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Correlation length and unusual corrections to entanglement entropy

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We study analytically the corrections to the leading terms in the Rényi entropy of a massive lattice theory, showing significant deviations from naive expectations. In particular, we show that finite size and finite mass effects give rise to different contributions (with different exponents) and thus violate a simple scaling argument. In the specific, we look at the entanglement entropy of a bipartite $XYZ$ spin-1/2 chain in its ground state. When the system is divided into two semi-infinite half-chains, we have an analytical expression of the Rényi entropy as a function of a single mass parameter. In the scaling limit, we show that the entropy as a function of the correlation length formally coincides with that of a bulk Ising model. This should be compared with the fact that, at criticality, the model is described by a $c = 1$ conformal field theory and the corrections to the entropy due to finite size effects show exponents depending on the compactification radius of the theory. We will argue that there is no contradiction between these statements. If the lattice spacing is retained finite, the relation between the mass parameter and the correlation length generates new subleading terms in the entropy, whose form is path dependent in phase space and whose interpretation within a field theory is not available yet. These contributions arise as a consequence of the existence of stable bound states and are thus a distinctive feature of truly interacting theories, such as the $XYZ$ chain.

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I. INTRODUCTION

In the past few years, there has been a growing interest in quantifying the degree of "quantumness" of a many-body state, which is usually taken as the ground state $|0\rangle$ of a given Hamiltonian.1–3 As the entanglement constitutes an intrinsically quantum property, one popular way to measure this is through bipartite entanglement entropy.4,5 To this end, the system is divided into two subsystems ($A$ and $B$) and one looks at the reduced density matrix, obtained by tracing out one of the two subsystems

$$\hat{\rho}_A \equiv \text{Tr}_B |0\rangle\langle 0|,$$

We will be interested in the Rényi entropies$^6$

$$S_\alpha \equiv \frac{1}{1-\alpha} \ln \text{Tr} \hat{\rho}_A^\alpha,$$ (2)

which, in the $\alpha \rightarrow 1$ limit, reduces to the Von Neumann entropy

$$S \equiv -\text{Tr} \hat{\rho}_A \log \hat{\rho}_A.$$ (3)

Varying the parameter $\alpha$ in (2) gives us access to a lot of information on $\hat{\rho}_A$, including its full spectrum.$^7,8$

For gapped systems, the entanglement entropy satisfies the so-called area law, which means that its leading contribution for sufficiently large subsystems is proportional to the area of the boundary separating system $A$ from $B$. In $1+1$ dimensional systems, the area law implies that the entropy asymptotically saturates to a constant (the boundary between regions being made just by isolated points).

Critical systems can present deviations from the simple area law. In one dimension, in particular, the entanglement entropy of systems in the universality class of a conformal field theory (CFT) is known to diverge logarithmically with the subsystem size.$^9,10$ From CFT, a lot is known also about the subleading corrections, which, in general, take the unusual form$^{11–14}$

$$S_\alpha(\ell) = \frac{c+\bar{c}}{12} \left( 1 + \frac{1}{\alpha} \right) \ln \frac{\ell}{a_0} + c'_\alpha + b_\alpha(\ell) \ell^{2h/a} + \cdots,$$ (4)

where $c$ is the central charge of the CFT, $\ell$ is the length of subsystem $A$, $a_0$ is a short distance cutoff, $c'_\alpha$ and $b_\alpha(\ell)$ are non-universal and the latter includes a periodic function of $\ell$ (with the period given by the Fermi momentum$^{12,14}$), and $h$ is the scaling dimension of the operator responsible for the correction (relevant or irrelevant, but not marginal since these operators generate a different kind of correction, which will be discussed later). This result is achieved using replicas, and thus, strictly speaking, requires $\alpha$ to be an integer. Moreover, it should be noted that in Ref. 13 the corrections are obtained from dimensionality arguments, by regularizing divergent correlations by an ultraviolet cutoff $a_0$. Thus, technically, the subleading contributions in (4) are extracted from scaling properties and are all of the form $\ell/a_0$.

Determining the exponents of the corrections is important both in fitting numerics (where often really large $\ell$ are unobtainable) and also for a better understanding of the model. For instance, the scaling exponent $h$ also determines the large $n$ limit of the entropy (single copy entanglement).11 Moreover, especially for $c = 1$ theories, $h$ provides a measure of the compactification radius of the theory$^{14}$ and thus of the decaying of the correlation functions. Up to now, this conjecture has been checked in a variety of critical quantum spin chains models.$^{15–17}$

Moving away from a conformal point, in the gapped phase universality still holds for sufficiently small relevant perturbations. Simple scaling arguments guarantee that the
leading terms survive, but with the correlation length $\xi$ replacing the infrared length-scale $\ell$. Recent results, based on exactly solvable models, indicate the appearance of the same kind of unusual corrections to the Rényi entropies, which are now functions of the correlation length $\xi$ with the same exponent $n^{11}$:

$$S_\alpha = \frac{c}{12} \left(1 + \frac{\alpha}{\alpha}ight) \ln \frac{\xi}{\alpha_0} + A_\alpha + B_\alpha \xi^{-h/\alpha} + \cdots.$$ (5)

There is a factor of 2 difference in each term between (4) and (5), due to the fact that the first is a bulk theory (with both chiralities in the CFT), while the latter is expected to be akin to a boundary theory, were only one chirality in the light-cone modes effectively survives.

In this paper we are going to investigate the subleading terms in the Rényi entropy of the one-dimensional XYZ model. In the scaling limit we find that the entropy is (modulo a multiplicative redefinition of the correlation length)

$$S_\alpha = \frac{1 + \alpha}{12 \alpha} \ln \frac{\xi}{\alpha_0} - \frac{1}{2} \ln 2 - \frac{1}{\alpha} \sum_{n=1}^{\infty} \sigma_{-1}(n) \left[ \left( \frac{\xi}{\alpha_0} \right)^{-2n} - \left( \frac{\xi}{\alpha_0} \right)^{-2n} \right] + \frac{\alpha}{1 - \alpha} \sum_{n=1}^{\infty} \sigma_{-1}(n) \left[ \left( \frac{\xi}{\alpha_0} \right)^{-2n} - \left( \frac{\xi}{\alpha_0} \right)^{-2n} \right],$$ (6)

where $\sigma_{-1}(n)$ is a divisor function, defined by (41). While the leading term correctly reproduces a $c = 1$ central charge, the interpretation of the scaling exponents in the subleading addenda is less straightforward: we will show that the operator content that can be extracted from (6) matches that of a bulk Ising model and thus the leading term can be equally interpreted as $\frac{c \xi}{12}$ with $c = \frac{c}{12}$.

Furthermore, if we include also lattice effects, which vanish in the strict scaling limit, additional corrections appear in (6) and, while they are less important than the dominant one for sufficiently large $\alpha$, they can be relevant for numerical simulations in certain ranges of $\alpha$. These corrections turn out to be path dependent (probably due to the action of different operators) and many kind of terms can arise, such as $\xi^{-2h}$, $\xi^{-2h/\alpha}$, $\xi^{-2(2-h)}$, $\xi^{-2(1+1/\alpha)}$, or even $1/\ln(\xi)$. In light of Ref. 13, some of these terms were to be expected, but the others still lack a field theoretical interpretation, which might be possible by applying a reasoning similar to that of Ref. 13 for a sine-Gordon model.

The paper is organized as follows: in Sec. II we introduce the XYZ model, its phase-diagram and elementary excitations. In Sec. III we discuss the structure of the reduced density matrix obtained by tracing out of the ground state half of the system and its formal equivalence with the characters of an Ising model. In Sec. IV we present the full expansion of the Rényi entropy and discuss how in the scaling limit this expansion coincides with that of a bulk Ising model. Then we discuss the lattice corrections both in the regime where the low-energy excitations are free particles and where they are bound states. In the latter case we show that different paths of approach to the critical point give rise to different sub-subleading corrections. Finally, in Sec. V we discuss our results and their meaning.

II. THE XYZ SPIN CHAIN

We will consider the quantum spin–$1/2$ ferromagnetic XYZ chain, which is described by the following Hamiltonian:

$$\hat{H}_{XYZ} = -J \sum_n [\sigma^x_n \sigma^x_{n+1} + \sigma^y_n \sigma^y_{n+1} + \sigma^z_n \sigma^z_{n+1}],$$ (7)

where the $\sigma^\mu_n (\mu = x, y, z)$ are the Pauli matrices acting on the site $n$ and the sum ranges over all sites $n$ of the chain; the constant $J$, which we take to be positive, is an overall energy scale while $(J_x, J_y)$ take into account the degree of anisotropy of the model.

In Fig. 1 we draw a cartoon of the phase diagram of the XYZ chain. The model is symmetric under reflections along the diagonals in the $(J_x, J_y)$ plane. The system is gapped in the whole plane, except for six critical half-lines/segments: $J_x = \pm 1$, $|J_y| \leq 1$; $J_x = \pm 1$, $|J_y| \leq 1$; and $J_x = \pm J_y$, $|J_y| \geq 1$. All of these lines correspond to the paramagnetic phase of an XXZ chain, but with the anisotropy along different directions. Thus, in the scaling limit they are described by a $c = 1$ CFT, with compactification radius varying along the line. We will use $0 \leq \beta \leq \sqrt{8\pi}$ (the sine-Gordon parameter of the corresponding massive theory) to parametrize the radius.

The critical segments meet three by three at four “tricritical” points. At these endpoints, $\beta$ is the same along each line, but the different phases have a rotated order parameter. Two of these points—$C_{1,2} = (1, -1), (-1, 1)$—are conformal points with $\beta^2 = 8\pi$; while the other two—$E_{1,2} = (1, 1), (-1, -1)$—
correspond to $\beta^2 = 0$ and are nonconformal. The former points correspond to an antiferromagnetic (AFM) Heisenberg chain at the BKT transition, while the latter describe the Heisenberg ferromagnet. Thus, at $E_{1,2}$ the system undergoes a transition in which the ground state passes from a disordered state to a fully aligned one. Exactly at the transition, the ground state is highly degenerate while the low-energy excitations are gapless magnons with a quadratic dispersion relation.

In studying the $XYZ$ chain, one takes advantage of the fact that (7) commutes with the transfer matrices of the the zero-field eight-vertex model (see, for example, Refs. 18 and 19) and thus the two systems can be solved simultaneously. The solution of the latter is achieved through the parametrization of $J_x, J_z$ in terms of elliptic functions

$$J_y = -\Delta \equiv \frac{\text{cn}(i\lambda)}{1 - k \text{sn}^2(i\lambda)},$$

$$J_z = -\Gamma \equiv \frac{1 + k \text{sn}^2(i\lambda)}{1 - k \text{sn}^2(i\lambda)},$$

(8)

where $(\Gamma, \Delta)$ are the well-known Baxter parameters, and $\text{sn}(x)$, $\text{cn}(x)$, and $\text{dn}(x)$ are Jacobian elliptic functions of parameter $k$. $\lambda$ and $k$ are parameters, whose natural domains are

$$0 < k < 1, \quad 0 \leq \lambda \leq I(k'),$$

(9)

$I(k')$ being the complete elliptic integral of the first kind of argument $k' = \sqrt{1 - k^2}$.

The definition of $(\Delta, \Gamma)$ itself is particularly suitable to describe the antiferroelectric phase of the eight-vertex model (also referred to as the principal regime), corresponding to $\Delta \leq 1$ and $|\Gamma| \leq 1$. However, using the symmetries of the model and the freedom under the rearrangement of parameters, it can be applied to the whole of the phase diagram of the spin Hamiltonian (for more details see Ref. 19). For the sake of simplicity, in this paper we will focus only on the rotated principal regime: $J_y \geq 1, |J_z| \leq 1$, see Fig. 1, and we defer to a different publication some interesting properties of the generalization to the whole phase diagram.

Before we proceed, it is more convenient to switch to an elliptic parametrization equivalent to (8):

$$l = \frac{2\sqrt{k}}{1 + k}, \quad \mu = \frac{\pi \lambda}{I(k')},$$

(10)

The elliptic parameter $l$ corresponds to a gnome $\tau = i \frac{l}{\mu l} = i \frac{l_{k'}}{l_{\mu l}},$ which is half of the original. The relation between $k$ and $l$ is known as Landen transformation. Note that $0 \leq \mu \leq \pi$.

In terms of these new parameters, we have

$$\Gamma = \frac{1}{\text{dn}[2\text{i}(l') \mu/\pi; l]}, \quad \Delta = -\frac{\text{cn}[2\text{i}(l') \mu/\pi; l]}{\text{dn}[2\text{i}(l') \mu/\pi; l]}.$$  

(11)

Curves of constant $l$ always run from the AFM Heisenberg point at $\mu = 0$ to the isotropic ferromagnetic point at $\mu = \pi$. For $l = 1$ the curve coincides with one of the critical lines discussed above, while for $l = 0$ the curve run away from the critical one to infinity and then back. In Fig. 1 we draw these curves for some values of the parameters.

For later convenience, we also introduce

$$x \equiv \exp \left[ -\pi \frac{\lambda}{2I(k)} \right] = e^{\mu \tau}.$$  

(12)

Using Jacobi's $\theta$ functions, we introduce the elliptic parameter $k_1$ connected to $x$, that is,

$$k_1 = \frac{\theta^2_2(0, x)}{\theta^2_2(0, x)} = \frac{x^\frac{1}{2} (-1; x)^\frac{1}{4}_\infty}{4 (-x; x)^2_\infty} \equiv k(x),$$

or, equivalently, $n \frac{I(k)}{I(k')} = -i \mu \tau$ (i.e., $l$ is to $\tau$ what $k_1$ is to $\mu \tau/\pi$). In (13) we also used the $q$-Pochhammer symbol

$$(a; q)_n \equiv \prod_{k=0}^{n-1} (1 - a q^k).$$

(14)

The correlation length and the low-energy excitations of the $XYZ$ chain were calculated in Ref. 20. There are two types of excitations. The first can be characterized as free quasiparticles (spinons). The lowest band is a two-parameter continuum with

$$\Delta E_{\text{free}}(q_1, q_2) = -J \frac{\text{sn}[2I(l') \mu/\pi; l]}{I(l)} I(k_1) \times \left( \sqrt{1 - k_1^2 \cos^2 q_1} + \sqrt{1 - k_1^2 \cos^2 q_2} \right).$$

(15)

The energy minimum of these state is achieved for $q_{1,2} = 0, \pm \pi$ and gives a mass gap

$$\Delta E_{\text{free}} = 2J \frac{1}{I(l)} \text{sn} \left[ 2I(l') \mu/\pi; l \right] I(k_1).$$

(16)

For $\mu > \pi/2$, in addition to the free states just discussed, some bound states become progressively stable. They are characterized by the following dispersion relation:

$$\Delta E_s(q) = -2J \frac{\text{sn}[2I(l') \mu/\pi; l]}{I(l)} \frac{I(k_1)}{\text{sn}[\mu; k_1]} \times \sqrt{1 - \text{dn}^2(\tau; k_1) \cos^2 \frac{q}{2}}$$

$$\times \sqrt{1 - \text{cn}^2(\tau; k_1) \cos^2 \frac{q}{2}},$$

(17)

where $\tau = i I(k_1) (\frac{\pi}{2} - 1)$ and $s$ counts the number of quasi-momenta in the string state. In the scaling limit, these bound states become breathers. The mass gap for the bound states is (setting $q = 0$ above)

$$\Delta E_s = \Delta E_{\text{free}} \text{sn}[\mu; k_1],$$

(18)

from which one sees that for $\mu > \pi/2$ the $s = 1$ bound state becomes the lightest excitation.

The correlation length for the $XYZ$ chain (Fig. 2) was also calculated in Ref. 20 and it is given by

$$\xi^{-1} = \frac{1}{a_0} \left\{ -\frac{1}{2} \ln k_2 \right\} \left\{ -\frac{1}{2} \ln \frac{k_1}{\text{dn}^2[2I(k_1) \mu/\pi]} \right\} \frac{\pi}{2} \leq \mu \leq \pi,$$

(19)
where \(a_0\) is a short distance cutoff, such as the lattice spacing, that sets the length unit and the new parameter \(k_2\) is the Landen transformed of \(k_1\):

\[
k_2 \equiv k(x^2) = \frac{1 - k_1'}{1 + k_1'}.
\]

(20)

The first behavior in (19) is due to the free particles states, while the \(s = 1\) bound state is responsible for the second.21

III. THE REDUCED DENSITY MATRIX

The bipartite entanglement entropy for the ground state of the XYZ chain was calculated in Refs. 22 and 23, in the limit where the infinite chain is partitioned in two (semi-infinite) half-lines. For this configuration, the reduced density matrix can be computed as the product of the four corner transfer matrices (CTM) of the corresponding eight-vertex model.24–26 In Ref. 22 it was shown that it can be written as

\[
\hat{\rho} = \frac{1}{Z} \prod_{j=1}^{\infty} \left( \begin{array}{cc} 1 & 0 \\ 0 & x^{2j} \end{array} \right),
\]

(21)

where \(Z \equiv (-x^2, x^2)_\infty\), that is, the partition function of the eight-vertex model, is the normalization factor that ensures that \(\text{Tr} \hat{\rho} = 1\). Thus we have

\[
\text{Tr} \hat{\rho}^\alpha = \frac{(-x^{2\alpha}; x^{2\alpha})_\infty}{(-x^2; x^2)^\alpha_\infty}
\]

(22)

and for the R\'enyi entropy

\[
S_\alpha = \frac{\alpha}{\alpha - 1} \sum_{j=1}^{\infty} \ln(1 + x^{2j}) + \frac{1}{1 - \alpha} \sum_{j=1}^{\infty} \ln(1 + x^{2j/\alpha}).
\]

(23)

The structure [Eqs. (21)–(23)] for the reduced density matrix of the half-line is common to all integrable, local spin-1/2 chains19 and thus the entanglement spectrum of these models is the same and only depends on \(x\), which in this context is usually parametrized as \(x = e^{-\epsilon}\). For the XYZ chain, \(\epsilon = -i\mu\tau\). In Ref. 23 we showed that \(\epsilon\) (and thus the entropy) has an essential singularity at nonconformal points, and thus its behavior differs dramatically from the conformal one.

From (23), one can see that the R\'enyi entropy is a monotonically decreasing function of \(\epsilon\):

\[
\lim_{\epsilon \to 0} S_\alpha = \infty, \quad \lim_{\epsilon \to \infty} S_\alpha = 0.
\]

(24)

Using (12) and19

\[
l = \sqrt{\frac{1 - \Gamma^2}{\Delta^2 - \Gamma^2}}, \quad \text{dn} \left[ 2 \text{I}(\mu\tau^2, \frac{\mu^2}{\pi}, \frac{l^2}{\Gamma}) \right] = \frac{1}{\Gamma}
\]

(25)

we can plot the entanglement entropy in the phase diagram of the XYZ model. In Fig. 3 we show a contour plot of the Von Neumann entropy in the \((J_z, J_x)\) plane, from which one can clearly see the different behavior of the conformal and nonconformal points.
\( q \) products of the form (22) give easy access to the spectral distribution of the reduced density matrix since

\[
(-q,q)_\infty = \prod_{k=1}^{\infty} (1 + q^k) = 1 + \sum_{n=1}^{\infty} p^{(1)}(n) q^n, \tag{26}
\]

where \( p^{(1)}(n) \) is the number of partitions of \( n \) in distinct positive integers. Also note that since

\[
\prod_{k=1}^{\infty} (1 + q^k) = \prod_{k=1}^{\infty} (1 - q^{2k-1})^{-1}, \tag{27}
\]

\( p^{(1)}(n) = p_{C,n} \), that is, the number of partitions of \( n \) into positive odd integers.

Moreover, one can recognize \( Z \) to be formally equal to the character of the spin field of the Ising CFT. To show this, we write

\[
Z(q = x^2) = \prod_{j=1}^{\infty} (1 + q^j) = \prod_{j=1}^{\infty} \frac{1 - q^{2j}}{1 - q^j}, \tag{28}
\]

and we use the Euler’s formula for pentagonal numbers (which is a consequence of the Jacobi triple-product identity)

\[
\prod_{j=1}^{\infty} (1 - q^{2j}) = \sum_{n=-\infty}^{\infty} (-1)^n q^{n(3n-1)} = \sum_{n=-\infty}^{\infty} [q^{2n(6n-1)} - q^{2(2n+1)(6n+2)}] \tag{29}
\]

to recognize that

\[
Z = x^{-\Delta} \chi^{\text{Ising}}_{1,2}(\xi/\pi), \tag{30}
\]

where \( \chi^{\text{Ising}}_{1,2}(\tau) \) is the character of the spin \( h_{1,2} = 1/16 \) operator of a \( c = 1/2 \) CFT.

\[
\chi^{\text{Ising}}_{1,2}(\tau) = \frac{q^{1/24}}{\prod_{j \in \mathbb{Z}} (1 - q^{j})} \sum_{n \in \mathbb{Z}} \left[ q^{i |p| \pi / \alpha} - q^{-i |p| \pi / \alpha} \right], \tag{31}
\]

with \( q = e^{2\pi \alpha} \) and \( (p, p') = (4,3) \) for the Ising minimal model. We have

\[
\text{Tr} \hat{\rho}^\alpha = \frac{\chi^{\text{Ising}}_{1,2}(i \alpha / \pi)}{[\chi^{\text{Ising}}_{1,2}(i / \pi)]^c}. \tag{32}
\]

As we discussed above, the critical line of the \( XXZ \) chain is approached for \( l \to 1 \), that is, for \( \tau \to 0 \) and \( x \to 1 \). On this line, excitations are gapless and in the scaling limit the theory can be described by a conformal field theory with central charge \( c = 1 \). To each \( 0 < \mu < \pi \) it correspond a point on the critical line, with sine-Gordon parameter \( \beta^2 = 8 \pi (1 - \frac{\mu}{\pi}) \). The two endpoints are exceptions since \( \mu = 0,\pi \) identify the same points for every \( l \). However, while in the conformal one we still have \( x \to 1 \), close to the ferromagnetic point, around \( \mu = \pi \), both \( x \) and \( q \) can take any value between 0 and 1. Hence a very different behavior of the entanglement entropy follows.

In order to study the asymptotic behavior of the entanglement entropy close to the conformal points, it is convenient to use the dual variable

\[
\tilde{x} \equiv e^{-i \pi / \alpha} = e^{-i \pi / 2}. \tag{33}
\]

which is such that \( \tilde{x} \to 0 \) as \( l \to 1 \).

Expressions like (22) involving \( q \) products can be written in terms of elliptic \( \theta \) functions. For instance, this was done for the entanglement entropy of the \( XYZ \) chain in Refs. 23 and 30. To study the conformal limit, one performs a modular transformation that switches \( x \to \tilde{x} \).

\[
k(\tilde{x}) = k'(x) = \frac{(x; x^2)^{\alpha}}{(-x; x^2)^{\alpha}}, \tag{34}
\]

and using (13) we have

\[
(-x^{2a}; x^{2a})_{\infty} = \left[ \frac{k^2(\tilde{x}^a)}{16x^a k'(\tilde{x})} \right]^{1/2} = \left[ \frac{k^2(\tilde{x}^{1/\alpha})}{16x^a k(\tilde{x})} \right]^{1/2} \tag{35}
\]
Thus

\[
\text{Tr} \hat{\rho}^\alpha = 2^{1/4} \tilde{x}^{-i\alpha} \left( \chi^{1/\alpha}_{1,2} / (\tilde{x}; x^2)^{\alpha} \right). \tag{36}
\]

The modular transformation that allowed us to switch from \( x \) to \( \tilde{x} \) is the same one that connects characters in minimal model of inverse temperature. For the spin operator of the Ising model we have

\[
\chi^{\text{Ising}}_{1,1}(\tau) = \frac{1}{\sqrt{2}} [\chi^{\text{Ising}}_{1,1}(\pi / \tau) - \chi^{\text{Ising}}_{1,1}(\pi / \tau)]. \tag{37}
\]

Using (31) and the identities (27) and (29) one can prove that

\[
\chi^{\text{Ising}}_{1,2}(i \pi / \alpha) = \frac{1}{\sqrt{2}} x^{-\alpha} (\tilde{x}; x^2)^{\alpha}, \tag{38}
\]

which agrees with (36) and implies

\[
\text{Tr} \hat{\rho}^\alpha = 2^{1/4} \chi^{\text{Ising}}_{1,1}(i \pi / \alpha) \chi^{\text{Ising}}_{1,2}(i \pi / \alpha). \tag{39}
\]

This agrees with what conjectured in Ref. 11, but with the important difference that the characters in (39) are \( c = 1/2 \) and do not belong to the infrared \( c = 1 \) bulk description of the \( XYZ \) chain. This Ising character structure for the CTM of the eight-vertex model was already noticed, see Ref. 32. We acknowledge that, once the formal equivalence (30) is understood, the content of the last page follows almost trivially, but we decided to provide a brief derivation here for the sake of completeness and because this result has consequences on the structure of the entanglement entropy, a fact which is not well known and will be discussed in the next paragraph. Finally, we notice that, being only a formal equivalence, Eq. (30) does not imply any underlying Virasoro algebra at work for CTM (as far as we know) and it is thus important to recognize that these manipulations stand on more general mathematical concepts.
IV. EXPANSIONS OF THE ENTANGLEMENT ENTROPY

Close to the conformal points, Eq. (23) is just a formal series since $\alpha \simeq 1$. However, using (36), it is straightforward to write a series expansion for the Rényi entropy (2) in powers of $\tilde{x} \ll 1$:

$$S_\alpha = -\frac{1 + \alpha}{24\alpha} \ln \tilde{x} - \frac{1}{2} \ln 2$$

$$- \frac{1}{1 - \alpha} \sum_{n=1}^{\infty} \sigma_{-1}(n)[\tilde{x}^2 - \alpha \tilde{x}^n - \tilde{x}^{2n}] + \frac{\alpha \tilde{x}^{2n}}{1 - \alpha},$$  \hspace{1cm} (40)

where the coefficients

$$\sigma_{-1}(n) \equiv \frac{1}{n} \sum_{j < k = 1}^{\infty} (j + k) + \sum_{j = 1}^{\infty} \frac{1}{j} = \frac{\sigma_1(n)}{n}$$  \hspace{1cm} (41)

is a divisor function and takes into account the expansion of the logarithm over a $q$ product and play a role similar to the partitions of integers in (26). It is worth noticing that the constant term $\ln(2^{-1/2}) \equiv \ln(\tilde{x}_{1/2})$—where $\tilde{x}_{1/2}$ is an element of the modular $\tilde{S}$ matrix of the Ising model—is the contribution to the entropy due to the boundary.34

The $\alpha \to 1$ yields the Von Neumann entropy:

$$S_\alpha = -\frac{1}{12} \ln \tilde{x} - \frac{1}{2} \ln 2$$

$$- \sum_{n=1}^{\infty} \sigma_{-1}(n)[n(\tilde{x}^n - 2\tilde{x}^{2n}) \ln \tilde{x} + \tilde{x}^n - \tilde{x}^{2n}]$$  \hspace{1cm} (42)

We see that, contrary to what happens for $\alpha > 1$, all subleading terms—which are powers of $\tilde{x}$—acquire a logarithmic correction, which strictly vanishes only at the critical points. A more specific analysis of this phenomenon, together with a quantitative study of what introduced in the next subsections, will be the subject of a future, partly numerical, publication.

A. Scaling limit

Comparing with (5) and coherently with (32), (40), and (42) can be identified with the expansion of a $c = 1/2$ theory. However, the parameter of this expansion $\tilde{x}$ has meaning only within Baxter’s parametrization of the model (8). To gain generality, the entropy is normally measured as a function of a universal parameter, such as the correlation length or the mass gap.

In the scaling limit, up to a multiplicative constant, one has

$$\tilde{x} \approx \left( \frac{\tilde{x}}{\alpha_0} \right)^{-2} \approx \left( \frac{\Delta E}{J} \right)^2$$  \hspace{1cm} (43)

so that, substituting this into (40), we get (6). Relation (43) is crucial in turning the leading coefficient in the entropy of a $c = 1/2$ entropy such as (40) into that of a $c = 1$ theory, but it also doubles all the exponents of the subdominant corrections. It is reasonable to assume that this $c = 1$ model is some sort of double Ising, but its operator content does not seem to match any reasonable $c = 1$ model since only even exponent states exist. Moreover, comparing (6) with (5), one would conclude that a $\hbar = 2$ operator is responsible for the first correction. It was argued in Ref. 13 that a marginal field gives rise to logarithmic corrections in the entropy, thus either this correction is due to descendant of the identity (namely, the stress-energy tensor), or we should think of it as a $2\hbar/\alpha$, with $\hbar = 1$.

In fact, we can write the partition function of the eight-vertex model as a bulk Ising model (i.e., quadratic in characters). Starting from (38), we have

$$Z = \frac{1}{\sqrt{2}} \pi^{-\frac{\pi}{2}} \pi^{-\frac{\pi}{2}} \prod_{k=1}^{\infty} (1 - \xi^{1-2k})(1 + \xi^{1-2k})$$

$$\approx \frac{x^{-\frac{\pi}{2}}}{\sqrt{2}} \left[ \chi_{1,1}^{\text{Ising}} \left( \frac{i}{\pi} \ln \xi \right) + \chi_{2,1}^{\text{Ising}} \left( \frac{i}{\pi} \ln \xi \right) \right]$$

$$\times \left[ \chi_{1,1}^{\text{Ising}} \left( \frac{i}{\pi} \ln \xi \right) - \chi_{2,1}^{\text{Ising}} \left( \frac{i}{\pi} \ln \xi \right) \right]$$

$$= \frac{x^{-\frac{\pi}{2}}}{\sqrt{2}} \left[ |\chi_0^{\text{Ising}}|^2 - |\chi_{1/2}^{\text{Ising}}|^2 - \chi_0^{\text{Ising}} \chi_{1/2}^{\text{Ising}} + \chi_{1/2}^{\text{Ising}} \chi_0^{\text{Ising}} \right].$$  \hspace{1cm} (44)

This formulation provides a simple explanation of the Renyi entropy expansion (6) and its operator content. In fact, it interprets the first correction as the Ising energy operator, and not as a descendant of the identity.

It also means that the prefactor in front of the logarithm in the entropy can be interpreted as $\frac{c}{\alpha^2}$ with $\alpha = \frac{1}{2}$.

No fundamental reason is known for which CTM spectra (and partition functions) of integrable models can be written as characters in terms of the mass parameter $x$ or $\tilde{x}$. This is the case also for Eq. (44). Thus, so far, we can only bring forth this observation while any connection with some underlying Virasoro algebra remains to be discovered. To the contrary, sufficiently close to a critical point, the CTM construction can be seen as a boundary CFT and thus its character structure as function of the size of the system is dictated by the neighboring fix point.

We are led to conclude that, in the scaling limit, the entropy can be written as a function of two variables: $S_\alpha(\tilde{x}, \tilde{E})$. When the inverse mass is larger that the subsystem size, we have the usual expansion of the form (4). But when the correlation length becomes the infrared cut-off scale, apparently a different expansion is possible, which, unlike (5), can contain terms with different exponents, like in (6). Hence, while the leading universal behavior has always the same numerical value and scales like the logarithm of the relevant infrared scale, the exponents of the corrections might be different for terms in $\tilde{E}$ and in $\tilde{E}$.

In the scaling limit, $\alpha_0 \to 0$, $J \to \infty$, and $\tilde{x} \to 0$ in such a way to keep physical quantities finite. In this limit, only the scaling relation (43) survives. However, at any finite lattice spacing $\alpha_0$, there will be corrections which feed back into the entropy and that can be relevant for numerical simulations. To discuss these subleading terms we have to consider two regimes separately.

B. Free excitations: $0 \leq \mu \leq \frac{\pi}{2}$

For $0 \leq \mu \leq \frac{\pi}{2}$ the lowest energy states are free, with dispersion relation (15). To express the entropy as a function
of the correlation length we need to invert (19). This cannot be
done in closed form. So we have to first expand (19), finding
\[
\frac{a_0}{\xi} = 4 \tilde{\xi}^{1/2} \sum_{n=0}^{\infty} \frac{\sigma_{-1}(2n+1)}{6n+1} \tilde{x}^n
\]
\[
= 4 \tilde{\xi}^{1/2} + \frac{16}{3} \tilde{x}^{3/2} + \frac{24}{5} \tilde{x}^{5/2} + \cdots
\]  
(45)
and then to invert this (by hand) to the desired order:
\[
\tilde{x} = \frac{1}{16} \left[ 1 - \frac{a_0^2}{\xi^2} + \frac{7}{144} \frac{a_0^4}{\xi^4} + O(\xi^{-6}) \right].
\]  
(46)
We get
\[
S_\alpha = \frac{1 + \alpha}{12\alpha} \ln \frac{\xi}{a_0} + \frac{1 - 2\alpha}{6\alpha} \ln 2
\]
\[
+ B_{\alpha} \xi^{-\tilde{\xi}} + C_{\alpha} \xi^{-\tilde{\xi}} + B_{\alpha}' \xi^{-\tilde{\xi}} + \cdots
\]
\[
- \alpha B_{\alpha} \xi^{-\tilde{\xi}} - \alpha B_{\alpha} \xi^{-\tilde{\xi}} + \cdots,
\]  
(47)
where the coefficients only depend on \( \alpha \) and contain the proper
power of \( a_0 \) to keep each term dimensionless (for instance \( B_{\alpha} = \frac{1}{\alpha} \tilde{\xi}^{3/2} \)). We note that a new term has appeared (and
more will be seen at higher orders) and that it is not of the
forms discussed in Ref. 12.

It is worth noticing that if we express the mass gap (16)
as function of \( \tilde{x} \), we would get a different series expansion
and thus different corrections to the entropy. These subleading
terms would have a different form, compared to (47), and even
be path dependent on how one approaches the critical point.
We prefer not to dwell into these details now, postponing
the description of this kind of path-dependent behavior with the
bound state’s correlation length to the next section.

C. Bound states: \( \tilde{\xi} < \mu < \pi \)

For \( \mu > \pi/2 \), bound states become stable, and the lightest
excitation becomes the \( s = 1 \) state with dispersion relation (17).
Accordingly, the expression for the correlation length is
different in this region from before. Using the dual variable \( \tilde{x} \)
and the formulation of elliptic functions as infinite products,
we can write (19) as
\[
\frac{a_0}{\xi} \equiv \ln \frac{-\tilde{x}^{\tilde{\xi}}; \tilde{x}^\infty}{(\tilde{x}^{\tilde{\xi}}; \tilde{x}^\infty)_{\infty}} - \frac{\pi^2}{2\mu} \sum_{k=1}^{\infty} \cos \left( \frac{\pi^2}{2\mu} (2k-1) \right) \tilde{x}^{(\infty-1)(2k-1)}.
\]  
(48)

The major difference in (48) compared to (45) is that the
bound state correlation length does not depend on \( \tilde{x} \) alone, but
separately on \( \mu \) and \( \tau \). This means that in inverting (48) to
find \( \tilde{x} \) as a function of \( \xi \), we have to first specify a relation between
\( \mu \) and \( \tau \), that is, to choose a path of approach to the critical
line. We will follow three different paths, that are shown in
Fig. 4.

(1) Renormalization group flow: The first natural path is
(represented by the blue line in Fig. 4)
\[
\tau = \text{is}, \quad \mu = \mu_0,
\]  
(49)
where \( s \to 0 \) guides our approach to the gapless point. This
path, keeping \( \mu \) fixed, corresponds to the RG flow. In the
scaling limit, the \( XYZ \) chain is described by a sine-Gordon
model, where \( \mu \) is proportional to the compactification radius.28 Thus, assuming (49) means changing the bare mass
scale, without touching \( \beta \). In the \((J_z,J_y)\) plane this path asympto-
tically crosses the critical line with slope \( m = -2/\cos \mu_0 \).
Substituting this in (48) we get
\[
\frac{a_0}{\xi} = 4g(\mu_0) \tilde{x}^{1/2} + \frac{16}{3} \tilde{x}^{3/2} + O(\tilde{x}^{5/2}),
\]  
(50)
where \( g(\mu) \equiv \cos \frac{\tau^2}{\mu} \). Comparing (50) with the free case (45)
we immediately conclude that the entropy retains an expansion
similar to (47), with the difference that all the coefficients now
depend on \( \mu_0 \) and thus change along the critical line:
\[
S_\alpha \simeq \frac{1 + \alpha}{12\alpha} \ln \xi + A_\alpha(\mu_0) + B_\alpha(\mu_0) \xi^{-\tilde{\xi}} + \cdots
\]
\[
- \alpha B_\alpha(\mu_0) \xi^{-\tilde{\xi}} + C_\alpha(\mu_0) \xi^{-\tilde{\xi}} + \cdots.
\]  
(51)

(2) Straight lines in \((J_z,J_y)\) plane: Let us now approach a
conformal critical point exactly linearly in the \((J_z,J_y)\) plane:
\[
J_z = 1 + m \cdot s, \quad J_y = s - \cos \mu_0.
\]  
(52)
This path corresponds to the following parametrization of \( \tau \)
and \( \mu \) (an example of which is the red line in Fig. 4):
\[
\tau = \frac{-1}{\ln(\xi)} + O\left( \frac{1}{\ln^2 s} \right), \quad \mu = \mu_0 + r(m,\mu_0) \cdot s + O(s^2),
\]  
(53)
where \( r(m,\mu) \equiv \frac{2+m \cos \mu}{2 \sin \mu} \). Thus, in the limit \( s \to 0 \), the
entropy parameter \( \tilde{x} \) vanishes like \( \tilde{x} \propto s^{3/2} \). Using (53) in
(48) we get
\[
\frac{a_0}{\xi} \simeq 4g(\mu_0) \tilde{x}^{1/2} + 4r(m,\mu_0) \tilde{x}^{3/2} + O(\tilde{x}^{5/2}) + \cdots
\]  
(54)
Inverting this relation, we arrive at the following expansion of the Rényi entropy along (52):
\[
S_\alpha \simeq \frac{1 + \alpha}{12\alpha} \ln \xi + A_\alpha(\mu_0)
\]
\[
+ B_\alpha(\mu_0) \xi^{-2/\alpha} + D_\alpha(m,\mu_0) \xi^{-2\mu_0/\alpha} \cdots.
\]  
(55)
We notice that the last term yields a new type of correction, with a nonconstant exponent, which varies with $\mu$. This term is of the form $\xi^{-(2-h)}$, where $h$ here is the scaling dimension of the vertex operator $e^{i\phi}$ of the underlying sine-Gordon theory. To the best of our knowledge, this is the first time that such a correction in the Rényi entropy of gapped systems is discussed and it also differs from those discussed in Ref. 12. It is surprising to see the appearance of the operator content corresponding to a changing of the compactification radius.

Moreover, the path one chooses to approach criticality selects a scaling limit in which irrelevant operators can be generated and these can modify the perturbative series that defines the correlation length, leading to something like we observed.

Putting (56) into (48) we have

$$\frac{d_0}{\xi} = 4g(\mu_0)\xi^{1/2} + 4r^2 \left( \frac{\mu_0}{\ln \xi} \right)^{1/2} + \frac{16}{3} \frac{g^3(\mu_0)}{\ln \xi} \xi^{3/2} + O \left( \frac{\xi^{1/2}}{\ln \xi}, \frac{\xi^{1/2}}{\ln \xi} \right).$$

We notice the appearance of a strange logarithmic correction in the expansion. Inverting (57) and plugging it into the entropy we get

$$S_\rho = \frac{1 + \alpha}{12\alpha} \ln \xi + A_\rho(\mu) + \frac{E_\rho(\ell, u)}{\ln \xi} + \cdots, \quad (58)$$

where $A_\rho(\mu)$ is a Majorana fermionic creation and annihilation operator for single particle states with eigenvalue $\epsilon_j = 2j\epsilon$ (note that $H_{\text{CTM}}$ is not the Hamiltonian of the subsystem A). This representation strongly supports the interpretation that the $c = 1$ theory is constructed in terms of $c = 1/2$ (Majorana) characters.

In Refs. 12 and 16 it was shown that the first correction in the Rényi entropy of a critical XXZ chain as a function of the subsystem size $L$ goes like $\ell^{2-2K/\alpha}$, where $K$ is the Luttinger parameter of the model. This fact has also been checked in many other critical $c = 1$ quantum spin chain models via DMRG simulations. When going to the corresponding massive model, assuming that the operators responsible for the corrections remain the same, the simple scaling prescription would give a term of the type $\xi^{-(2K/\alpha)}$. The results presented here would then indicate an improbable fixed value for the Luttinger parameter $K = 2$. This exponent for the massive XXZ chain was observed before (take, for instance, Ref. 11), but its nature has not been discussed. Instead, consistently with Ref. 16, we found in Sec. IV that the operator responsible for this correction is the energy of the underlying bulk Ising model. As pointed out in Ref. 13, the leading correction in $\ell$ is of the form $\ell^{2K/\alpha}$ in the one-interval case and $\ell^{-K/\alpha}$ for the half-life, whereas for two intervals, in the Ising case, the exponent acquires an additional factor of 2, which counts the number of twist fields at the edge of the interval. It would be interesting to perform a calculation for one interval with two boundary points in our case too, to check whether a doubling of the exponent in the correlation length would happen in.

**V. CONCLUSIONS AND OUTLOOKS**

By using the example of the integrable $XYZ$ chain, we proved that, for a massive model, the study of the corrections to the entanglement entropy as a function of the correlation length requires a separate analysis from the one that yields the entropy as function of the subsystem size.

For the bipartite Rényi entropy of the $XYZ$ model of a semi-infinite half-line we found, in the scaling limit and as a function of the correlation length, the universal form (6), where all subleading contributions are explicitly written, thanks to a novel formulation of the reduced density matrix in terms of $q$ products. We argued that these corrections are best interpreted in light of a previously unnoticed bulk Ising structure of the CTM formulation of the model. This means that corrections as a function of the correlation length have different exponents compared to those depending on the length of the subsystem, unlike what was expected from previous studies. This also implies that the coefficient $\frac{1}{\ell^{(2K/\alpha)}}$ of the logarithmic leading term has the same value both for $c = 1$ and $c = 1/2$ of the bulk Ising formulation in the mass parameter and for the $c = 1$, $\bar{c} = 0$ of the critical chiral free boson model in the subsystem size.

In this respect, it is also interesting to note that the reduced density matrix $\hat{\rho}$ of (21) can be written as

$$\hat{\rho} \propto e^{-H_{\text{CTM}}}, \quad H_{\text{CTM}} = \sum_{j=1}^{\infty} 2\epsilon_j \eta_j^\dagger \eta_j, \quad (59)$$

where $(\eta_j, \eta_j^\dagger)$ are (Majorana) fermionic creation and annihilation operators for single particle states with eigenvalue $2\epsilon_j = 2j\epsilon$ (note that $H_{\text{CTM}}$ is not the Hamiltonian of the subsystem A).
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