightarrow E^{22}$ and $E^{12} \leftrightarrow E^{21}$.

One can characterize the precise 2^n terms that will appear in the expression for the permutation operator through a set of four simple rules:

Rules 2.1 *The operator $\mathcal{T}_i$ is the sum of each possible term, with coefficient 1, that is a product of matrices $E^{\epsilon_\alpha,\epsilon'_\alpha}_{\alpha,i}$, $\alpha = 1, \ldots, n$ respecting the following rules:*

1. *a matrix $E^{11}_{\alpha,i}$ can only be followed in the product by $E^{11}_{\alpha+1,i}$ or $E^{21}_{\alpha+1,i}$,*
2. *a matrix $E^{22}_{\alpha,i}$ can only be followed in the product by $E^{22}_{\alpha+1,i}$ or $E^{12}_{\alpha+1,i}$,*

3. *a matrix* $E^{12}_{\alpha,i}$ *can only be followed in the product by* $E^{21}_{\alpha+1,i}$ *or* $E^{11}_{\alpha+1,i}$,

4. *a matrix* $E^{21}_{\alpha,i}$ *can only be followed in the product by* $E^{12}_{\alpha+1,i}$ *or* $E^{22}_{\alpha+1,i}$

(with $n+1 \equiv 1$ *and where the rules apply cyclically in the product: the first factor follows the last factor).*

This restricts greatly the type of terms that will emerge. For example there will never be terms which involve both matrices E^{11} and E^{22} and no other type, although the terms $E^{11}_{1,i}E^{11}_{2,i}\cdots E^{11}_{n,i}$ and $E^{22}_{1,i}E^{22}_{2,i}\cdots E^{22}_{n,i}$ are allowed and always appear, as we can see for $n = 2, 3, 4$ above. Similarly, the number of matrices E^{12} and E^{21} in a given product is always the same. In fact, the rules prescribe the following simple structure for the elementary matrices at any given site along the n copies: strings of any number (including zero) of E^{11} and E^{22} are separated by E^{21} (in the junctions from E^{11} to E^{22}) and by E^{12} (in the junctions from E^{22} to E^{11}), with a condition of periodicity. This point of view will be very useful in explicit calculations below.

The rules above immediately give an expression for the permutation operator of the form

$$\mathcal{T}_i = \sum_{\epsilon_1,\ldots\epsilon_n=1}^{2} E^{\epsilon_2\epsilon_1}_{1,i} E^{\epsilon_3\epsilon_2}_{2,i} E^{\epsilon_4\epsilon_3}_{3,i} \cdots E^{\epsilon_1\epsilon_n}_{n,i}. \tag{2.18}$$

This reveals the structure of the trace of some matrix. More precisely, if we introduce an auxiliary space $V_{\text{aux}} \cong \mathbb{C}^2$ as well as the operators

$$T_{\alpha,i;\text{aux}} = \sum_{\epsilon,\epsilon'=1}^{2} E^{\epsilon\epsilon'}_{\text{aux}} E^{\epsilon'\epsilon}_{\alpha,i} = \begin{pmatrix} E^{11}_{\alpha,i} & E^{21}_{\alpha,i} \\ E^{12}_{\alpha,i} & E^{22}_{\alpha,i} \end{pmatrix}_{\text{aux}}, \tag{2.19}$$

which acts non-trivially both on the auxiliary space, and at site i, copy α, then the permutation operator at site i can be written as the following trace

$$\mathcal{T}_i = \text{Tr}_{\text{aux}}\left(T_{1,i;\text{aux}} T_{2,i;\text{aux}} \cdots T_{n,i;\text{aux}}\right) = \text{Tr}_{\text{aux}}\left(\prod_{\alpha=1}^{n} T_{\alpha,i;\text{aux}}\right) \tag{2.20}$$

where the product is, by convention, ordered from left to right in order of increasing α. It is easy to obtain (2.15), (2.16) and (2.17) from (2.20) by setting $n = 2, 3$ and 4, respectively. As it should be, $\mathcal{T}_i$ reduces to the identity matrix for $n = 1$.

We note that the operator $T_{\alpha,i;\text{aux}}$ is simply a permutation operator exchanging the auxiliary space with the space (α, i). The form (2.20) of the cyclic permutation operator is something that is well-known in the context of integrable quantum spin chains solved by means of algebraic Bethe ansatz. In this context, the L-matrix is, at a certain value of the spectral parameter, simply a permutation operator exchanging an auxiliary space and the space associated to a given site of the quantum chain (see, e.g., [30]). The monodromy matrix is the trace of the product of L-matrices, exactly of the form (2.20), and is identified, at this special value of the spectral parameter, with the translation operator along the periodic chain. In our context, however, the operator that we obtain permutes the *copies* of a replica model at a given site, rather than the sites of the chain.

In fact, this connection between our expression (2.20) and the algebraic Bethe ansatz becomes very explicit if one employs the solutions to the inverse scattering problem found in [31] to express the operators $E^{\epsilon\epsilon'}_{\alpha,i}$ in terms of the entries of the monodromy matrix. We suspect that this relationship could be useful in the future for studying the properties of the replica permutation operator within the Bethe ansatz framework.

2.2 Exchange relations

In the derivation above, it is clear that the Rules 2.1, the expression (2.18), and the trace expression (2.20) are equivalent. A careful analysis of the permutation action (2.8) would also give rise to the four rules stated. Here, for completeness, we will show explicitly that equation (2.8) is a consequence of (2.20). In order to do so, we will show that the main exchange property of replica permutation operators (the property that constitutes the starting point for the definition of twist fields in QFT) is satisfied by the operator (2.20).

Given a 2 by 2 matrix $\mathcal{O}$, let $\mathcal{O}_{\alpha,i}$ be the operator on the quantum chain that acts as $\mathcal{O}$ on site i, copy α, and as the identity operator everywhere else. Then, we have the following:

Lemma 1 *The operators $\mathcal{T}_i$ defined by (2.20) satisfy the relations*

$$\mathcal{T}_i \mathcal{O}_{\alpha,i} = \mathcal{O}_{\alpha-1,i} \mathcal{T}_i \tag{2.21}$$

(with $\mathcal{O}_{0,i} \equiv \mathcal{O}_{n,i}$) for all $i = 1, \ldots, N$, all $\alpha = 1, \ldots, n$, and all $\mathcal{O}$.

Proof. This relation follows from the trace expression (2.20) along with two identities. Denoting by $\mathcal{O}_{\rm aux}$ the operator acting non-trivially as $\mathcal{O}$ on the auxiliary space and as the identity operator everywhere else, we only have to show that

$$T_{\alpha,i;\rm aux} \mathcal{O}_{\alpha,i} = \mathcal{O}_{\rm aux} T_{\alpha,i;\rm aux}, \quad T_{\alpha,i;\rm aux} \mathcal{O}_{\rm aux} = \mathcal{O}_{\alpha,i} T_{\alpha,i;\rm aux}. \tag{2.22}$$

The first identity can be derived as follows. With

$$\mathcal{O} = \begin{pmatrix} o_{11} & o_{12} \\ o_{21} & o_{22} \end{pmatrix}, \tag{2.23}$$

we have

$$\begin{aligned} T_{\alpha,i;\rm aux} \mathcal{O}_{\alpha,i} &= \begin{pmatrix} E^{11}_{\alpha,i} & E^{21}_{\alpha,i} \\ E^{12}_{\alpha,i} & E^{22}_{\alpha,i} \end{pmatrix}_{\rm aux} \begin{pmatrix} \mathcal{O}_{\alpha,i} & 0 \\ 0 & \mathcal{O}_{\alpha,i} \end{pmatrix}_{\rm aux} = \begin{pmatrix} E^{11}_{\alpha,i}\mathcal{O}_{\alpha,i} & E^{21}_{\alpha,i}\mathcal{O}_{\alpha,i} \\ E^{12}_{\alpha,i}\mathcal{O}_{\alpha,i} & E^{22}_{\alpha,i}\mathcal{O}_{\alpha,i} \end{pmatrix}_{\rm aux} \\ &= \begin{pmatrix} o_{11}E^{11}_{\alpha,i} + o_{12}E^{21}_{\alpha,i} & o_{11}E^{21}_{\alpha,i} + o_{12}E^{22}_{\alpha,i} \\ o_{21}E^{11}_{\alpha,i} + o_{22}E^{12}_{\alpha,i} & o_{21}E^{21}_{\alpha,i} + o_{22}E^{22}_{\alpha,i} \end{pmatrix}_{\rm aux}, \end{aligned} \tag{2.24}$$

which is equal to

$$\begin{aligned} \mathcal{O}_{\rm aux} T_{\alpha,i;\rm aux} &= \begin{pmatrix} o_{11} & o_{12} \\ o_{21} & o_{22} \end{pmatrix}_{\rm aux} \begin{pmatrix} E^{11}_{\alpha,i} & E^{21}_{\alpha,i} \\ E^{12}_{\alpha,i} & E^{22}_{\alpha,i} \end{pmatrix}_{\rm aux} \\ &= \begin{pmatrix} o_{11}E^{11}_{\alpha,i} + o_{12}E^{21}_{\alpha,i} & o_{11}E^{21}_{\alpha,i} + o_{12}E^{22}_{\alpha,i} \\ o_{21}E^{11}_{\alpha,i} + o_{22}E^{12}_{\alpha,i} & o_{21}E^{21}_{\alpha,i} + o_{22}E^{22}_{\alpha,i} \end{pmatrix}_{\rm aux}. \end{aligned} \tag{2.25}$$

The second relation of (2.22) follows in a similar way. ∎

The defining property (2.8) is essentially a consequence of (2.21).

Lemma 2 *The operators $\mathcal{T}_i$ defined (2.20) satisfy the relations (2.8).*

Proof. We start by writing the quantum state of the spin-$\frac{1}{2}$, n-copy quantum spin chain at site i in terms of elementary matrices $E^{\epsilon_1\epsilon_2}_{\alpha,i}$. Let $|0\rangle_i$ be a reference state at site i for which all spins of all n-copies are up ($s_1 = \cdots = s_n = \uparrow$). Any other of the 2^n possible spin configurations can be generated by acting on this reference state with a combination of elementary matrices. For example, if we want to lower the spin of copy 1, we just have to compute $E^{21}_{1,i}|0\rangle_i$, whereas acting

with $E^{11}_{1,i}$ will leave the state unchanged and the action of $E^{22}_{1,i}$ and $E^{12}_{1,i}$ gives zero. Therefore, a generic state is written as

$$|s_1 s_2 \dots s_n\rangle_i = \left(\prod_{\alpha=1}^{n} E^{j_{s_\alpha}1}_{\alpha,i}\right)|0\rangle_i, \quad j_{s_\alpha}=1 \quad \text{for} \quad s_\alpha =\uparrow \quad \text{and} \quad j_{s_\alpha}=2 \quad \text{for} \quad s_\alpha =\downarrow, \quad (2.26)$$

and from the expression (2.18), we have $\mathcal{T}_i|0\rangle = |0\rangle$ since the only non-zero summand is the one where $\epsilon_\alpha = 1$ for all α. We now evaluate the action of the permutation operator on this state by successively employing (2.21),

$$\begin{aligned}\mathcal{T}_i|s_1, s_2, \dots, s_n\rangle_i &= \mathcal{T}_i\left(\prod_{\alpha=1}^{n} E^{j_{s_\alpha}1}_{\alpha,i}\right)|0\rangle_i \\ &= \left(\prod_{\alpha=1}^{n} E^{j_{s_\alpha}1}_{\alpha-1,i}\right)\mathcal{T}_i|0\rangle_i = \left(\prod_{\alpha=1}^{n} E^{j_{s_\alpha}1}_{\alpha-1,i}\right)|0\rangle_i = |s_2, \dots, s_n, s_1\rangle_i. \quad (2.27)\end{aligned}$$

This establishes (2.8). ∎

2.3 The conjugate permutation operator $\tilde{\mathcal{T}}$

Other permutation operators, $\tilde{\mathcal{T}}_i$ at each site i, take us from copy α to copy $\alpha - 1$. We can simply obtain $\tilde{\mathcal{T}}_i$ by reversing the order of the replicas, that is

$$\tilde{\mathcal{T}}_i = \mathrm{Tr}_{\mathrm{aux}}\left(T_{n,i;\mathrm{aux}} T_{n-1,i;\mathrm{aux}} \cdots T_{1,i;\mathrm{aux}}\right), \quad (2.28)$$

or, alternatively, taking the trace,

$$\tilde{\mathcal{T}}_i = \sum_{\epsilon_1,\dots\epsilon_n=1}^{2} E^{\epsilon_2\epsilon_1}_{n,i} E^{\epsilon_3\epsilon_2}_{n-1,i} E^{\epsilon_4\epsilon_3}_{n-2,i} \cdots E^{\epsilon_1\epsilon_n}_{1,i}, \quad (2.29)$$

One may check this explicitly by showing that $\tilde{\mathcal{T}}_i\mathcal{T}_i = \mathbf{1}$. This can be done by using the following property of the elementary matrices:

$$E^{\epsilon_1,\epsilon_2}_{\alpha,i} E^{\epsilon_3\epsilon_4}_{\alpha,i} = \delta_{\epsilon_2,\epsilon_3} E^{\epsilon_1\epsilon_4}_{\alpha,i}. \quad (2.30)$$

Employing the representations (2.18) and (2.29) for the permutation operators (including some extra matrices in the products for clarity) we have

$$\begin{aligned}\tilde{\mathcal{T}}_i\mathcal{T}_i &= \sum_{\epsilon_1,\dots\epsilon_n=1}^{2} E^{\epsilon_2\epsilon_1}_{n,i} E^{\epsilon_3\epsilon_2}_{n-1,i} E^{\epsilon_4\epsilon_3}_{n-2,i} \cdots E^{\epsilon_{n-1}\epsilon_{n-2}}_{3,i} E^{\epsilon_n\epsilon_{n-1}}_{2,i} E^{\epsilon_1\epsilon_n}_{1,i} \\ &\quad \times \sum_{\epsilon'_1,\dots\epsilon'_n=1}^{2} E^{\epsilon'_2\epsilon'_1}_{1,i} E^{\epsilon'_3\epsilon'_2}_{2,i} E^{\epsilon'_4\epsilon'_3}_{3,i} \cdots E^{\epsilon'_{n-1}\epsilon'_{n-2}}_{n-2,i} E^{\epsilon'_n\epsilon'_{n-1}}_{n-1,i} E^{\epsilon'_1\epsilon'_n}_{n,i} \\ &= \sum_{\epsilon_1,\dots\epsilon_n=1}^{2} \sum_{\epsilon'_1,\dots\epsilon'_n=1}^{2} \delta_{\epsilon_1,\epsilon'_1} E^{\epsilon_2\epsilon'_n}_{n,i} \delta_{\epsilon_2\epsilon'_n} E^{\epsilon_3\epsilon'_{n-1}}_{n-1,i} \dots \delta_{\epsilon_{n-1}\epsilon'_3} E^{\epsilon_n\epsilon'_2}_{2,i} \delta_{\epsilon_n\epsilon'_2} E^{\epsilon_1\epsilon'_1}_{1,i} \\ &= \sum_{\epsilon_1,\dots\epsilon_n=1}^{2} E^{\epsilon_2\epsilon_2}_{n,i} E^{\epsilon_3\epsilon_3}_{n-1,i} E^{\epsilon_4\epsilon_4}_{n-2,i} \dots E^{\epsilon_{n-1}\epsilon_{n-1}}_{3,i} E^{\epsilon_n\epsilon_n}_{2,i} E^{\epsilon_1\epsilon_1}_{1,i} = \mathbf{1}. \quad (2.31)\end{aligned}$$

The last equality follows from the fact that all matrices $E^{\epsilon\epsilon}_{\alpha,i}$ are diagonal, so that each product above is a diagonal matrix with a single non-vanishing entry 1. The sum over all such matrices (there are exactly 2^n of them) is the identity.

2.4 Replica permutation operators for higher spin chains

We can now generalize the results above to more general spin chains, with arbitrary spin representations living at each site of the chain. Indeed the exchange relations (2.21) which we have just proven can be employed as a starting point for finding a realization of the permutation operator which is valid for higher spin chains. It can be shown that, assuming a dimension-d representation lives at site i of the quantum spin chain, the permutation operator $\mathcal{T}_i$ can be expressed exactly as in (2.20) with $T_{\alpha,i;\text{aux}}$ given by

$$T_{\alpha,i;\text{aux}} = \begin{pmatrix} E^{11}_{\alpha,i} & E^{21}_{\alpha,i} & \cdots & E^{d1}_{\alpha,i} \\ E^{12}_{\alpha,i} & E^{22}_{\alpha,i} & \cdots & E^{d2}_{\alpha,i} \\ \vdots & \vdots & \ddots & \vdots \\ E^{1d}_{\alpha,i} & E^{2d}_{\alpha,i} & \cdots & E^{dd}_{\alpha,i} \end{pmatrix}_{\text{aux}} . \tag{2.32}$$

It is not too difficult to show that all properties established in the previous section for spin-$\frac{1}{2}$ also hold for the general case. We will not dwell on such proofs here as in the remainder of this paper we will concentrate on the spin-$\frac{1}{2}$ case.

2.5 Local-unitary operators and twist fields

Since the operator $\mathcal{T}_i$ is real, we immediately find, from (2.20) and (2.28), that

$$\tilde{\mathcal{T}}_i = \mathcal{T}_i^\dagger .$$

Hence, $\mathcal{T}_i$ is a unitary operator. It is of course the local element of the unitary operator associated with the cyclic replica permutation symmetry of the n-copy Hamiltonian

$$H^{(n)} = \sum_{i=1}^{N} h_i^{(n)} = \sum_{i=1}^{N} \sum_{\alpha=1}^{n} h_{\alpha,i} \tag{2.33}$$

(where $h_{\alpha,i}$, for $\alpha = 1,\ldots,n$ and $i = 1,\ldots,N$, acts as h_i on $\otimes_{j=1}^{N} V_{\alpha,j}$, and as the identity on $\otimes_{j=1}^{N} V_{\alpha',j}\ \forall\ \alpha' \neq \alpha$). More precisely, the unitary operator that is the product of $\mathcal{T}_i$ over all sites i, i.e. $\mathcal{T}_{\{1,\ldots,N\}} = \prod_{i=1}^{N} \mathcal{T}_i$, implements the cyclic replica permutation of the chain, and commutes with the n-copy Hamiltonian. A unitary operator that can be written as a product of single-site unitary operators is sometimes called a *local-unitary* operator.

In fact, the local-unitary operator $\mathcal{T}_{\{1,\ldots,N\}}$ commutes also with the energy density,

$$\left[\mathcal{T}_{\{1,\ldots,N\}}, h_i^{(n)}\right] = 0. \tag{2.34}$$

In general, it is expected that any unitary operator associated to an internal symmetry, i.e. that is local-unitary, commutes not only with the Hamiltonian, but also with the energy density. To such an internal symmetry, one may then associate *twist fields*; e.g. in the case of $\mathcal{T}_i$,

$$\mathtt{T}_i = \mathcal{T}_{\{i,i+1,\ldots,N\}} = \prod_{j=i}^{N} \mathcal{T}_i .$$

A standard example is the twist field involved in the construction of fermion operators on the Ising spin chain. Quantum chain twist fields give rise to the usual QFT twist fields in the scaling limit. Twist fields have the property of being local "in the bulk": their commutators with the

energy density vanish for large enough separations (and away from the end of the chain N), by virtue of their association with an internal symmetry transformation. In the case of the replica permutation symmetry:

$$[\mathtt{T}_i, h_j^{(n)}] = 0 \quad \text{for } j \text{ far enough from } i \text{ and from } N. \tag{2.35}$$

This has important implications in QFT, and is likely to have important implications as well in the context of integrable quantum spin chains. We will not investigate further here such implications.

Consider the permutation operators $\mathcal{T}_i$ and their twist fields $\mathtt{T}_i$. In the scaling limit, this of course gives rise to branch-point twist fields, associated with branch-point singularities on the surface where the QFT is defined. Like in QFT, the entanglement entropy (and likewise the Rényi entropy) of a region A of the quantum chain can be expressed via a correlation function of as many pairs of twist fields $\mathtt{T}_i$, $\mathtt{T}_i^\dagger$ as there are connected sub-regions. For instance, for a single connected region A starting at site i and ending at site j, we have

$$S_A^{\text{Rényi}} = \frac{1}{1-n} \log \left(\frac{\langle \Psi | \mathtt{T}_i \mathtt{T}_j^\dagger | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right).$$

2.6 Local-unitary invariance

One of the properties of the entanglement and Rényi entropies is that they are invariant under local-unitary transformations (transformation of the state by a local-unitary operator). The precursor of this invariance is of course that the replica permutation operators $\mathcal{T}_A$ are invariant under tensor-powers of local-unitary transformations[‡], $U^{\otimes n} \mathcal{T}_A (U^\dagger)^{\otimes n} = \mathcal{T}_A$ for U a local-unitary operator on $\mathcal{H}$. In general, we expect that if two quantum states have the same Rényi entropies, then they are related by a local-unitary transformation.

3 The XXZ Heisenberg spin-$\frac{1}{2}$ chain: main features

In order to illustrate the technique proposed, we now choose the XXZ Heisenberg spin-$\frac{1}{2}$ chain as a benchmark. It is one of the most studied quantum chains and includes other interesting theories as special cases. The XXZ Heisenberg spin-$\frac{1}{2}$ finite chain of length N is characterized by the Hamiltonian

$$H_\Delta = \sum_{j=1}^{N} \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta(\sigma_j^z \sigma_{j+1}^z - 1) \right), \tag{3.36}$$

where $\sigma_j^{x,y,z}$ are the Pauli matrices associated to site j of the chain and acting on the two-dimensional space $V_j \cong \mathbb{C}^2$, a spin-1/2 module. We consider periodic boundary conditions $\sigma_{N+1}^{x,y,z} \equiv \sigma_1^{x,y,z}$, and for simplicity we restrict to N being even. The parameter Δ is known as the anisotropy parameter and, depending on its value, the physical properties of the model can change dramatically. In this paper, we will be looking at the region $-1 < \Delta \leq 1$. In this region, the model is antiferromagnetic and preserves the z-component of the total spin: its ground state has total z-spin equal to zero. As $N \to \infty$, the model is massless: the gap between the unique ground state and the first excited state tends to 0. For $\Delta = 1$ the model becomes what is

[‡]The set of (products of) replica permutation operators associated with all permutation elements spans the space of local-unitarily invariant operators (but these operators are not all linearly independent).

known as the XXX model or Heisenberg spin chain, whereas for $\Delta = 0$ it reduces to the XX model, which possesses a free fermion description. For $\Delta = -1$, the ground state of the model is very different. It is unitarily related to the ground state of the ferromagnetic Heisenberg spin chain, and is not unique. In all cases, the ground state is invariant under translations (cyclic permutations of the sites along the chain). The anisotropy parameter is commonly expressed in terms of another parameter η as

$$\Delta = \cosh(\eta), \tag{3.37}$$

with $0 \leq \eta < \pi$.

The characterization of the physical states, including the ground state, of this and many other integrable quantum spin models can be carried out very effectively by means of the algebraic Bethe ansatz approach [32, 30]. The details of the approach can be found in many places (a particularly good review can be found in [30]) and we will not review those here. The entanglement entropy is a function of the correlation functions of the model. The evaluation of correlation functions has been performed in the literature by various methods: using the algebraic Bethe ansatz [33, 30, 34] with the solution to the inverse scattering problem [31, 35, 36], and through a computation of form factors [37, 38, 39] in quantum spin chains of infinite length via q-deformed vertex operators.

We will denote by $|\psi\rangle_\Delta$ the ground state of the Hamiltonian (3.36). We will also use the notation $E_i^{\epsilon\epsilon'}$ for the operator on $\mathcal{H}$ acting as the elementary matrix (2.13) at site i and as the identity elsewhere. Instead of considering correlation functions of Pauli matrices, we will consider *fundamental blocks*, correlation functions of (i.e. quantum averages of products of) elementary matrices in the ground state $|\psi\rangle_\Delta$. We will use the following notation (with implicit dependence on Δ):

$$\langle \prod_{i\in A} E_i^{\epsilon_i\epsilon_i'} \rangle := \frac{{}_\Delta\langle\psi| \prod_{i\in A} E_i^{\epsilon_i,\epsilon_i'} |\psi\rangle_\Delta}{{}_\Delta\langle\psi|\psi\rangle_\Delta}, \tag{3.38}$$

where $A \subset \{1, 2, \ldots, N\}$ is an index set.

We will denote by $|\Psi\rangle$ (with implicit dependence on Δ) the vector in the replica model $\mathcal{H}^{(n)}$ corresponding to the tensor product $|\psi\rangle_\Delta^{\otimes n}$ of the ground state. This is of course the ground state of the n-copy Hamiltonian $H^{(n)}$. By factorisation, we have, for instance,

$$\frac{\langle\Psi|E_{1,i}^{\epsilon_1\epsilon_1'} E_{2,i}^{\epsilon_2\epsilon_2'} \ldots E_{n,i}^{\epsilon_n\epsilon_n'}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \prod_{\alpha=1}^{n} \langle E_i^{\epsilon_\alpha\epsilon_\alpha'}\rangle. \tag{3.39}$$

We note that it is a simple matter to verify the general locality property (2.35) of the twist fields $\mathtt{T}_i$ in the present case. With $h_j = \sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y + \Delta(\sigma_j^z\sigma_{j+1}^z - 1)$ and $h_j^{(n)}$ defined as in (2.33), we find

$$[\mathtt{T}_i, h_j^{(n)}] = \delta_{i-1,j}\mathtt{T}_i \sum_{\alpha=1}^{n} \Big(\sigma_{\alpha,i-1}^x(\sigma_{\alpha,i}^x - \sigma_{\alpha+1,i}^x) + \sigma_{\alpha,i-1}^y(\sigma_{\alpha,i}^y - \sigma_{\alpha+1,i}^y) + \Delta\sigma_{\alpha,i-1}^z(\sigma_{\alpha,i}^z - \sigma_{\alpha+1,i}^z)\Big)$$

for $j \neq N$.

3.1 Entanglement entropy of one and two sites

We now perform simple computations of the entanglement entropy between one or two sites and the rest of the chain using the permutation operator technique. This illustrates how the

technique directly gives the combinatorics for evaluating the trace of the reduced density matrix in terms of correlation functions (avoiding the explicit diagonalisation of the matrix).

The one-site computation can be thought of as a consistency check of our formalism, since the outcome is known a priori. This is because the ground state of the spin-$\frac{1}{2}$ XXZ chain is characterized by equal numbers of spins up and down. Hence if we pick one spin in the chain, its projection in the z-direction is entirely determined by the values of that projection for the remaining spins in the chain. In other words, the entanglement between one spin and the rest is maximal and it is well known that this maximum value is exactly $\log(2)$.

The entropy that we want to compute is

$$S_{\{i\}} = -\lim_{n\to 1} \frac{d}{dn} \left(\frac{\langle \Psi | \mathcal{T}_i | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right). \tag{3.40}$$

In order to evaluate this, we note that

$$\langle E_i^{12} \rangle = \langle E_i^{21} \rangle = 0, \tag{3.41}$$

and

$$\langle E_i^{11} \rangle = \langle E_i^{22} \rangle = \frac{1}{2}. \tag{3.42}$$

The first equality (3.41) is due to the fact that the operators E_i^{12} and E_i^{21} have the effect of reversing the spin at site i, turning the quantum average above into the scalar product of the ground state with another orthogonal state. The second equality (3.42) is due to the fact that the quantum averages involved represent the probability of finding the spin at site i up, and that of finding it down. These probabilities are exactly $\frac{1}{2}$ due to the nature of the ground state.

Factorisation (3.39) and the expression (2.18) mean that we have to evaluate a sum of products of one-point functions. Because of (3.41), the only non-vanishing contributions to the quantum average of $\mathcal{T}_i$ will come from the two terms that involve only matrices E^{11} or E^{22}. That is:

$$\frac{\langle \Psi | \mathcal{T}_i | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \langle E_i^{11} \rangle^n + \langle E_i^{22} \rangle^n = 2^{1-n}. \tag{3.43}$$

The entanglement entropy is therefore, as expected

$$S_{\{i\}} = -\lim_{n\to 1} \frac{d}{dn} 2^{1-n} = \lim_{n\to 1} 2^{1-n} \log(2) = \log(2). \tag{3.44}$$

We now consider the computation of the entanglement entropy of spins sitting at sites 1 and $m+1$ with respect to the rest of the chain:

$$S_{\{1,m+1\}} = -\lim_{n\to 1} \frac{d}{dn} \left(\frac{\langle \Psi | \mathcal{T}_1 \mathcal{T}_{m+1} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right) \tag{3.45}$$

(this is the same as $S_{\{i,m+i\}}$ thanks to translation invariance).

Given the factorization property (3.39), we know that $S_{\{1,m+1\}}$ will be given in terms of two-point functions involving pairs of operators $E_1^{\epsilon_1 \epsilon_1'} E_{m+1}^{\epsilon_2, \epsilon_2'}$. However, as before, many of these correlation functions are vanishing. More precisely, they do so whenever an operator E^{12} or E^{21} appears in combination with E^{11} or E^{22}. There are only six non-vanishing two-point functions:

$$\langle E_1^{11} E_{m+1}^{11} \rangle = \langle E_1^{22} E_{m+1}^{22} \rangle, \qquad \langle E_1^{11} E_{m+1}^{22} \rangle = \langle E_1^{22} E_{m+1}^{11} \rangle, \tag{3.46}$$

and

$$\langle E_1^{12} E_{m+1}^{21} \rangle = \langle E_1^{21} E_{m+1}^{12} \rangle, \tag{3.47}$$

where the equalities are again due to spin reversal symmetry. This means that although the operator $\mathcal{T}_1\mathcal{T}_{m+1}$ is a sum of 4^n terms, each of which involving $2n$ matrices E^{ij}, inside the correlation function most of these terms will give a vanishing contribution.

We may evaluate the correlation function by using Rules 2.1, recalling the structure mentioned there. Here, we may consider a square lattice of cylindrical topology, with 2 columns, n rows, and periodicity along the columns. Each cell is occupied by an elementary matrix: this represents a term in the product $\mathcal{T}_1\mathcal{T}_{m+1}$. Rules 2.1 imply that in order to determine a column, we only need to provide the positions of matrices E^{12} and E^{21}, with the condition of alternation, unless there are none. In the latter case, there are only two possibilities: whether the column is filled with E^{11}, or it is filled with E^{22}. On the other hand, the constraints about non-vanishing correlation functions imply that on a row, if a E^{12} is present then a E^{21} must also be present. This implies that in order to determine a term, we only need to determine the positions of matrices E^{12} and E^{21} along one column only – say the first column – unless there are none.

Suppose that along the first column there are s matrices E^{22}, and q pairs of matrices E^{12} and E^{21}. Then there are $n-s-2q$ matrices E^{11}. In the case where $q=0$, by the discussion above not all values of s are available, and there are exactly four terms:

$$\langle E_1^{11}E_{m+1}^{11}\rangle^n + \langle E_1^{22}E_{m+1}^{22}\rangle^n + \langle E_1^{11}E_{m+1}^{22}\rangle^n + \langle E_1^{22}E_{m+1}^{11}\rangle^n.$$

For $q>0$, all values q from 1 to $[n/2]$ (where $[\cdot]$ means integer part) occur, and all values of s from 0 to $n-2q$ occur. By factorisation, every term characterised by such s and q gives rise to the same product of correlation functions:

$$\langle E_1^{11}E_{m+1}^{22}\rangle^{n-s-2q}\langle E_1^{22}E_{m+1}^{11}\rangle^s\langle E_1^{12}E_{m+1}^{21}\rangle^q\langle E_1^{21}E_{m+1}^{12}\rangle^q.$$

In order to count the number of such terms, consider two possibilities: whether the jump from n to 1 along the column breaks a string of (possibly a vanishing number of) matrices E^{22}, or it breaks a string of matrices E^{11}. In the first case, the number of terms is $p_{q+1}(s)p_q(n-s-2q)$, and in the second, it is $p_{q+1}(n-s-2q)p_q(s)$, where $p_q(s)$ represents the number of partitions of s into a sum of q parts, with the number 0 is also included as a possible part. Hence, the number of such terms is

$$C_n(s,q) = p_{q+1}(s)p_q(n-s-2q) + p_{q+1}(n-s-2q)p_q(s). \tag{3.48}$$

A formula for $p_q(s)$ can be easily obtained by noticing that the function $(1-x)^{-n}$ is precisely the generating function of such coefficients, namely

$$\frac{1}{(1-x)^q} = \sum_{s=0}^{\infty} p_q(s)x^s = \sum_{s=0}^{\infty}\left(\begin{array}{c} q+s-1 \\ q-1 \end{array}\right)x^s, \tag{3.49}$$

where $\left(\begin{array}{c} a \\ b \end{array}\right) = \frac{a!}{b!(a-b)!}$ is the binomial coefficient. We can easily show that the coefficient (3.48) can be written as

$$C_n(s,q) = \frac{n}{n-s-q}\left(\begin{array}{c} q+s-1 \\ q-1 \end{array}\right)\left(\begin{array}{c} n-s-q \\ q \end{array}\right). \tag{3.50}$$

Employing this result and from the discussion above, we find that the correlation function that we want to compute is

$$\begin{aligned}\frac{\langle\Psi|\mathcal{T}_1\mathcal{T}_{m+1}|\Psi\rangle}{\langle\Psi|\Psi\rangle} &= \sum_{q=1}^{[\frac{n}{2}]}\sum_{s=0}^{n-2q} C_n(q,s)\langle E_1^{11}E_{m+1}^{22}\rangle^{n-s-2q}\langle E_1^{22}E_{m+1}^{11}\rangle^s\langle E_1^{12}E_{m+1}^{21}\rangle^q\langle E_1^{21}E_{m+1}^{12}\rangle^q \\ &\quad +\langle E_1^{11}E_{m+1}^{11}\rangle^n + \langle E_1^{22}E_{m+1}^{22}\rangle^n + \langle E_1^{11}E_{m+1}^{22}\rangle^n + \langle E_1^{22}E_{m+1}^{11}\rangle^n. \end{aligned}\tag{3.51}$$

The sum above is relatively complicated to compute. However, it simplifies greatly if we employ the equalities (3.46)-(3.47). We then obtain

$$\begin{aligned}\frac{\langle\Psi|\mathcal{T}_1\mathcal{T}_{m+1}|\Psi\rangle}{\langle\Psi|\Psi\rangle} &= \sum_{q=1}^{[\frac{n}{2}]}\langle E_1^{11}E_{m+1}^{22}\rangle^{n-2q}\langle E_1^{12}E_{m+1}^{21}\rangle^{2q}\sum_{s=0}^{n-2q}C_n(q,s)\\ &\quad +2\langle E_1^{11}E_{m+1}^{11}\rangle^n+2\langle E_1^{11}E_{m+1}^{22}\rangle^n. \end{aligned} \tag{3.52}$$

It is now possible to carry out the sum. The sum in s yields simply

$$\sum_{s=0}^{n-2q}C_n(q,s)=2\left(\begin{array}{c} n \\ 2q \end{array}\right). \tag{3.53}$$

Finally, the sum in q gives

$$\begin{aligned}&2\sum_{q=1}^{[\frac{n}{2}]}\left(\begin{array}{c} n \\ 2q \end{array}\right)\langle E_1^{11}E_{m+1}^{22}\rangle^{n-2q}\langle E_1^{12}E_{m+1}^{21}\rangle^{2q}\\ &=-2\langle E_1^{11}E_{m+1}^{22}\rangle^n+\left(\langle E_1^{11}E_{m+1}^{22}\rangle+\langle E_1^{12}E_{m+1}^{21}\rangle\right)^n+\left(\langle E_1^{11}E_{m+1}^{22}\rangle-\langle E_1^{12}E_{m+1}^{21}\rangle\right)^n \end{aligned} \tag{3.54}$$

Therefore, the final expression for the two-point function of permutation operators is

$$\frac{\langle\Psi|\mathcal{T}_1\mathcal{T}_{m+1}|\Psi\rangle}{\langle\Psi|\Psi\rangle}=\left(\langle E_1^{11}E_{m+1}^{22}\rangle+\langle E_1^{12}E_{m+1}^{21}\rangle\right)^n+\left(\langle E_1^{11}E_{m+1}^{22}\rangle-\langle E_1^{12}E_{m+1}^{21}\rangle\right)^n+2\langle E_1^{11}E_{m+1}^{11}\rangle^n, \tag{3.55}$$

and the entropy becomes

$$\begin{aligned}S_{\{1,m+1\}} &= -(\langle E_1^{11}E_{m+1}^{22}\rangle+\langle E_1^{12}E_{m+1}^{21}\rangle)\log\left[\langle E_1^{11}E_{m+1}^{22}\rangle+\langle E_1^{12}E_{m+1}^{21}\rangle\right]\\ &\quad -(\langle E_1^{11}E_{m+1}^{22}\rangle-\langle E_1^{12}E_{m+1}^{21}\rangle)\log\left[\langle E_1^{11}E_{m+1}^{22}\rangle-\langle E_1^{12}E_{m+1}^{21}\rangle\right]\\ &\quad -2\langle E_1^{11}E_{m+1}^{11}\rangle\log\langle E_1^{11}E_{m+1}^{11}\rangle. \end{aligned} \tag{3.56}$$

Note that in (3.55) we can immediately read-off the eigenvalues of the reduced density matrix (the three quantities that are taken to the power n) and their degeneracies (the integer coefficients of these powers).

It is simple to rewrite this expression in terms of Pauli matrices. Employing the short-hand notation $\langle\sigma_1^z\sigma_{m+1}^z\rangle=z(m)$ and $\langle\sigma_1^+\sigma_{m+1}^-\rangle=s(m)$, we have

$$\begin{aligned}S_{\{1,m+1\}} &= -\frac{(1-z(m)+4s(m))}{4}\log\left[\frac{(1-z(m)+4s(m))}{4}\right]\\ &\quad -\frac{(1-z(m)-4s(m))}{4}\log\left[\frac{(1-z(m)-4s(m))}{4}\right]\\ &\quad -\frac{(1+z(m))}{2}\log\left[\frac{1+z(m)}{4}\right]. \end{aligned} \tag{3.57}$$

From here let us specialise to the case of infinite length, $N\to\infty$. This makes sense because correlation functions of local operators have finite limits. Then, one feature of the expression above is that for $m\to\infty$ the correlation functions $s(m),z(m)\to 0$ by large-distance factorisation, and therefore the entropy at large distances saturates to its maximum value

$$\lim_{m\to\infty}S_{\{1,m+1\}}=2\log(2), \tag{3.58}$$

which is exactly twice the entanglement entropy of a single spin computed above, as expected. One can now evaluate the entanglement entropy of two spins for a great variety of spin-$\frac{1}{2}$ models for which the correlation functions are known.

We will conclude this subsection by providing some numerical results for the entanglement entropy $S_{\{1,m+1\}}$ at particular values of m and Δ. Although the general expressions for the two-point functions involved in (3.57) are given in general in terms of complicated multiple integral representations [39, 38, 37, 40], those integrals have been done at least for small values of m and different values of the anisotropy parameter. Very useful tables listing explicit values of the two-point functions for many values of Δ and $m = 1, 2$ and 3 can be found in [41, 42]. Employing those results, it is possible to evaluate the entropy for various values of the anisotropy parameter as shown in Fig. 2(a). In addition, the two-point functions of spin operators admit a simple form for special values of the anisotropy parameter. One such value is $\Delta = 0$ or $\eta = \frac{\pi}{2}$ which is commonly known as the free Fermion point (see Fig. 2(b)).

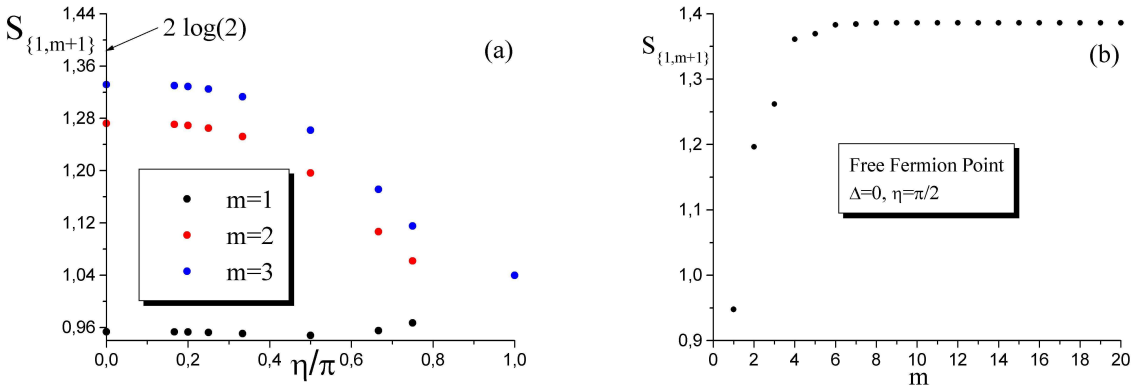

Figure 2: (a) The entanglement entropy of two spins $S_{\{1,m+1\}}$ in the XXZ chain for different values of the anisotropy parameter and $m = 1, 2, 3$. We observe how the entropy tends to grow with m until reaching the value $2\log(2)$ for very large m. An exception to this is the case $\eta = \pi$. In this case the entropy takes the value $\frac{3}{2}\log(2)$ irrespectively of m. This is due to the very special nature of this point, for which the two point function $s(m)$ oscillates between the values $\pm\frac{1}{4}$ as $m \to \infty$ (rather than vanishing). The limit $\eta \to \pi^-$ or $\Delta \to -1^+$ will be discussed at length in Section 5. (b) The entanglement entropy of two spins $S_{\{1,m+1\}}$ at the Free Fermion point, where the correlation functions (see e.g. [43] for a derivation) are given by: $\langle\sigma_1^z\sigma_{m+1}^z\rangle = \frac{2((-1)^m-1)}{\pi^2 m^2}$ and $\langle\sigma_1^+\sigma_{m+1}^-\rangle = \frac{(-1)^m}{2}\prod_{k=1}^{[\frac{m}{2}]}\frac{\Gamma(k)^2}{\Gamma(k-\frac{1}{2})\Gamma(k+\frac{1}{2})}\prod_{k=1}^{[\frac{m+1}{2}]}\frac{\Gamma(k)^2}{\Gamma(k-\frac{1}{2})\Gamma(k+\frac{1}{2})}$.

Finally, we note that the correction terms for the asymptotic behaviour of the entanglement entropy at large m and generic values of the anisotropy parameter can be obtained by employing the results of [44]. In this paper, the asymptotic behaviour of the two-point functions $\langle\sigma_1^z\sigma_{m+1}^z\rangle$ and $\langle\sigma_1^x\sigma_{m+1}^x\rangle$ was obtained using perturbed CFT techniques (the results of [44] were even more general, as they considered time-dependent correlation functions).

Using

$$A = \frac{1}{2(1-\frac{\eta}{\pi})^2}\left(\frac{\Gamma\left(\frac{\eta}{2\pi-2\eta}\right)}{2\sqrt{\pi}\Gamma\left(\frac{\pi}{2\pi-2\eta}\right)}\right)^{\frac{\eta}{\pi}} \exp\left[-\int_0^\infty \frac{dt}{t}\left(\frac{\sinh(\frac{\eta}{\pi}t)}{\sinh t\cosh(1-\frac{\eta}{\pi})t} - \frac{\eta}{\pi}e^{-2t}\right)\right], \quad (3.59)$$

we obtain the following leading asymptotic expression for the entropy:

$$S_{\{1,m+1\}} \sim 2\log(2) - \frac{16A^2}{m^{\frac{2\eta}{\pi}}} - \frac{512A^4}{8m^{\frac{4\eta}{\pi}}} + \mathcal{O}(m^{-\frac{6\eta}{\pi}}, m^{-\frac{\eta}{\pi}-\frac{4\pi}{\eta}+4}, m^{-\frac{\pi}{\eta}}, m^{-2}), \quad (3.60)$$

for $\eta \in (0,\pi)$.

4 Quantum states for chains of infinite length

Infinite-length chains can be described using Hilbert spaces. However, contrarily to the case of finite-length chains, the infinite-dimensional Hilbert spaces $\mathcal{H}_\Delta$ occurring in the limit $N \to \infty$ depend, in a sense, on the parameter Δ characterising the Hamiltonian (3.36)[§]. More precisely, $\mathcal{H}_\Delta$ is formed by the completion of the set of finite-energy eigenvectors of the Hamiltonian H_Δ, and these are sets of very different vectors for different values of Δ. In particular, the Hilbert spaces $\mathcal{H}_\Delta$, $\mathcal{H}_{\Delta'}$ are orthogonal for $\Delta \neq \Delta'$; e.g. in the limit of infinite volume, the overlap ${}_\Delta\langle\psi|\psi\rangle_{\Delta'}/\sqrt{{}_\Delta\langle\psi|\psi\rangle_\Delta\,{}_{\Delta'}\langle\psi|\psi\rangle_{\Delta'}}$ between the two ground states tend to zero. Due to this, the description of infinite-length quantum chains via Hilbert spaces is not very well adapted to the study of quantum averages of localised observables. Indeed, the quantum average of an operator that factorises to the identity on all sites except finitely many is well defined on the Hilbert spaces $\mathcal{H}_\Delta$ for any Δ (in the range $-1 < \Delta \leq 1$ considered), and smooth as a function of Δ. The Hilbert space description does not provide any natural topology in agreement with continuity in Δ. The study of the limit $\Delta \to -1^+$ requires a more adapted description.

For Hilbert spaces of finite dimension, knowing all quantum averages uniquely fix the quantum state. From this, one way of describing quantum states (pure or mixed) that is more convenient when considering the infinite-volume limit, is through linear functionals representing quantum averages. Let us consider the infinite set of vector spaces $\{V_i : i \in \mathbb{Z}\}$: this is the set of sites of the chain as usual, except that the index can be both positive and negative (i.e. there is no boundary). For any finite block of sites A, let us consider the complex vector space $\mathcal{E}_A$ of operators supported on A: the space $\otimes_{i\in A}\mathrm{End}(V_i)$ with action like the identity on all sites $j \notin A$. Let us further consider the complex vector space $\mathcal{E} = \cup_A \mathcal{E}_A$ of finitely-supported operators; explicitly, these are the finite linear combinations of finite products of elementary matrices $E_i^{\epsilon\epsilon'}$.

Definition 4.1 *The space of quantum states on the infinite-length chain, which we will denote by $\mathcal{F}$, is the space of all linear functionals $\psi : \mathcal{E} \to \mathbb{C}$ that are real-linear:*

$$\psi(E)^* = \psi(E^\dagger) \quad (E \in \mathcal{E}) \quad (4.61)$$

and normalised

$$\psi(1) = 1. \quad (4.62)$$

[§]Of course, as a Hilbert space, the space with an infinite countable basis is unique.

The physical meaning of $\psi(E)$, for hermitian E, is simply the average of the observable E in the physical state represented by ψ.

For infinite length, this definition of a quantum state is extremely useful, because it puts in a common space the quantum states of any quantum chain with well-defined correlation functions: for instance, the XXZ chains for $-1 < \Delta \leq 1$. Indeed, to every ray $\{a|\psi\rangle : a \in \mathbb{C}\}$ lying in the Hilbert space $\mathcal{H}_\Delta$ for some Δ, we associate a quantum state in $\mathcal{F}$ defined by

$$\psi(E) := \frac{\langle\psi|E|\psi\rangle}{\langle\psi|\psi\rangle}, \quad E \in \mathcal{E}. \tag{4.63}$$

This definition of the space of quantum states is also very natural from the viewpoint of the Rényi entropies $S_A^{\text{Rényi}}(n)$ for integer n. Given a quantum state $\psi \in \mathcal{F}$, we can construct the linear functional $\Psi := \psi^{\otimes n}$ on $\mathcal{E}^{\otimes n}$, and the Rényi entropy of ψ with respect to a finite set of sites A is expressed using our replica permutation operators:

$$S_A^{\text{Rényi}}(n) = \frac{1}{1-n} \log\left(\Psi\left(\mathcal{T}_A\right)\right). \tag{4.64}$$

Note that indeed, the permutation operator $\mathcal{T}_A$ associated with a finite block of sites A is a finitely-supported operator. Naturally, since the density matrix ρ_A is completely determined by the fundamental blocks on the sites A, it can also be defined in the infinite-volume case. In particular, we have

$$\mathrm{Tr}\left(\rho_A^n\right) = \Psi\left(\mathcal{T}_A\right). \tag{4.65}$$

Recall the concept of local-unitary transformations introduced in section 2. This concept can naturally be included into the infinite-length setting. Given disjoint blocks of sites A_k, $k = -\infty, \ldots, \infty$, a *block-defined transformation* is a doubly-infinite sequence $U = (U_k : k \in \mathbb{Z})$ of elements $U_k \in \mathcal{E}_{A_k}$ that are invertible, $U_k^{-1} \exists\ \forall\ k$. To any such U we can associate an adjoint action on $\mathcal{E}$, given by $\mathrm{Ad}\, U(E) := \prod_k U_k^{-1} E U_k$, $E \in \mathcal{E}$. The product is finite, hence this is a well-defined action. This gives rise to an action on quantum states, defined by $U \cdot \psi = \psi \circ \mathrm{Ad}\, U$ for any $\psi \in \mathcal{F}$. A local-unitary transformation is a block-defined transformation, where $A_k = \{k\}$ all U_k are unitary. It stays true in the infinite-length setting that $\mathcal{T}_A$ is local-unitarily invariant.

In order to discuss convergence of quantum states in $\mathcal{F}$, we define a topology (in fact, a geometry), via compact convergence of fundamental blocks. This topology in fact works (and will be used) more generally for linear functionals without the normalisation condition ($\psi(1) = 1$). This is inspired by the usual compact convergence topology in function theory. Consider a sequence of functions on $\mathcal{F}$ parametrised by an integer $k \geq 0$, defined by

$$d_k(\psi_1, \psi_2) := \sqrt{\sum_{\{\epsilon_i, \epsilon_i' : i = -k, \ldots, k\}} \left| \psi_1\left(\prod_{i=-k}^{k} E_i^{\epsilon_i \epsilon_i'}\right) - \psi_2\left(\prod_{i=-k}^{k} E_i^{\epsilon_i \epsilon_i'}\right)\right|^2} \quad (\psi_1,\ \psi_2\ \in \mathcal{F}).$$

This is a natural definition, because it is invariant under a change of orthonormal basis in the space of linear operators on the subchain of $2k+1$ sites centered at 0 (with the inner product given by $(E, E') = \mathrm{Tr}(E^\dagger E')$). Consider then the distance function

$$d(\psi_1, \psi_2) := \sum_{k=0}^{\infty} \frac{2^{-k} d_k(\psi_1, \psi_2)}{1 + d_k(\psi_1, \psi_2)}. \tag{4.66}$$

Definition 4.2 *The compact convergence topology on the space of quantum states $\mathcal{F}$ is that of open balls induced from the distance function (4.66).*

This topology is the most convenient when considering finitely-supported observables. Indeed, by the usual arguments of compact convergence, one can see that every Cauchy sequence $(\psi_j \in \mathcal{F} : j = 1, 2, \ldots)$ gives rise, for any finitely-supported operator E, to a Cauchy sequence $(\psi_j(E) : j = 1, 2, \ldots)$. In other words, the limit of a Cauchy sequence in $\mathcal{F}$ is in $\mathcal{F}$: the space of quantum states is complete. Moreover, again by standard arguments of compact convergence, if, for a sequence $(\psi_j \in \mathcal{F} : j = 1, 2, \ldots)$, all fundamental blocks $\psi_j\left(\prod_{i=m_1}^{m_2} E_i^{\epsilon_i \epsilon'_i}\right)$ converge as $j \to \infty$, then the sequence converges, and the limit is a quantum state whose action on elementary matrices agrees with the limit of the fundamental blocks. That is, this is the topology that associate convergence of quantum states to convergence of averages of all finitely-extended observables.

We remark that this topology also allows us to describe the infinite-length limit of quantum chains. Indeed, to any sequence of vectors $|\psi\rangle^{(k)}$ in the space spanned by the sites from $-k$ to k, for $k = 1, 2, 3, 4, \ldots$, we can associate a sequence ψ_k of elements in $\mathcal{F}$, by $\psi_k(E) = {}^{(k)}\langle\psi|E|\psi\rangle^{(k)}$ if $E \in \mathcal{E}_{\{-k,\ldots,k\}}$, and $\psi_k(E) = 0$ otherwise. If $|\psi\rangle^{(k)}$ describe ground states, and if the infinite-volume limit of the chain exists, then this sequence converges, hence define a state $\lim_{k\to\infty} \psi_k \in \mathcal{F}$. The same procedure can be applied for any sequence of linear functionals on spaces $\mathcal{E}_{A_k}$ with growing A_k such that $\lim_{k\to\infty} A_k = \mathbb{Z}$. Let us also note that in this context, there is no *a priori* clear distinction between pure states and mixed states in infinite volume. Indeed, for any density matrix ρ on a finite number of sites, it is always possible to construct a pure state on twice as many sites, such that the reduced density matrix equals ρ. Hence, to a sequence of density matrices leading to a converging sequence of quantum states, we can associate a sequence of vectors giving rise to the same limit quantum state (and vice versa).

5 The limit $\Delta \to -1^+$

We now wish to study the state occurring in the limit $\Delta \to -1^+$ of the infinite-length XXZ model in compact convergence topology. Using the calculation Rules 2.1, as well as exact results for fundamental blocks of the XXZ models found in the literature, we provide a full description of the reduced density matrix associated to any finite subset of sites. Our main result is that the reduced density matrix associated with a number m of sites (no matter what their positions are) has only $m + 1$ non-vanishing eigenvalues which are given by

$$\lambda_k = \frac{1}{2^m} \begin{pmatrix} m \\ k \end{pmatrix} \qquad \text{with} \qquad k = 0, \ldots, m. \tag{5.67}$$

Therefore, for m odd each eigenvalue is twice degenerate, whereas for m even all eigenvalues but one are twice degenerate.

5.1 The XXZ quantum state in the limit $\Delta \to -1^+$

From the explicit formulas obtained in [39, 38, 37, 40], it follows that the limit $\Delta \to -1^+$ of the fundamental blocks associated with the ground state of the Hamiltonian (3.36) exists and is finite. More precisely, specializing the multiple integral formulae obtained in [39, 38, 37, 40], we find that in the limit $\Delta \to -1^+$, the non-vanishing fundamental blocks associated to an index set $A = \{j_1, j_2, \ldots, j_m\}$ (with $j_k \neq j_{k'}$ for $k \neq k'$) reduce to

$$\lim_{\Delta\to-1^+} \langle E_{j_1}^{\epsilon_1\epsilon'_1} E_{j_2}^{\epsilon_2\epsilon'_2} \cdots E_{j_m}^{\epsilon_m\epsilon'_m} \rangle = \frac{1}{2^m} \prod_{j\in B} (-1)^j, \tag{5.68}$$

where B is the subset of sites at which either an operator E^{12} or an operator E^{21} sits:

$$B = \{j_k : \epsilon_k \neq \epsilon'_k\} \subset A.$$

Note that the indices $j_1, \ldots, j_m$ in formula (5.68) are not necessarily consecutive, contrarily to the formula for fundamental blocks in [37, 36]. It is simple to check that (5.68) is consistent with the relation $\mathbf{1} = E^{11}_j + E^{22}_j$.

Let us consider the ground state $|\psi\rangle_\Delta$ of the Hamiltonian H_Δ. For $\Delta \in (-1, 1]$, the corresponding quantum states ψ_Δ all lie in $\mathcal{F}$. Moreover, by formula (5.68), all fundamental blocks converge in the limit where Δ tends to -1 from above. Hence, the limit $\lim_{\Delta\to -1^+} \psi_\Delta$ exists and is a quantum state of the infinite-volume chain. We will denote this limit by

$$\psi_- := \lim_{\Delta\to -1^+} \psi_\Delta \ \in \mathcal{F}. \tag{5.69}$$

This quantum state is completely characterised by formula (5.68):

$$\psi_-\left(E^{\epsilon_1\epsilon'_1}_{j_1} E^{\epsilon_2\epsilon'_2}_{j_2} \cdots E^{\epsilon_m\epsilon'_m}_{j_m}\right) = \begin{cases} \dfrac{1}{2^m}\displaystyle\prod_{j\in B}(-1)^j & \text{equal numbers of } E^{12} \text{ and } E^{21} \\ 0 & \text{otherwise.} \end{cases} \tag{5.70}$$

We would now like to study this state by computing its Rényi and von Neumann entanglement entropies. As is clear from (5.70), a very special feature of this state is that its correlation functions are extremely simple. Hence, we will be able to find analytic expressions for the Rényi entropies and deduce the exact eigenvalues and degeneracies of the reduced density matrices; these are inaccessible for generic values of Δ.

5.2 Rényi and von Neumann entanglement entropies of the state ψ_-

The Rényi entropy (1.3) can be evaluated using the replica permutation operators via (4.64). The present subsection provides a proof of the following proposition, which is in agreement with the first point stated at the beginning of this section, equation (5.67).

Proposition 1 *Consider the state ψ_-, obtained in the limit $\Delta \to -1^+$ of the ground state ψ_Δ in the compact convergence topology. Its Rényi and von Neumann entanglement entropies associated with any set of m sites are given by*

$$S^{\text{Rényi}}_A(n) = -\frac{nm\log 2}{1-n} + \frac{1}{1-n}\log\left(\sum_{k=0}^{m}\binom{m}{k}^n\right) \tag{5.71}$$

and

$$S_A = m\log 2 - \frac{1}{2^m}\sum_{k=0}^{m}\binom{m}{k}\log\binom{m}{k}. \tag{5.72}$$

The large-m asymptotics of these quantities are given by

$$S^{\text{Rényi}}_A(n) = \frac{1}{2}\log\left(\frac{\pi m}{2}\right) + \frac{\log(n)}{2(n-1)} + O\left(m^{-1}\right), \quad S_A = \frac{1}{2}\log\left(\frac{\pi m}{2}\right) + \frac{1}{2} + O\left(m^{-1}\right). \tag{5.73}$$

The leading term in the asymptotics of the Rényi entropy is therefore independent of n.

Let us start with the simplest non-trivial case $n = 2$. The specialisation of (2.18) to $n = 2$ immediately gives the formula

$$\mathrm{Tr}\left(\rho_A^2\right) = \sum_{\epsilon_i', \epsilon_i = 1}^{2} \psi_- \left(E_{j_1}^{\epsilon_1 \epsilon_1'} E_{j_2}^{\epsilon_2 \epsilon_2'} \cdots E_{j_m}^{\epsilon_m \epsilon_m'}\right) \psi_- \left(E_{j_1}^{\epsilon_1' \epsilon_1} E_{j_2}^{\epsilon_2' \epsilon_2} \cdots E_{j_m}^{\epsilon_m' \epsilon_m}\right). \tag{5.74}$$

Notice that many of the correlation functions in this sum are vanishing: a fundamental block is non-zero if and only if it involves equal numbers of matrices E^{12} and E^{21}.

Given the structure of the product (5.74) it is easy to see that the products of $(-1)^j$ in (5.68) will not play a role, as matrices E^{12} and E^{21} appear at exactly the same sites in both correlation functions, so that all phase factors cancel out. Therefore, the sum (5.74) reduces to

$$\mathrm{Tr}\left(\rho_A^2\right) = \frac{\text{number of non-vanishing m-site fundamental blocks}}{2^{2m}}. \tag{5.75}$$

The number of non-vanishing m-site blocks can be easily obtained by simple combinatoric arguments. A generic non-vanishing fundamental block will have s operators E^{11}, q pairs of operators E^{12} and E^{21}, and $m - s - 2q$ operators E^{22} at the remaining sites. The total number of such blocks is simply

$$\frac{m!}{s!(q!)^2(m-s-2q)!}, \tag{5.76}$$

therefore

$$\mathrm{Tr}\left(\rho_A^2\right) = \frac{1}{2^{2m}} \sum_{q=0}^{[\frac{m}{2}]} \sum_{s=0}^{m-2q} \frac{m!}{s!(q!)^2(m-s-2q)!} = \frac{\Gamma\left(\frac{1}{2}+m\right)}{\sqrt{\pi}\Gamma\left(1+m\right)}. \tag{5.77}$$

The Rényi entropy (1.3) is given by

$$S_m^{\text{Rényi}}(2) = -\log\left(\frac{\Gamma\left(\frac{1}{2}+m\right)}{\sqrt{\pi}\Gamma\left(1+m\right)}\right), \tag{5.78}$$

and, for m large behaves asymptotically as

$$S_m^{\text{Rényi}}(2) = \frac{1}{2}\log(\pi m) + O(m^{-1}). \tag{5.79}$$

The calculation can be extended to higher values of n. The Rényi entropy for generic n will be obtained form a sum over an n-fold product of m-site fundamental blocks. A feature of Rules 2.1 is that for every site, there must be as many matrices E^{12} as there are matrices E^{21} distributed amongst the n copies. Hence, as in the $n = 2$ case, the $(-1)^j$ factors in (5.68) all cancel out when multiplying the n fundamental blocks together, because any possible factor -1 will always be present an even number of times. This means that once more, the computation reduces to combinatorially working out the number of non-vanishing products of fundamental blocks that occur.

A simplification to this combinatorial calculation is obtained from two general consequences of Rules 2.1. First, once a choice of elementary matrices has been made for the first $n-1$ fundamental blocks, the choice for the n^{th} one exists and is unique. This is because the rules say if, on any given site, we have the elementary matrices $E^{\epsilon_+ \epsilon_+'}$ at copy $\alpha + 1$ and $E^{\epsilon_- \epsilon_-'}$ at copy $\alpha - 1$, then the elementary matrix at copy α is fixed to be $E^{\epsilon_+' \epsilon_-}$. Second, if the first $n-1$ fundamental blocks are non-vanishing and satisfy the rules, then the unique choice of the last block also is non-vanishing. This is because there is the same number of matrices E^{12} as there

is of E^{21} in total in the first $n-1$ blocks (since this is true in every block). Since at every site there can only be, in the $n-1$ first copies, an equal number of E^{12} and E^{21} or a surplus by one of either E^{12} or E^{21}, then the number of sites where there is a surplus of E^{12} must be the same as that where there is a surplus of E^{21}. Hence, Rules 2.1 imply that on the last block, there will be the same numbers of E^{12} and E^{21}. Therefore, putting these three observations together, in order to count the number of non-vanishing products of n fundamental blocks occurring, we only need to count the number of choices of elementary matrices for the first $n-1$ fundamental blocks that make these blocks non-vanishing and that satisfy Rules 2.1.

Let us now analyse the case $n=3$, where the quantity $\mathrm{Tr}\left(\rho_A^3\right)$ is given by a sum over triple products of m-site fundamental blocks. We can depict Rules 2.1 through diagrams such as

1st fundamental block		E_j^{11}				E_j^{12}	
2nd fundamental block	$\swarrow$ E_j^{11} $\downarrow$	or	$\searrow$ E_j^{21} $\downarrow$		$\swarrow$ E_j^{11} $\downarrow$	or	$\searrow$ E_j^{21} $\downarrow$
3rd fundamental block	E_j^{11}	or	E_j^{12}		E_j^{21}	or	E_j^{22}

and similarly for E_j^{22} and E_j^{21} by exchanging super-indices $1,2$ everywhere.

Let us consider the first fundamental block. Let it contain s matrices E^{11}, q pairs of matrices E^{12}, E^{21}, and $m-s-2q$ matrices E^{22}. Each such fundamental block can appear in conjunction with various choices of the second fundamental block. According to the rules above, every matrix E^{11} or E^{12} in the first can be followed by a matrix E^{11} or E^{21} in the second. Similarly, every matrix E^{22} or E^{21} in the first can be followed by a matrix E^{22} or E^{12} in the second. The number of second fundamental blocks containing a pairs of matrices E^{12} and E^{21} is given by

$$\left(\begin{array}{c} s+q \\ a \end{array}\right)\left(\begin{array}{c} m-s-q \\ a \end{array}\right). \tag{5.80}$$

Summing over all possible values of a gives

$$\sum_{a=0}^{\min(s+q,m-s-q)} \left(\begin{array}{c} s+q \\ a \end{array}\right)\left(\begin{array}{c} m-s-q \\ a \end{array}\right) = \left(\begin{array}{c} m \\ s+q \end{array}\right). \tag{5.81}$$

Therefore, the total number of distinct triple products leads to

$$\begin{aligned} \mathrm{Tr}\left(\rho_A^3\right) &= \frac{1}{2^{3m}} \sum_{q=0}^{[\frac{m}{2}]} \sum_{s=0}^{m-2q} \frac{m!}{s!(q!)^2(m-s-2q)!} \left(\begin{array}{c} m \\ s+q \end{array}\right) \\ &= \frac{\Gamma\left(\frac{1}{2}+m\right)}{2^m\sqrt{\pi}\,\Gamma\left(1+m\right)}\, {}_3F_2\left(\left\{\frac{1}{2}-m,-m,-\frac{m}{2}\right\},\left\{1,\frac{1}{2}-m\right\};1\right). \end{aligned} \tag{5.82}$$

The leading asymptotic behaviour of the Rényi entropy can be extracted by exploiting the fact that for large m

$$\begin{aligned} &{}_3F_2\left(\left\{\frac{1}{2}-m,-m,-\frac{m}{2}\right\},\left\{1,\frac{1}{2}-m\right\};1\right) \sim {}_3F_2\left(\left\{-m,-m,-\frac{m}{2}\right\},\left\{1,-m\right\};1\right) \\ &= {}_2F_1\left(\left\{-\frac{m}{2},-\frac{m}{2}\right\},\left\{1\right\};1\right) = \frac{m!}{\Gamma\left(1+\frac{m}{2}\right)^2}. \end{aligned} \tag{5.83}$$

Substituting this into (5.82) and employing Stirling's approximation for the Gamma functions we obtain,

$$S_m^{\text{Rényi}}(3) = \frac{1}{2}\log(\frac{\pi m}{2}) + O(1, m^{-1}). \tag{5.84}$$

Unfortunately, the approximation above is too crude and does not allow to extract the correct constant $1/4\log(3)$ as predicted by (5.73). This is the same leading behaviour as in (5.79) which is incompatible with the CFT prediction according to which the coefficient of $\log(m)$ should be a function of n.

It is possible to extend the previous combinatorial arguments to higher (generic) values of n. Again, from Rules 2.1, we know that it is from the set of matrices E^{11} and E^{21} in the fundamental block of copy α that emerge all matrices E^{11} and E^{12} in the copy $\alpha+1$. The same is true if all super-indices 1,2 are exchanged. Let us consider the α^{th} fundamental block, for $\alpha = 1, 2, \ldots, n-1$. Let it contain s_α matrices E^{11}, q_α pairs of matrices E^{12}, E^{21}, and $m - s_\alpha - 2q_\alpha$ matrices E^{22} (with $s := s_1$ and $q := s_1$). Since $q_{\alpha+1}$ matrices E^{21} are chosen from the $s_\alpha + q_\alpha$ matrices E^{11} and E^{12}, the rest must be all matrices E^{11}, so we must have

$$s_{\alpha+1} = s_\alpha + q_\alpha - q_{\alpha+1}. \tag{5.85}$$

Hence, we find

$$s_{\alpha+1} + q_{\alpha+1} = s_\alpha + q_\alpha \;\Rightarrow\; s_\alpha + q_\alpha = s + q \;\forall\, \alpha. \tag{5.86}$$

Therefore, from expression (5.80), the number of fundamental blocks at copy α is given by

$$\left(\begin{array}{c} s+q \\ q_\alpha \end{array}\right)\left(\begin{array}{c} m-s-q \\ q_\alpha \end{array}\right). \tag{5.87}$$

Summing over all possible values of q_α for $\alpha = 2, \ldots, n-1$ and using formula (5.81) gives

$$\text{Tr}\,(\rho_A^n) = \frac{1}{2^{nm}} \sum_{q=0}^{[\frac{m}{2}]} \sum_{s=0}^{m-2q} \frac{m!}{s!(q!)^2(m-s-2q)!} \left(\begin{array}{c} m \\ s+q \end{array}\right)^{n-2}. \tag{5.88}$$

From the definition (1.3) it is clear that the formula above should give exactly the sum over all n-powers of the eigenvalues of the density matrix associated to the state ψ^-. However, this is not obvious from (5.88) in its present form. In order to make this structure clearer it is useful to rewrite (5.88) in a slightly different way. We will introduce the new variable $k = s + q$ and write the binomial coefficient to the power $n-2$ as a product of powers n and -2. The sum becomes,

$$\text{Tr}\,(\rho_A^n) = \frac{1}{2^{nm}} \sum_{q=0}^{[\frac{m}{2}]} \sum_{k=q}^{m-q} \frac{(k!(m-k)!)^2}{(k-q)!(q!)^2(m-k-q)!m!} \left(\begin{array}{c} m \\ k \end{array}\right)^n. \tag{5.89}$$

Exchanging the two sums we find the equivalent expression:

$$\text{Tr}\,(\rho_A^n) = \frac{1}{2^{nm}} \sum_{k=0}^{m} \sum_{q=0}^{m-k} \frac{(k!(m-k)!)^2}{(k-q)!(q!)^2(m-k-q)!m!} \left(\begin{array}{c} m \\ k \end{array}\right)^n = \frac{1}{2^{nm}} \sum_{k=0}^{m} \left(\begin{array}{c} m \\ k \end{array}\right)^n, \tag{5.90}$$

where the last equality follows from the remarkable identity

$$\sum_{q=0}^{m-k} \frac{(k!(m-k)!)^2}{(k-q)!(q!)^2(m-k-q)!m!} = 1. \tag{5.91}$$

The result (5.90) clearly identifies the non-vanishing eigenvalues of the density matrix as (5.67) and provides a much simpler expression for the von Neumann and Rényi entropies, given by (5.71) and (5.72).

Even though we have not been able to carry out the sums explicitly, it is possible to extract the leading behaviour of (5.71) and (5.72) for large m. First, we transform the last sum in (5.90) into a multiple integral using a generating function procedure:

$$\begin{aligned}\mathrm{Tr}\,(\rho_A^n) &= \frac{1}{2^{mn}}\frac{1}{(2\pi i)^{n-1}}\oint_0 \prod_{j=1}^{n-1}\frac{dx_j}{x_j}\ \prod_{j=1}^{n-1}(1+x_j)^m\ \left(1+\prod_{j=1}^{n-1}x_j^{-1}\right)^m \\ &= \frac{1}{(2\pi)^{n-1}}\int_{-\pi}^{\pi}\prod_{j=1}^{n-1}d\theta_j\ \prod_{j=1}^{n-1}\cos^m\left(\frac{\theta_j}{2}\right)\ \cos^m\left(\sum_{j=1}^{n-1}\frac{\theta_j}{2}\right). \qquad (5.92)\end{aligned}$$

Then, we evaluate the large-m asymptotic using a saddle-point analysis. The main contribution to the integral at large-m will be obtained when the integrand is evaluated at $\theta_j \sim 0$ for all j. The leading asymptotics is evaluated by using $\cos(\theta/2) = e^{-\theta^2/2+O(\theta^4)}$:

$$\begin{aligned}\mathrm{Tr}\,(\rho_A^n) &\sim \frac{1}{(2\pi)^{n-1}}\int_{-\infty}^{\infty}\prod_{j=1}^{n-1}d\theta_j\ \exp\left[-\frac{m}{8}\left(\sum_{j=1}^{n-1}\theta_j^2+\left(\sum_{j=1}^{n-1}\theta_j\right)^2\right)\right] \qquad (5.93)\\ &= \frac{1}{(2\pi)^{n-1}}\int_{-\infty}^{\infty}\prod_{j=1}^{n-1}d\theta_j\ \exp\left[-\frac{m}{8}\left(n\theta_1^2+\sum_{j=2}^{n-1}\theta_j^2\right)\right] \\ &= \frac{1}{\sqrt{n}}\left(\frac{2}{\pi m}\right)^{\frac{n-1}{2}}. \qquad (5.94)\end{aligned}$$

Corrections coming from the $O(\theta^4)$ terms in the exponential give rise to a factor $1+O(m^{-1})$.

5.3 Discussion

In order to discuss the results of Proposition 1, we construct the state ψ_- in a different way. Let $\mathbb{P}_z$ be the operation, on the space of finitely-supported operators, that projects onto those keeping the z component of the spin:

$$\begin{aligned}\mathbb{P}_z : \qquad \mathcal{E} &\to \mathcal{E} \quad \text{(linearly)} \\ \prod_{j\in A}E_j^{\epsilon_j,\epsilon'_j} &\mapsto \delta_{0,\sum_{j\in A}(\epsilon_j-\epsilon'_j)}\prod_{j\in A}E_j^{\epsilon_j,\epsilon'_j}. \qquad (5.95)\end{aligned}$$

Further, let U be the following local-unitary operator:

$$U = \prod_{j\in 2\mathbb{Z}+1}\sigma_j^z, \qquad (5.96)$$

and let $\psi_{\hat{e}_x}$ be the following quantum state:

$$\psi_{\hat{e}_x} = \bigotimes_{j\in\mathbb{Z}}\psi_{\hat{e}_x;j}, \qquad (5.97)$$

where $\psi_{\hat{e}_x;j} : \mathcal{E}_{\{j\}} \to \mathbb{C}$ is the average, on site j, obtained from the vector $|\psi_{\hat{e}_x}\rangle_j := (|\uparrow\rangle_j + |\downarrow\rangle_j)/\sqrt{2}$ representing a spin pointing in the positive x direction (this is the eigenvector of σ_j^x

with eigenvalue 1). Note that the right-hand side of (5.97) is a converging doubly-infinite tensor product in the compact convergence topology. Then, it is a simple matter to see that

$$\psi_- = U \cdot \psi_{\hat{e}_x} \mathbb{P}_z. \tag{5.98}$$

Indeed, from (5.97) we notice that $\psi_{\hat{e}_x;j}\left(E_j^{\epsilon,\epsilon'}\right) = 1/2$ for all ϵ, ϵ'. Using that $\mathrm{Ad}\, U\left(E_j^{\epsilon,\epsilon'}\right) = (-1)^j E_j^{\epsilon,\epsilon'}$ for $\epsilon \neq \epsilon'$, and that $\mathrm{Ad}\, U\left(E_j^{\epsilon,\epsilon'}\right) = E_j^{\epsilon,\epsilon'}$ for $\epsilon = \epsilon'$, we immediately find that the right-hand side of (5.98) reproduces formula (5.70). Note that in (5.98), the order of the operations $U\cdot$ and $\mathbb{P}_z$ is irrelevant, since they commute (i.e. $[\mathrm{Ad}\, U\,,\, \mathbb{P}_z] = 0$).

The form (5.98) of the state ψ_- points to the following construction. For each $k = 0, 1, 2, \ldots$, consider the Hilbert space $\otimes_{i=-k}^{k} V_i$, and the vectors where all spins point in the positive x direction: $|\psi_{\hat{e}_x}\rangle^{(2k+1)} := \prod_{i=-k}^{k} |\psi_{\hat{e}_x}\rangle_i$. Of course, these vectors can be written as linear combinations of vectors with spins pointing in z directions (here, we use the standard values $\pm 1/2 \equiv \uparrow, \downarrow$ for the spin variables s_i, instead of the numbers $1, 2$ respectively):

$$|\psi_{\hat{e}_x}\rangle^{(2k+1)} = \frac{1}{(\sqrt{2})^{2k+1}} \sum_{\{s_i = \pm\frac{1}{2} : i = -k, \ldots, k\}} \bigotimes_{i=-k}^{k} |s_i\rangle_i.$$

Now consider the Hilbert space $\otimes_{i=-k}^{k} V_i \otimes V_{\mathrm{env}}$ with $V_{\mathrm{env}} \cong \mathbb{C}^{2k+2}$. The space V_{env} can be though of as a spin-$(k+1/2)$ module, with orthonormal basis vectors $|S\rangle_{\mathrm{env}}$, $S \in \{-k-1/2, \ldots, k+1/2\}$ of spins $S/2$. Take the vectors $|\psi_k\rangle$ as follows:

$$|\psi_k\rangle = \frac{1}{(\sqrt{2})^{2k+1}} \sum_{\{s_i = \pm\frac{1}{2} : i = -k, \ldots, k\}} \bigotimes_{i=-k}^{k} |s_i\rangle_i \otimes \left| -\sum_{i=-k}^{k} s_i \right\rangle_{\mathrm{env}}. \tag{5.99}$$

Essentially, we have adjoined to every vector in the sum an additional degree of freedom with a spin exactly opposite to the total spin of the original chain (the sites from $-k$ to k), in such a way that all vectors have total spin 0 (in the z direction). In the sub-sum of vectors where the original chain has a given total spin, the adjoined vector just factorises out, so that when calculating averages, the resulting sub-sum of matrix elements is unchanged. Hence, the average in $|\psi_k\rangle$ of any product $\prod_{j=-k}^{k} E_j^{\epsilon_j,\epsilon'_j}$ that preserve the total spin of the original chain is exactly equal to the average in $|\psi_{\hat{e}_x}\rangle^{(2k+1)}$. However, the average of such elementary matrices in $|\psi_k\rangle$ is zero if they do not preserve the total spin.

As usual, from $|\psi_k\rangle$ we can form a linear functional ψ_k on $\mathcal{E}_{\{-k,\ldots,k\}}$. By the discussion above, we have

$$\psi_k\left(\prod_{j=-k}^{k} E_j^{\epsilon_j,\epsilon'_j}\right) = \begin{cases} {}^{(2k+1)}\langle\psi_{\hat{e}_x}| \prod_{j=-k}^{k} E_j^{\epsilon_j,\epsilon'_j} |\psi_{\hat{e}_x}\rangle^{(2k+1)} & \text{total } z \text{ component preserved} \\ 0 & \text{otherwise.} \end{cases}$$

We may now take the limit

$$\psi_\infty := \lim_{k\to\infty} \psi_k. \tag{5.100}$$

Since the averages in the states $|\psi_{\hat{e}_x}\rangle^{(2k+1)}$ are stable as k increases, and since the linear functionals act on increasing subsets of the chain whose limit is the whole chain, we find that the limit exists in the compact convergence topology. We have $\psi_\infty = \psi_{\hat{e}_x}\, \mathbb{P}_z$, hence

$$\psi_- = U \cdot \psi_\infty. \tag{5.101}$$

The state $\psi_{\hat{e}_x}$ is factorisable, hence has entanglement entropy equal to 0. The higher entanglement entropy of (5.98) (in particular, the diverging behaviour at large m) comes from the interplay between this factorised state where spins point in x directions, and the condition of having a total z-component equal to 0.

Construction (5.99), (5.100), (5.101) gives some insight into this interplay. It makes it clear that the extra entanglement entropy generated by the presence of the operator $\mathbb{P}_z$, i.e. by the condition of preserving the z-component, is due to an extra entanglement with the additional degree of freedom V_{env}. This degree of freedom can be interpreted as an "environment", which couples with the "system", the sites from $-k$ to k, via the z-component of the total spin. The system can be seen as a random collection of spins up and down, all configurations having equal probabilities. Such a state has zero entanglement entropy with respect to any subsystem. However, the coupling generates entanglement between the system and the environment, which is picked up when measuring the entanglement between a subsystem and the rest. Since the environment is infinite-dimensional in the infinite-k limit, its capacity for entanglement is infinite, hence as the number of sites m of the subsystem increases, the entanglement entropy increases. On the other hand, since the environment does not couple to each individual spin separately, the entanglement entropy increases at a rate that is less than linear in m. The number of blocks of system states that couple to separate environment states is the number of possible values of the z-component of the total spin. For m sites, this is $m+1$, hence we can indeed expect a logarithmic behaviour in m for the entanglement entropy at large m. Since the blocks have different sizes, they have different probabilities of occurring, hence we may indeed expect $b \log m$ for some $b < 1$. In fact, the size of a block with total z-spin equal to $k - m/2$, for k between 0 and m, is simply the binomial coefficient $\begin{pmatrix} m \\ k \end{pmatrix}$. This explains the eigenvalues of the reduced density matrix, from which we derived the $(1/2)\log m$ behaviour.

Besides explaining the features of the entanglement entropy of the state ψ_-, this construction also gives an insight into the way the ground state ψ_Δ of the XXZ model tends to ψ_- as $\Delta \to -1^+$. First, note that $U \cdot \psi_{\hat{e}_x}$ is a ground state of the XXZ model at $\Delta = -1$, because (as is well known) the Hamiltonian of this model is simply obtained from a U transform of the Hamiltonian of the *ferromagnetic* XXX model – the ground state energy of the latter is highly degenerate, and $\psi_{\hat{e}_x}$ is a possible ground state. We expect that as $\Delta \to -1^+$, there is an increasing characteristic length ξ such that: 1) on scales much below ξ, sites are essentially randomly up and down (in the z-direction), with appropriate coefficients so that they locally reproduce the ground state $U \cdot \psi_{\hat{e}_x}$ of the XXZ model at $\Delta = -1$; and 2) on scales above ξ, the total spin is more likely to be zero, as it should be for the XXZ model for $-1 < \Delta \leq 1$. As $\Delta \to -1^+$, the "inner" sites, on any finite scales, are described by the state $U \cdot \psi_{\hat{e}_x}$, and the "outer" sites, beyond $\xi \to \infty$, are collectively described by the single degree of freedom V_{env}, whose entanglement with the inner sites, necessary to keep the total spin to zero, projects onto spin-preserving operators.

An immediate feature of large-m scaling of the Rényi entropy of the state ψ_- is that it is in disagreement with the predictions coming from conformal invariance of critical points. For instance, for a region A of m consecutive sites, CFT predicts

$$S_A^{\text{Rényi}}(n) \overset{CFT}{=} \frac{c}{6}(1 + n^{-1}) \log m + O(1)$$

where c is the central charge. This is different from (5.73), which is independent of n. Yet, the scaling (5.73) is logarithmic, hence there is a similar type of scale invariance (or covariance): a region twice bigger sees its entanglement entropy added by half a "unit", $1/2 \log(2)$. The

scale ξ should give rise to a new universal function interpolating between this non-conformal scale-invariant behaviour, and the conformal scaling. That is, it should be possible to define a new scaling limit, looking at the entanglement entropy for a region of length m that scales like $m = \alpha\xi$ while the limit $\Delta \to -1^+$ is taken. The result is likely to be $f(\alpha) \log m$, for a function $f(\alpha)$ interpolating between $f(0) = 1/2$ and the coefficient predicted by CFT, e.g. $f(\infty) = c/3$ for the von Neumann entanglement entropy of a connected region, with the central charge $c = 1$.

Another important feature of the entanglement entropy of the state ψ_- is that it does not depend on the actual positions of the sites of the region A. As will be clear from our future work [29], this is a feature of any ground state of the XXZ model at $\Delta = -1$. It turns out that the state ψ_- is just one of these ground states. The field theory interpretation is that the twist field has dimension 0 (corresponding to a central charge 0), but that there is an entanglement entropy contribution coming from the degeneracy.

6 Conclusions and outlook

In this paper we have described in detail a new approach to the computation of the bi-partite entanglement entropy of quantum spin chain models. Our approach employs the "replica trick" widely used in the CFT context [15, 16] and also, more recently, for integrable QFTs [24]. This approach consists of considering a "replica" version of the theory for which one wants to compute the entropy, that is, a new theory consisting of n non-interacting copies of the original model. It turns out that computations of the entropy are often more feasible in the replica model than in the original seemingly simpler theory. The reason for this is the existence of new symmetries of the replica model which enable extra fields (in the QFT case) or extra local operators (in the quantum spin chain case) to exist in the n-copy model. These fields (operators) are related to the symmetry of the replica theory under cyclic permutations of the n-copies.

For integrable QFTs the fields referred to above were introduced in [24] and named branch point twist fields. It was shown that the entanglement entropy can be expressed in terms of their two-point functions which lead to various computation of the entropy which have been summarized in the review [28].

In this paper we have identified the basic operators in terms of which the spin chain equivalent of the QFT twist field can be expressed: they are *local cyclic replica permutation operators*. Each operator $\mathcal{T}_i$ acts on one site of the chain i by cyclicly permuting the spins of the n-copies at that particular site. Ground state correlation functions of products of such operators over different sites of the chain play the same role as two (or higher)-point functions of branch point twist fields in QFT.

We have described a representation of the replica permutation operators for quantum spin chains of general spin in terms of fundamental 2×2 matrices $E^{\epsilon\epsilon'}_{\alpha,i}$ acting at site i, copy α of the chain and proved that such representation does reproduce the cyclic permutation action on quantum states described above. We have also shown that the permutation operators satisfy exchange relations with respect to other local operators of the chain, in much the same way as the twist field in QFT. In fact, as in QFT, these exchange relations can be used as starting point for the construction of the permutation operator in quantum spin chains.

We have demonstrated the working of our approach by evaluating the bi-partite entanglement entropy of one and two spins in an infinitely long spin-$\frac{1}{2}$ quantum spin chain characterized by an antiferromagnetic ground state. We find that the computation of the entropy is recast into combinatorial problems, which become less tractable as the number of spins is increased. It will be very interesting to address this problem in the future and to establish whether or not our approach may be useful for the study of the entanglement entropy of large subsystems.

From our approach it is clear that the larger the subsystem the more operators will be involved in the correlation functions which enter the expressions of the entropy, so that advancement in the understanding of the large-distance behaviour of such correlation functions (see [45] for recent progress) goes hand in hand with the success of our approach to evaluate the large size asymptotics of the entropy.

Despite the difficulties emphasized above we have been able to identify a particular quantum state for which both the von Neumann and Rényi entropies are non-trivial but can still be explicitly computed for any subsystem size and any values of n. This quantum state, which we denoted by ψ_-, is defined by its correlation functions which are obtained as the $\Delta \to -1^+$ limit of those of the spin-$\frac{1}{2}$ XXZ quantum spin chain in the antiferromagnetic regime [39, 38, 37, 40]. Our analysis has allowed us to identify all the eigenvalues of the density matrix associated to this quantum state and to find the exact large subsystem asymptotics of both the von Neumann and Rényi entropies. In both cases the leading term scales with the logarithm of the size of the subsystem as for critical systems. However the coefficient of this logarithmic term is independent of n for the Rényi entropy in direct contrast with the well-known dependence found for CFTs.

It is tempting to speculate that this logarithmic but non-conformal behaviour may be somehow related to the unusual behaviour at $\Delta = -1$ encountered in [5]. In this recent work it is argued that such unusual features are characteristic of essential singularities. We must however stress that the quantity evaluated in [5] and in the present work are rather different in nature, as well as the characterization of the quantum state of the chain, so that the unusual features observed in both cases are not a priori related in an obvious way. Yet, it is possible that the description that we gave of how the ground state approaches the $\Delta = -1$ point from the region $\Delta > -1$ may be of use in understanding the results of [5]. For instance, it may be that the characteristic length ξ could be replaced by the correlation length in describing the approach of the point $\Delta = -1$ in [5]. The analysis of the limit $\Delta \to -1$, and the results of [5], naturally beg the question as to the entanglement entropies of the infinitely-many ground states of the XXZ model at $\Delta = -1$. As we said, it turns out that the state ψ_- is just one of these ground states, although a very particular one, highly entangled. Likewise, it is possible to construct a ground state for every possible finite asymptotic value of the entanglement entropy and it may be that behaviours observed in [5] result from approaching these various ground states. We will come back to the study of the entanglement entropies of $\Delta = -1$ ground states in a later work [29].

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