Critical properties and Rényi entropies of the spin-3/2 XXZ chain

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I. INTRODUCTION

Since their first introduction 11 quantum spin chains have been an incredibly fertile field for theoretical physicists. They are in fact interesting for various reasons: first of all because of their one-dimensional (1D) nature, that enhances the importance of quantum fluctuations and forbids the application of mean-field or other ordinary perturbative approaches; secondarily because of the integrability of some of them and the possibility of giving a descriptions of their low-energy sector by means of effective quantum field theories; lastly because of the availability of some numerical techniques that appear to be particularly powerful in these cases.

Spin-1/2 quantum spin chains with nearest neighbor interaction 12 have been widely considered in literature and, among them, the XXZ spin-1/2 chain is by far the most studied, both analytically and numerically. Being integrable via Bethe Ansatz 13 it represents a yardstick for non-exact techniques. Also, the physics of its low-energy sector is described in the continuum limit by a special class of Conformal Field Theories (CFTs) 13, with conformal charge \( c = 1 \), the so called Tomonaga-Luttinger Liquids (TLLs) 14, which represent a paradigm for all those models whose excitations are of bosonic nature. 15

Higher spin XXZ chains are also very interesting, because they constitute examples of models for which, despite being non-integrable, one can provide quite well known established field theory description. 14,15 Moreover, their properties may be quantitatively determined with good accuracy by means of numerical simulations based on several efficient methods such as exact diagonalization, quantum Monte Carlo, and Density-Matrix-Renormalization-Group (DMRG). 16 Thus, they represent a decisively indicative and efficient test in order to establish the validity of properties that, up to now, have been verified mainly in integrable systems. In addition, the physics of these models can also be studied experimentally: for example, the spin-3/2 isotropic case is thought to model the behaviour of some kind of quasi-1D antiferromagnets of magnetic ions, such as CsVCl 3,17 and AgCrP 2S 3,17, whereas various spin models may be now engineered in cold matter setups of trapped ion 18,19 and have promising future implementation with ultracold atoms and molecules in strongly anisotropic optical lattices. 20,21 and Rydberg atoms. 22

In recent times, much attention has been devoted to the connection between Quantum Phase Transitions and entanglement properties in strongly correlated systems. 23,24 In particular, whenever the effective theory describing a system is conformal, it is well known that a fruitful way to get physical information from numerical simulations, especially from DMRG calculations, is to look at quantities known as Rényi Entanglement Entropies (REs) 25. More specifically, as it will be recalled in the following, for TLLs the knowledge of the REs yields a very careful estimation not only of the central charge of the underlying critical theory, 25 but also of the decay exponents of correlation functions, 26 which are encoded in the so called Luttinger parameter \( K \).

The main aim of this work is to present a complete investigation of critical and entanglement properties of the \( S = 3/2 \) XXZ model all over its gapless regime, and to compare the accuracy of different analysis methods employed to extrapolate thermodynamic quantities from finite-size numerical calculations based on the DMRG algorithm. In the first part, we will fully exploit the low-energy field theory of XXZ model and determine its relevant quantities by considering different, independent observables; then, we will present a investigation of the entanglement entropies for bipartite intervals, considering both ground and excited states and systematically comparing the numerical findings with CFT predictions. The paper is structured as follows: in Sec. 1 we briefly review the main features of spin-\( S \) XXZ chains from a field theoretical viewpoint, focusing on the TLL universality class emerging in the half-integer \( S \) case. We present our DMRG calculations and results on the \( S = 3/2 \) model in Sec. 2 together with a brief resumé of all applied techniques. In Section 3 we perform a systematic investigation of the Rényi entropies of both the ground and excited states and compare the numerical findings with...
the predictions based on CFTs. Finally, we summarize the results and draw our conclusions in Sec. V.

II. MODEL HAMILTONIAN

The spin-$S$ anisotropic Heisenberg model, also known as XXZ chain, is described by the following Hamiltonian:

$$H_{XXZ} = \sum_{i=1}^{L} (S_{i}^{x}S_{i+1}^{x} + S_{i}^{y}S_{i+1}^{y} + \Delta S_{i}^{z}S_{i+1}^{z})$$  \hspace{1cm} (1)

where $S_{i}^{x,y,z}$ is a spin-$S$ operator relative to the $i$-th site and $\Delta$ is the anisotropy coefficient. Here, $S$ can take positive half-odd-integer or integer values. In the simplest case $S = 1/2$, the model is integrable by Bethe ansatz\cite{22,23} if it is critical for $|\Delta| \leq 1$, and, in the interval $-1 < \Delta \leq 1$ its low-energy physics is effectively described by a conformal field theory with central charge $c = 1$.

The picture becomes more puzzling as one moves away from the integrable $S = 1/2$ case. At the isotropic point $\Delta = 1$, chains with integer spin display a finite gap, whereas in the half-integer case the system is gapless and still described by a $c = 1$ CFT, as has been proved in a series of analytical and numerical studies\cite{24,25,26,27,28,29,30,31,32,33,34,35,36}.

In such gapless regime, which persists in the finite range of interactions $-1 < \Delta \leq 1$, the low-energy spectrum is universally described by a TLL Hamiltonian:

$$H = \frac{v_s}{2\pi} \int dx \left[ \left( \frac{\partial_x \vartheta}{2} \right)^2 / K + K \left( \frac{\partial_x \varphi}{2} \right)^2 \right]$$  \hspace{1cm} (2)

where $\vartheta$ and $\varphi$ are conjugated density and phase bosonic fields, while the two interaction-dependent parameters $v_s$ and $K$ are called sound velocity and Luttinger parameter respectively. Both the long-distance decay of correlation functions and spectral properties are determined by $v_s$ and $K$: however, since no exact solution is known except for $S = 1/2$, one has to resort to unbiased numerical methods in order to quantitatively estimate the dependence of such parameters with respect to $\Delta$. For the $S = 3/2$ case, that we are going to extensively study in the following, various numerical studies have been reported in literature, based on both exact diagonalization of small systems and simulations based on the DMRG algorithm\cite{37,38,39,40,41}.

We will systematically refer and compare our results to the known ones in the remainder of the paper.

III. NUMERICAL RESULTS: CRITICAL PROPERTIES

In this section, we provide a complete study of the quantum critical regime $-1 < \Delta \leq 1$ for the $S = 3/2$ XXZ model employing the DMRG technique, which allows to estimate both ground state and excited state properties with notable accuracy. Being interested in various physical quantities such as entropies, correlation functions and spectral properties, we employ simulations with both open (OBC) and periodic (PBC) boundary conditions. While the former guarantee better accuracy in the DMRG procedure, the latter are not affected by boundary effects; providing estimates in both configuration represents a good check for our final results. In order to accurately determine all relevant quantities of interest, we perform calculations with up to $512$ (1156) states per block for OBC (PBC), together with up to 5 sweeps for each intermediate size during the infinite-size algorithm; in such a setting, typical discarded weights are of order $10^{-8}$ ($10^{-6}$) during the last iteration.

Reliable estimates of the relevant physical quantities, $v_s$ and $K$, may be obtained with different numerical analysis. In the following, we will employ three alternative methods based on independent quantities: energy scaling in the low-energy spectrum, entanglement entropy and spin fluctuations. A detailed account on how such quantities are related to the sound velocity and the Luttinger parameter is given in each of the following subsections.

A. Central charge

As a first step in our study, we extract the central charge of the system from the scaling of the block Von Neumann Entropy (VNE), which is defined as

$$S_1(l, L) = -\text{Tr}_A \rho_A \log_2 \rho_A$$  \hspace{1cm} (3)

Here, the system of total length $L$ is bipartite in two sub-systems $A, B$ of length $l, L - l$ respectively, and $\rho_A$ denotes the reduced density matrix of $A$ with respect to $B$. In a CFT, one has\cite{42,43,44,45,46}

$$S_1(l, L) = \frac{c}{3\eta} \log_2 \left[ L \sin(\pi l/L) / \pi \right] + s_1 + S_1^{osc}$$  \hspace{1cm} (4)

where the coefficient $\eta = 1.2$ for PBC/OBC, $s_1$ is a model-dependent constant and $S_1^{osc}$ represents finite-size oscillating corrections.\cite{47,48} In a finite system under PBC, the central charge can be determined by fitting the half-lattice entropy

$$S_1(L/2, L) = \frac{c}{3} \log_2 (L/\pi) + s_1$$  \hspace{1cm} (5)

as a function of the system size $L$ by assuming a scaling form of the type $c(L) = c_0 + a_0 L^a$. Typical results are plotted in Fig. 4, a best fit of Eq. 5 for $L \in [28, 60]$ gives an excellent agreement with the expected value, as $c_0 = 1.00$ up to a 2% error over the entire parameter range; for negative values of $\Delta$, an even better agreement is reached. Alternative techniques to extract $c$ via finite-size scaling\cite{49,50} lead to comparable results. A good estimate of the central charge represents a reliable check of our numerical calculations, and is also required to consistently perform a level spectroscopy analysis without targeting excitations in momentum space.\cite{51,52}
result extracted by targeting the first excited states at finite magnetic phase transition, the velocity of the sound excitations seems to approach zero. On the other hand, \( v_s \) was estimated by employing the previously found values of the central charge. The large number of system sizes considered in our calculations allows to safely perform a four-parameter fit of the form \( \epsilon_{gs}(L) = a_0 + a_1/L^2 + a_2/L^4 \); typical fitting results are shown in the inset of Fig. 2. At the antiferromagnetic point \( \Delta = 1 \), our results are in good agreement with a previous DMRG study\(^{39} \), where \( v_s \) was extracted by targeting the first excited states at finite momentum, and in sharp disagreement with the spin wave result\(^{49} \), \( v_s^{SW} = 3 \), in which quantum fluctuations are only approximately treated. Including logarithmic corrections according to Wess-Zumino-Novikov-Witten\(^{30,31} \) theory does not lead to appreciable differences.

The complete dependence of \( v_s \) versus \( \Delta \) is plotted in Fig. 2 and suggests how, once approaching the ferromagnetic phase transition, the velocity of the sound excitations seems to approach zero. On the other hand, \( v_s \) reaches its maximum value at the Berezinskii-Kosterlitz-Thouless point\(^{47} \), in full analogy with the \( S = 1/2 \) case\(^{39} \). We thus apply the same fitting procedure of Ref. 39 which takes into account logarithmic corrections as ensuing from the underlying SU(2) Wess-Zumino-Novikov-Witten field theoretical structure\(^{41,42} \), obtaining \( K = 0.499 \pm 0.005 \) at the critical point, in good agreement with previous numerical\(^{39} \) and analytical findings\(^{42} \). A summary of the so obtained results all over the critical regime is presented in Fig. 8 and will be discussed at the end of this subsection.

\[ \epsilon_{gs}(L) = \epsilon_0 + \frac{v_s c \pi}{6L^2} + \ldots \] (6)

\[ \epsilon_0 \] being the energy density in the thermodynamic limit, and employing the previously found values of the central charge. The long-distance decay of all correlation functions and thus which susceptibilities are the most relevant in the microscopic model\(^{10} \). We will thus employ three complementary methods to extract such a quantity from numerical simulations. This procedure allows to systematically check the validity of each method in various parameter regimes, and, close to the antiferromagnetic point, indicates which type of estimate is more affected by the well known logarithmic corrections.

As a first way to estimate \( K \), we make use of the previously calculated \( v_s \) and apply the level spectroscopy method by targeting the first excited state with total magnetization \( \langle \sum_i S_i^z \rangle = 1 \) under PBC. Given its energy density \( \epsilon_{gs}(L) = L(\epsilon_{gs}(L) - \epsilon_{+1}(L)) \) scales to zero in the thermodynamic limit as\(^{10,29} \),

\[ \Delta_g(L) = \frac{\pi v_s}{2KL} + \ldots \] (7)

We thus performed a least-square regression fit as a function of \( 1/L^2 \) and a non-linear fit of the form \( \Delta_g(L) = b_0/L^2 + b_1/L^b_2 \) in order to estimate the effect of higher-order corrections, which turns out to be negligible if \( |\Delta| \leq 0.9 \), as can be inferred from typical finite-size scalings shown in Fig. 3. At the antiferromagnetic point, however, the quality of the best fit with just algebraic contributions turns out to be insufficient due to the presence of strong logarithmic corrections\(^{10} \). We thus apply the method by targeting the first excited state with total magnetization \( \langle \sum_i S_i^z \rangle = 1 \) under PBC. Given its energy density \( \epsilon_{gs}(L) = L(\epsilon_{gs}(L) - \epsilon_{+1}(L)) \) scales to zero in the thermodynamic limit as\(^{10,29} \),
The second way of getting $K$ is the one introduced by the authors in Ref. [30] based on the finite size corrections of the bipartite Rényi entropies:

$$S_\alpha(l, L) = \frac{1}{1 - \alpha} \log_2 \text{Tr}_A \rho_A^\alpha$$

whose scaling, for a CFT with $c = 1$, follows [35]:

$$S_\alpha(l, L) = \frac{c(1 + \frac{1}{\alpha})}{6\eta} \log_2 [L \sin(\pi l/L) / \pi] + s_\alpha + S_\alpha^{\text{osc}}(l, L)$$

where for $\alpha \to 1$ one recovers the von Neumann entropy [4]. The influence of the Luttinger parameter on such entanglement entropies is encoded in the oscillating factor,

$$dS_\alpha(L) = S_\alpha \left( \frac{L}{2}, L \right) - S_\alpha \left( \frac{L}{2} - \frac{\pi}{2 k_F}, L \right)$$

which, for $L \gg 1$, reduces to [30]:

$$dS_\alpha(L) = \frac{\pi^4 (1 + \frac{1}{\alpha})}{48\eta \ln 2 k_F^2 L^2} \left( \frac{c(k_F L)}{L^{4/5}} \right) a + O \left( \frac{1}{L} \right)$$
The finite size scaling of $dS_\alpha$ with respect to the system size $L$ allows to precisely estimates $K$ under both OBC and PBC, as discussed in detail in Ref. [28,60]. Since it has been noticed that the oscillation amplitude is very small for Heisenberg chains with $S > 1/2$ and $\alpha \approx 2$, we employed REs with larger values of $\alpha$ in order to get a reliable estimate from the DMRG results. In particular, our estimate of $K$ are mostly based on the $\alpha = 10$ REs, as these data represent a good compromise between small oscillation amplitude and slow oscillation decay.

Typical results from both PBC and OBC with systems sizes $L \in [28, 60] (L \in [100, 180])$ are presented in Figs. 5 and 6. We notice that even though it considerably decreases close to the ferromagnetic transition, the magnitude of the oscillation is still large enough to perform accurate finite-size scaling. For $\Delta = 0$, comparable results may be obtained even with smaller $\alpha$’s. However, close to the antiferromagnetic point, different types of corrections arise and the quality of the fitting procedure rapidly decreases. Thus, extracting $K$ beyond $\Delta = 0.7$ turns out to be numerically challenging. As can be seen from Fig. 5 data points obtained via $dS_\alpha$ significantly deviates (of about a $5-15\%$ discrepancy) from other estimates in this regime. Finally, let us point out that, for $\Delta = -0.9$, the decay exponent for PBC is so large that oscillations are strongly dumped for large system sizes, so that an accurate estimate of $K$ is not possible; for OBC instead, being the exponent smaller by a factor of 2, the estimate is still in very good agreement with all other methods even for $\Delta = -0.9$.

The third way we estimate $K$ is through spin fluctuations. For a bipartition as the one used to define the von Neumann entropy, we define the quantity $F = \left(\langle \sum_{i \in A} S_i^z \rangle^2 - \langle \sum_{i \in A} S_i^z \rangle^2\right)^2$. For a TLL under PBC, spin fluctuations behave as

$$F(L, L) = K \frac{\pi^2}{\alpha^2} \ln \left[ \frac{\pi L}{\sin \left( \frac{\pi L}{L} \right)} \right] + A_1 + O(l^{2K}) \quad (13)$$

and provide a quantitative estimation of $K$. We employ such method by fitting the half-lattice spin fluctuation $F(L/2, L)$ as a function of the system size in the interval $L \in [28, 60]$; typical fitting results are illustrated in Fig. 7. At the antiferromagnetic point $\Delta = 1$, logarithmic corrections to correlation functions severely modify Eq. 13, strong oscillations, not captured by a quadratic TLL theory, emerge with respect to the parity of $L$, preventing a reliable estimate of $K$.

The results obtained in this section are all shown in Fig. 8, from which one can see that they agree over almost the whole anisotropy parameter range. In general, the level spectroscopy method leads to more accurate estimates, as the quantities it relies on are very accurately estimated with DMRG, and additional finite size corrections seems to play a minor role; on the contrary, REs estimates, which are extremely precise for $\Delta < 0.6$, may indeed suffer from both larger truncation errors and stronger finite-size dependences close to the antiferromagnetic point, resulting in a worst mutual agreement with fluctuations and LS. Finally, all results are compared with a previously stated conjecture based on exact calculations on small system sizes which relates the Luttinger parameter $K_S$ of a spin-$S$ Heisenberg chain with $S = 1/2$ case in the $\Delta < 0$ regime:

$$K(\Delta)_S = 2SK(\Delta)_{1/2}.$$

Remarkably, as it can be seen from Fig. 8, this conjecture appears to be in a semi-quantitative agreement with the numerical results even well beyond its original validity regime. Discrepancies among the results emerge mainly close to the antiferromagnetic point, where logarithmic corrections differently affect the techniques we have presented: in this regime, level spectroscopy turns out to be the most reliable method to extract the Luttinger parameter, as field theoretical instruments allow to perform more accurate scaling hypothesis with respect to methods based on REs and fluctuations. Nevertheless, the picture suggests that a deeper theoretical insight on the analytical properties of both REs and fluctuations close to critical point with logarithmic corrections may in principle enlarge their regime of applicability.

IV. NUMERICAL RESULTS: ENTANGLEMENT ENTROPIES AND CONNECTION WITH CFTS

A. Rényi entropies of excited states

In recent times, an analytical formula for the REs of low-energy excited states in a CFT was derived and numerically verified for various quantum spin chains. In particular, it has been predicted that the trace of the reduced density matrix $\rho_{A,T}$ of excited states generated by primary operators $T$ of conformal weights $h$, $\bar{h}$ satis-
fies the following relation:

\[ \alpha^{2\alpha(h+h)} \text{Tr}_{A}\rho^\alpha_{A,Y} = \left( \frac{Z(\alpha)}{(1)\alpha^\alpha} \right) \frac{\langle \prod_{j=0}^{\alpha-1} \mathcal{Y}(2\pi j/\alpha)\mathcal{Y}^\dagger(2\pi(j+l)/\alpha) \rangle_{\text{cy}}}{\langle \mathcal{Y}(0)\mathcal{Y}^\dagger(2\pi l) \rangle_{\text{cy}}} \] (15)

Here, \( \alpha \) is assumed to be a positive integer, but the result can be analytically continued all \( \alpha \geq 1 \); \( Z(\alpha) \) is the partition function on a torus of dimensions \( 2\pi \alpha \) and \( 2\log_2[L/\pi\sin(\pi l/L)] \); \( \langle \cdots \rangle_{\text{cy}} \) denotes expectation value on the vacuum state on a cylinder of length \( 2\pi \). In particular, if \( \mathcal{Y} \) is a vertex operator, formula (15) predicts that the VNE (and, up to oscillating terms, all REs) of the excited state generated by \( \mathcal{Y} \) should be equal to the one of the ground state. This finding has been numerically verified in a series of exactly solvable spin models in Refs. 15, 16. In order to further strengthen it, we considered the REs of the state generated by applying a vertex operator on the ground state (which belongs to the \( S_{\text{ex}}^z = \sum_{l=1}^{L} S_{l}^z = 0 \) sector) thus obtaining the ground state in the \( S^z = 1 \) sector. Spanning the entire critical region and employing PBC, we found excellent agreement with the CFT prediction for both von Neumann and \( \alpha > 1 \) REs. In the former case, the entropy of excited and ground state coincide within numerical uncertainty up to a constant shift of order \( 10^{-2} \), as can be seen from typical data presented in the upper panel of Fig. 9 for small systems up to \( L = 12 \), we further checked this behavior with exact diagonalization.

We afterwards checked the relation between the oscillation corrections and the Luttinger parameter as extracted in the previous section by considering REs with \( \alpha > 1 \). Even in this case, the agreement with the predicted behavior is remarkable, except at the ferromagnetic point where the quality of the fit significantly decreases. Results of \( S_{\alpha}^z(l, 60) \) as a function of \( l \) are plotted in Fig. 9, lower panel, and suggest that the amplitude of the oscillations follows a similar behavior as in the ground state case, namely oscillations are more pronounced when approaching the antiferromagnetic point.

\[ \Delta = \Delta_0, \Delta = \Delta_0 + 0.5, \Delta = \Delta_0 + 1 \]

B. Entanglement behavior of Heisenberg chains with different \( S \)

In a recent paper, Ref. 29, an interesting property concerning entanglement entropies of XXZ chains was conjectured. Based on numerical DMRG simulations, it was
shown that, under both OBC and PBC, the von Neumann entropy of XXZ spin chains with different half-odd-integer $S \geq 5/2$ satisfies the following relation:

$$\ln(2) \Delta S_1(S) \equiv S_1(l, L)_S - S_1(l, L)_{S-1} = \frac{1}{2S-1} + \epsilon_S$$  \hspace{1cm} (16)

where $\epsilon_S \to 0$ in the $L \to \infty$ limit. Such relation implies that, independently on the anisotropy $\Delta$, the non-universal constant contribution acquires a universal form; interestingly, it scales as the inverse of the difference between the one-site Hilbert space dimension of the $S$ case minus the $S = 1/2$ one.

We systematically investigated the behavior of $\Delta S_1(3/2)$ as a function of $\Delta$ by employing PBC in order to get rid of the oscillation contribution, which, as noticed in literature and confirmed in the previous section, is extremely different for different values of $S$. As a preliminary check, we compared our value of $\Delta S_1(3/2)$ at $\Delta = 1/2$ with the one reported in Ref.\textsuperscript{29}, finding indeed very good agreement up to the different logarithmic basis employed here. Due to a very slight $l$-dependence of $\Delta S_1(3/2)$, we mostly considered its mean value in the interval of block length $l \in [11, 29]$ in systems with up to $L = 60$ sites. A schematic plot of the entropy difference at $L = 58$ is presented in Fig. 10: $\Delta S_1(3/2)$ displays a notable non-monotonic $\Delta$-dependence. Similar plots are obtained with different $L$. In summary, our results firmly confirm that Eq. (16) does not hold for $S = 3/2$, in accordance with Ref.\textsuperscript{29}.

\section*{V. CONCLUSIONS}

In this work, we analyzed critical and entanglement properties of the spin-3/2 anisotropic XXZ chain. By means of DMRG simulations, we systematically calculated the sound velocity and the Luttinger parameter in the entire critical region with a variety of methods such as level spectroscopy, entropy analysis and spin-fluctuations. At the antiferromagnetic point, logarithmic corrections prevent an accurate estimate of the Luttinger parameter via spin-fluctuations and entropy oscillations, whilst level spectroscopy, where such corrections may be systematically introduced, still provide reliable results. Such findings benchmark the use of level spectroscopy techniques, which stem as preferable over correlation function methods based on fluctuations and Rényi entropies when approaching and determining phase transition points with logarithmic corrections. Away from such delicate regimes, all methods give compatible results, in agreement with previous studies, although REs usually require more accurate calculations since their absolute value is very small in our case study.

Finally, we investigated in detail the behavior of Rényi entropies of both ground and excited states. In the former case, we compared the REs of the $S = 1/2$ and $S = 3/2$ cases, proving that they are not connected by general relations as in the $S > 3/2$ case. Then, we provided evidence that recent results on the RE of certain excited states in a conformal field theory are verified in the model of interest, presenting the first numerical evidence of such expected behavior in non-integrable models. Even though the leading corrections to REs of excited states and those of the ground state display the same type of behaviour\textsuperscript{31,46}, whether the combination of the two may allow for a precise determination of physical quantities of interest still stands as an open question.

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34 Notice that in the limiting cases were no oscillations are present, such method cannot be trivially applied. However, in the context of spin chains in Luttinger liquid regimes, a finite $k_F$ usually ensures the applicability of such criterion.
35 A large value of $\alpha$ requires larger system sizes to get a reliable estimate of the oscillation decay exponent.