Rényi entropy and parity oscillations of anisotropic spin-s Heisenberg chains in a magnetic field

J. C. Xavier[1,2] and F. C. Alcaraz[2]

[1]*Instituto de Física, Universidade Federal de Uberlândia, Caixa Postal 593, 38400-902 Uberlândia, MG, Brazil*

[2]*Instituto de Física de São Carlos, Universidade de São Paulo, Caixa Postal 369, 13560-970 São Carlos, SP, Brazil*

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Using the density matrix renormalization group, we investigate the Rényi entropy of the anisotropic spin-s Heisenberg chains in a z-magnetic field. We considered the half-odd-integer spin-s chains, with $s = 1/2$, $3/2$, and $5/2$, and periodic and open boundary conditions. In the case of the spin-$1/2$ chain we were able to obtain accurate estimates of the new parity exponents $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$ that gives the power-law decay of the oscillations of the α-Rényi entropy for periodic and open boundary conditions, respectively. We confirm the relations of these exponents with the Luttinger parameter K, as proposed by Calabrese *et al.* [Phys. Rev. Lett. **104**, 095701 (2010)]. Moreover, the predicted periodicity of the oscillating term was also observed for some nonzero values of the magnetization m. We show that for $s > 1/2$ the amplitudes of the oscillations are quite small and get accurate estimates of $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$ become a challenge. Although our estimates of the new universal exponents $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$ for the spin-$3/2$ chain are not so accurate, they are consistent with the theoretical predictions.

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I. INTRODUCTION

The observation that entanglement may play an important role at a quantum phase transition has motivated many studies on the characterization of the critical phenomena by using quantum information concepts.[1–7] Quantum spin chains have been proven as useful laboratories to investigate the interconnection of entanglement and quantum criticality.[1–7] Although does not exist yet an universal measure that quantifies the entanglement,[8] the von Neumann entropy and the Rényi entropies are the most commonly used measures since they are sensitive to the long-distance quantum correlations of critical systems.

In this paper, we study the Rényi entropy in the critical region of the anisotropic spin-s Heisenberg models for $s = 1/2$, $3/2$, and $5/2$. Consider a one-dimensional system of size L and composed by two subsystems A and B of sizes l and $L - l$, respectively. The Rényi entropy is defined as

$$S_\alpha(L,l) = \frac{1}{1-\alpha} \ln Tr\left(\rho_A^\alpha\right), \tag{1}$$

where ρ_A is the reduced density matrix of the subsystem A. The von Neumann entropy is given by the limiting case $\alpha = 1$.

In the past few years a great effort has been made to understand the asymptotic behavior of $S_\alpha(L,l)$. It is expected that the ground state of critical one-dimensional systems gives a Rényi entropy that behaves as

$$S_\alpha(L,l) = S_\alpha^{\rm CFT}(L,l) + S_\alpha^{\rm osc}(L,l). \tag{2}$$

The first term, in this equation, is the conformal field theory (CFT) prediction in the scaling regime ($L \gg l \gg 1$) and is given by[3,6,9–11]

$$S_\alpha^{\rm CFT} = \frac{c}{6}\left(1+\frac{1}{\alpha}\right) \ln\left[\frac{L}{\pi}\sin\left(\frac{\pi l}{L}\right)\right] + c_1^{(p)} \tag{3}$$

for periodic boundary conditions (PBC) and

$$S_\alpha^{\rm CFT} = \frac{c}{12}\left(1+\frac{1}{\alpha}\right) \ln\left\{\frac{4(L+1)}{\pi}\sin\left[\frac{\pi(2l+1)}{2(L+1)}\right]\right\} + c_1^{(o)} \tag{4}$$

for open boundary conditions (OBC), where c is the central charge and $c_1^{(p)}$ and $c_1^{(o)}$ are nonuniversal constants. The expression (4) for OBC has a small modification that is absorbed in the constant $c_1^{(o)}$, as compared with the standard CFT expression.[6,9–11] We chose this expression since, as shown in Ref. 12, in the case of the XX model, it is accurate up to order $(1/l)$ (see also Ref. 13). It is interesting to mention that a generalization of the above equations for the excited states was proposed recently.[14]

The second term in Eq. (2) seems to originate in the strong antiferromagnet correlations, as first argued by Laflorencie *et al.* in the case of the spin-1/2 Heisenberg chain with OBC.[15] In open chains, since translation invariance is broken, the energy density as a function of the site l also shows a similar decaying alternating term $E^{\rm osc}$. In Ref. 15, by using bosonization techniques, this oscillating term was calculated and compared with numerical evaluations of the entropy suggesting that $S_1^{\rm osc}(l) \sim E^{\rm osc} \sim [\frac{L}{\pi}\sin(\frac{\pi l}{L})]^K$, where K is the Luttinger parameter. In fact, these strong oscillations for the open chains were observed by several authors.[12,13,15–25]

More recently, Calabrese *et al.* in Ref. 23 (see also Ref. 24) investigate the anisotropic spin-1/2 Heisenberg chain with periodic boundary conditions and verified that even in this case those oscillations are still present if the Rényi index $\alpha > 1$. For the XX chain in a magnetic field with PBC/OBC, Calabrese and collaborators obtained exactly $S_\alpha^{\rm osc}$ and observed a universal behavior of this oscillating term.[12,23,24] Based on these exact results and on numerical calculations of the spin-1/2 XXZ chain with PBC at zero magnetic field, Calabrese and collaborators conjectured that $S_\alpha^{\rm osc}$ has the following universal behavior[12,23,24] (see also Ref. 15)

$$S_\alpha^{\rm osc} = \frac{g_\alpha^{(p)}}{L^{p_\alpha^{(p)}}} \cos(2lk_F)\left|\sin\left(\pi\frac{l}{L}\right)\right|^{-p_\alpha^{(p)}} \tag{5}$$

for PBC and

$$S_\alpha^{\rm osc} = \frac{g_\alpha^{(o)}}{L^{p_\alpha^{(o)}}} \sin\left[(2l+1)k_F^{(o)}\right]\left|\sin\left[\frac{\pi(2l+1)}{2(L+1)}\right]\right|^{-p_\alpha^{(o)}} \tag{6}$$

for OBC. The constants $g_\alpha^{(p)}$ and $g_\alpha^{(o)}$ are nonuniversal and the critical exponents governing the decaying of the amplitudes of the oscillations are $p_\alpha^{(p)} = 2p_\alpha^{(o)} = \frac{2K}{\alpha}$. In the PBC case [Eq. (5)] the period of the oscillations depends on the Fermi momentum k_F, while in the OBC case [Eq. (6)] it depends on $k_F^{(o)} = \frac{L}{L+1}k_F + \frac{\pi}{2(L+1)}$.

The origin of the exponents $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$, as observed by Cardy and Calabrese in Ref. 26, are the conical spacial-time singularities produced in the conformal mapping used to describe the reduced density matrix ρ_A in the CFT. There are two important ingredients in the oscillatory behavior of Eqs. (5) and (6): the nonuniversal constants $g_\alpha^{(p)}$ and $g_\alpha^{(o)}$ and the Luttinger parameter K [that gives the exponents $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$]. Unfortunately, there is no prediction for $g_\alpha^{(p)}$ and $g_\alpha^{(o)}$ and as we are going to verify, in the case of the spin-s anisotropic Heisenberg model, they decrease dramatically as we increase the spin size s.

Our aim in the present paper is to verify the above conjectures more extensively for the spin-1/2 XXZ, as well for the critical regions of the spin $s > 1/2$ anisotropic Heisenberg model in the presence of an external z-magnetic field. The inclusion of the magnetic field is interesting because the magnetization and the Luttinger parameter K depend on its value. We have then more possibilities to verify the conjectures (5) and (6). The parameter K in the case of the spin-1/2 XXZ chain can be calculated exactly from the Bethe ansatz solution of the model. For $s > 1/2$ the model is not exactly integrable but this parameter can be calculated numerically by exploring the consequences of the conformal invariance of the quantum chain in the bulk limit. In the following we present some important relations that will be used to evaluate the Luttinger liquid parameter K.

The ground-state energy of a system of size L, as $L \to \infty$, behaves as[27,28]

$$\frac{E_0}{L} = e_\infty + \frac{f_\infty}{L} - \frac{v_s \pi c}{\delta 6 L^2} + o(L^{-2}), \qquad (7)$$

where $\delta = 1 (\delta = 4)$ for the system with periodic (open) boundary condition, v_s is the sound velocity, e_∞ is the bulk ground-state energy per site, and f_∞ is the surface free energy that vanishes for the systems with PBC.

The mass gap amplitudes of the finite-size corrections of the higher energy states, for a system with periodic (open) boundary conditions, are related to the anomalous dimensions x_{bulk}^β (surface exponents x_s^β). In the periodic case there are, for each primary operator O_β $(\beta = 1,2,\ldots)$ in the CFT, a tower of states $E_{j,j'}^\beta(L)$ in the spectrum of the Hamiltonian with asymptotic behavior[29]

$$E_{j,j'}^\beta(L) - E_0(L) = \frac{2\pi v_s}{L}\left(x_{\text{bulk}}^\beta + j + j'\right) + o(L^{-1}), \quad (8)$$

where $j,j' = 0,1,2,\ldots$. For the chains with OBC the tower of states have energies[30]

$$E_j^\beta(L) - E_0(L) = \frac{\pi v_s}{L}(x_s^\beta + j) + o(L^{-1}), \qquad (9)$$

with $j = 0,1,2,\ldots$.

For models described by a Luttinger liquid CFT, which are the present cases, the Luttinger liquid parameter K is given by $K = \frac{1}{4x_p}$, where x_p is the lowest anomalous dimension obtained by using in Eq. (8) the lowest excited state in the sector whose magnetization is increased by one unit with respect to that of the ground state.

II. THE MODEL

We consider the anisotropic spin-s Heisenberg chain, also known as the spin-s XXZ chain, in the presence of a magnetic field h with Hamiltonian given by

$$H = \sum_j \left(s_j^x s_{j+1}^x + s_j^y s_{j+1}^y + \Delta s_j^z s_{j+1}^z\right) - h\sum_j s_j^z, \qquad (10)$$

where $\vec{s}_j = (s_j^x, s_j^y, s_j^z)$ are the spin-s SU(2) operators and $\Delta = \cos\gamma$ is the anisotropy.

We investigate the above model, using the density matrix renormalization group (DMRG)[31] method with OBC and PBC, keeping up to $\tilde{m} = 4000$ states per block in the final sweep. We have done ∼6–11 sweeps, and the discarded weight was typically 10^{-7}–10^{-12} at that final sweep. In our DMRG procedure the center blocks are composed of $(2s + 1)$ states.

Let us first present some known results *in the absence of the magnetic field*, i.e, $h = 0$. It is well known that this model at the isotropic point $\Delta = 1$ or $\gamma = 0$ is gapless (gapful) for half-odd-integer (integer) spins.[32,33] The anisotropic chains are critical and conformal invariant for $-1 < \Delta \leqslant 1$ with central charge $c = 1$ for half-odd-integer spins.[34–37] On the other hand, in the case of integer spins a critical phase appears for $-1 \leqslant \Delta \leqslant \Delta_c(s)$, where $\Delta_c(s) < 1$ is a critical anisotropy.[36]

The spin-1/2 XXZ chain is exactly soluble[38,39] and for this reason some exact results are known on its critical region $-1 \leqslant \Delta = \cos\gamma \leqslant 1$. In particular, the anomalous dimension (surface exponent) associated to the lowest eigenenergy, in the sector with total spin z-component $S_T^z = \sum_j s_j^z = 1$, is given by $x_p = \frac{\pi-\gamma}{2\pi}$ $(x_s = 2x_p)$ and the sound velocity is $v_s = \frac{\pi \sin\gamma}{2\gamma}$.[38–42] The exact solution of the spin-1/2 chain has also been explored in the context of the entanglement calculations.[43–47] Although exactly integrable, in this context, only some few issues were explored in the spin-1/2 XXZ chain. This is due to the difficulty in extracting analytically results from its exact solution.

For $h \neq 0$ the model is in a critical and conformal invariant phase for $h_c < |h| < 1 + \Delta$. The critical field $h_c = 0$ for $|\Delta| \leqslant 1$, and for $\Delta > 1$, $h_c = h_c(\Delta)$ depends continuously on Δ. In this phase the model is described by a Luttinger liquid phase whose parameter $K = \frac{1}{4x_p}$ depends on the values of the magnetization per site $m = m(h) = \frac{S_T^Z}{L}$ of the ground state, and the anisotropy Δ. The exact solution of the model allows us to obtain the exponents $x_p = x_p(m)$. This is done by solving a set of nonlinear integral equations that, for the sake of brevity, we refer to Ref. 48. It is expected that for the half-odd spins s, with $s > 1/2$, similar phases emerge when a magnetic field is applied.

III. RESULTS

As mentioned earlier, we need to calculate the anomalous dimension x_p in order to verify if the oscillating term of the Rényi entropies [Eqs. (5) and (6)] decays with the new exponents $p_\alpha^{(p)} = 2p_\alpha^{(o)} = \frac{2K}{\alpha}$. For the spin-1/2 case and $h=0$, we know that $x_p(m=0) = \frac{\pi-\gamma}{2\pi}$. For $h \neq 0$ we can still determine $x_p(m)$ exactly by solving numerically a set of nonlinear integral equations given in Ref. 48. On the other hand, for $s > 1/2$ there are no exact results for x_p.

In order to verify the dependence of the exponents $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$ with the Luttinger parameter K (or x_p), we need to use independent estimates for them. The independent estimates can be obtained from the mass gap of the eigenspectrum and from the α-Rényi entropies. We are going to calculate these quantities using the DMRG technique. The estimate of x_p will be obtained by following basically the same procedure used by one of us in Ref. 22. We consider the Hamiltonian defined in Eq. (10) with PBC to determine the anomalous dimension x_p. The value of $x_p(m)$ is obtained from the limit $L \to \infty$ of the finite-size sequences

$$x_p(m,L) = \frac{L\left[E\left(L,S_T^z+1\right) - E\left(L,S_T^z\right)\right]}{2\pi v_s}, \tag{11}$$

where, as before, $S_T^z = \sum_j s_j^z$.

We estimated the sound velocity v_s using Eq. (7) with $c=1$. We also assume that $x_p(m,L)$ behaves asymptotically as

$$x_p(m,L) = x_p(m) + a_1/L^\omega + a_2/L^2, \tag{12}$$

where $\omega = \frac{2}{x_p} - 4$. These corrections are expected from the finite-size perturbation of the critical models (see Ref. 38). We use a simple fit procedure to obtain $x_p(m)$ by considering typically system of sizes $L = 16$–96.

A. $s = 1/2$

As a benchmark test, we consider first the spin-1/2 XXZ chain. In Table I, we present the estimated values of x_p for some values of magnetization m and anisotropy Δ obtained from Eqs. (11) and (12). We see on this table a clear agreement between our numerical results, obtained via DMRG, and the exact values shown between the parentheses. We thus see that this procedure gives accurate estimates of x_p (similar results was found in Ref. 22 for $m=0$). As mentioned before, for $\Delta > 1$ the model is still critical in the region where the magnetic field produces a nonzero magnetization ($0 < m < 1/2$).[49–52]

TABLE I. The anomalous dimension x_p for the spin-1/2 XXZ chain with PBC and some values of the magnetization m and anisotropy Δ. The values in between the parentheses are the exact ones (see text).

Δ	$m=0$	$m=1/6$	$m=1/4$	$m=3/10$
0	0.2500	0.2499	0.2498	0.2498
	(0.25)	*(0.25)*	*(0.25)*	*(0.25)*
0.5	0.3333	0.3111	0.2956	0.2863
	(0.3333)	*(0.3118)*	*(0.2959)*	*(0.2863)*
$\sqrt{2}/2$	0.3752	0.3319	0.3106	0.2963
	(0.375)	*(0.3334)*	*(0.3101)*	*(0.2967)*
0.9980	0.464	0.358	0.327	0.309
	(0.49)	*(0.3599)*	*(0.3264)*	*(0.3086)*
2.0	—	0.422	0.363	—
	—	*(0.4233)*	*(0.3626)*	—

Unfortunately, for some values of Δ in this region, we observed that the DMRG is not stable. In particular, for systems with OBC and $m \gtrsim 3/10$ we observed that the DMRG is not stable for any Δ. For this reason, we were able to estimate x_p only for $\Delta \lesssim 2$ and $m < 3/10$.

Now, let us estimate the exponents $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$. Recently Calabrese *et al.* in Ref. 23 (see also Ref. 24) calculated exactly these exponents for the spin-1/2 XX chain ($\Delta = 0$) with PBC. They also verified indirectly, through the DMRG algorithm, that $p_\alpha^{(p)} = \frac{1}{2x_p\alpha}$ for $\Delta \neq 0$ and $h = 0$. Fagotti and Calabrese in Ref. 12 also obtained p_α^o exactly for the spin-1/2 XX chain in a magnetic field with OBC. We also include in our analysis the chains with OBC to show, indeed, that the conjecture holds for $\Delta \neq 0$. Here, instead of just verifying that the oscillating term S_α^{osc} is consistent with a universal decay mediated by the exponents $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$, as done in Ref. 23, we are going to estimate *directly* these exponents. We obtain our estimates from the direct fit of the numerical data to the functions (5) and (6).

In Figs. 1 and 2, we present the Rényi entropy $S_\alpha(L,l)$ as a function of l for the anisotropic spin-1/2 Heisenberg chains with PBC/OBC and for some values of m. The symbols (circle, squares, etc.) are the numerical data and the solid lines [with the exception of Fig. 2(a)] connect the fitted points using Eq. (2) with $c = 1$. We show $S_\alpha(L,l)$ only for $l \leqslant L/2$ since $S_\alpha(L,L-l) = S_\alpha(L,l)$. As shown in Fig. 1(a), the amplitudes of the oscillations increase with the value of α. Similar results were also observed in Ref. 23. It is important to stress that if $\alpha > 1$ we can only get a reasonable fit of the numerical data by considering the oscillating term S_α^{osc}, in addition to the standard term S_α^{CFT} predicted by CFT.

Note, from Eqs. (5) and (6), that the periodicity of the oscillating term S_α^{osc} depends on the value of the Fermi momentum k_F. On the other hand, k_F depends of the value of the magnetization, namely $k_F = (1/2 - m)\pi$. Therefore, if we change the magnetization, a change in the periodicity of the oscillations of S_α should be observed. According to Eqs. (5) and (6), the period of oscillations is $\Delta l^* = \pi/k_F$ for PBC and $\Delta l^* = \pi/k_F^o$ for OBC. Our results presented in Figs. 1 and 2, are in perfect agreement with these predictions [see also Fig. 3(d)].

In Fig. 2, we show the Rényi entropy for $\Delta > 1$ and some values of m. For $|\Delta| > 1$ and $m = 0$ the Rényi entropies tend to a constant,[3,6] since the system is gapped. On the other hand, for nonzero magnetization ($0 < m < 1/2$) the system is critical,[49–52] therefore it is expected that S_α behaves as Eq. (2). Indeed, we have observed these two behaviors, as illustrated in Figs. 2(a)– 2(c).

The numerical values of $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$ obtained from the fitting together with the corresponding predicted exact values are presented in the Tables II and III. As we can see in these tables, the values found are very close to the expected ones [with the exception of $\Delta = \cos(\pi/50) = 0.9980$ and $m = 0$] which strongly suggest that the amplitudes of the oscillating terms decay as predicted and observed previously.[12,15,23,24] The fact that the estimated values of $p_\alpha^{(p)}$ for $\Delta = 0.9980$ and $m = 0$ are not so accurate is not a surprise since, at the isotropic point, logarithmic corrections are present. Consequently, the finite-size estimates

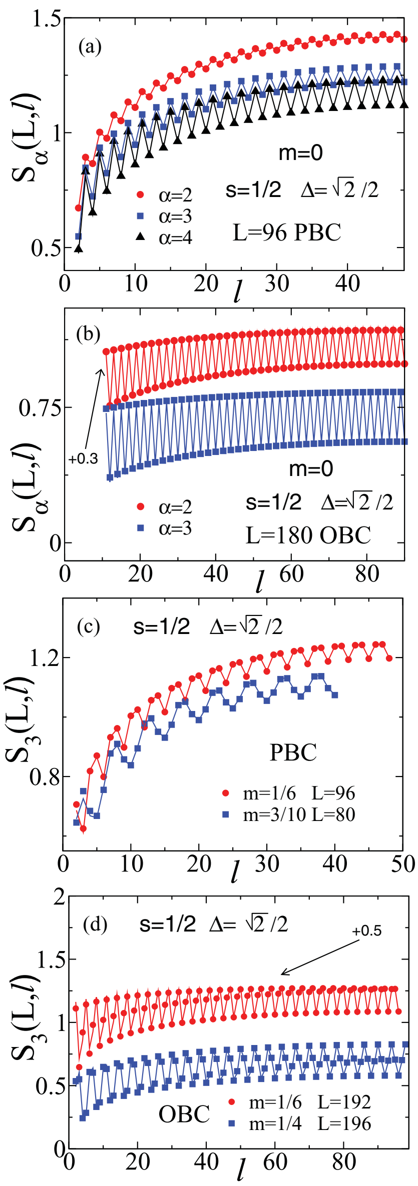

FIG. 1. (Color online) The Rényi entropy $S_\alpha(L,l)$ as a function of l for the spin-1/2 XXZ chain with $\Delta = \sqrt{2}/2$. (a) $L = 96$, PBC, $m = 0$ and three values of α (see legend). (b) $L = 180$, OBC, $m = 0$, and two values of α (see legend). We added 0.3 in the values of the entropy for $\alpha = 2$ in order to see both data in the same figure. (c) $L = 96$ with $m = 1/6$, and $L = 80$ with $m = 3/10$. In both bases $\alpha = 3$ and PBC (d) $L = 192$ with $m = 1/6$, and $L = 196$ with $m = 3/10$. In both bases $\alpha = 3$ and OBC.

have a very slow convergence for anisotropies close to $\Delta = 1$.

B. $s > 1/2$

Now, let us consider the case of spins $s > 1/2$. As we will see below, it is not simple to confirm that the oscillating term decays with the exponents $p_\alpha^{(p)} = 2p_\alpha^{(o)} = \frac{2K}{\alpha}$. The difficulty of extracting $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$ is mainly due to the small amplitude of the oscillations of S_α^{osc}, as we are going to see below. In order to get some idea of their order of the magnitude, let us

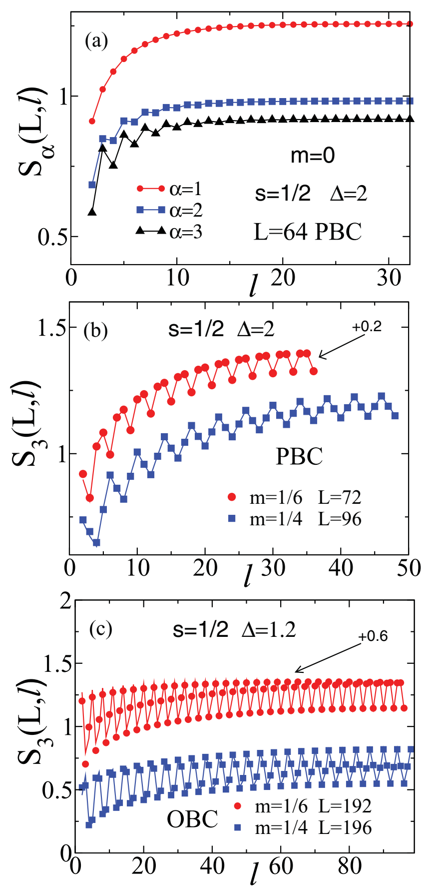

FIG. 2. (Color online) The Rényi entropy $S_\alpha(L,l)$ as a function of l for the spin-1/2 XXZ chain for $\Delta > 1$. (a) $L = 96$, $\Delta = 2$, PBC, and three values of α (see legend). (b) $S_3(L,l)$ for chains with PBC, $\Delta = 2$, and two values of magnetization m (see legend). (c) $S_3(L,l)$ for chains with OBC, $\Delta = 1.2$ and two values of m (see legend).

consider the oscillations in the region around the middle of the chains. According to Eqs. (5) and (6) the amplitudes are $A_s^{(p)} \sim g_\alpha^{(p)}(\Delta,s)/L^{p_\alpha^{(p)}(\Delta,s)}$ and $A_s^{(o)} \sim g_\alpha^{(o)}(\Delta,s)/L^{p_\alpha^{(0)}(\Delta,s)}$. However, our numerical results indicate that $g_\alpha^{(p)}$ and $g_\alpha^{(o)}$are practically independent of the anisotropy value. The amplitudes $A_s^{(p)}$ and $A_s^{(o)}$ are then expected to be smaller as $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$ decrease or, equivalently, as x_p increases. For example, for $\Delta = \sqrt{2}/2$ ($\gamma = \pi/4$), the exponents are $x_p = 0.333, 0.099$, and 0.057 for $s = 1/2, 3/2$, and $5/2$, respectively.[22] Therefore, we expect, at this anisotropy, a decreasing of the amplitude of the oscillations as s increases. This can be observed when we compare Fig. 1(a) with the curves of Fig. 3(a) at $\Delta = \sqrt{2}/2$. Actually, our results indicate that for $s = 3/2$ and $s = 5/2$ the amplitudes of the oscillations are approximately one and two order of magnitude smaller, as compared with those of the $s = 1/2$ at $\Delta = \sqrt{2}/2$, respectively. With such small amplitudes it is quite difficult to extract, at the anisotropy $\Delta = \sqrt{2}/2$, accurate values of $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$ for the spin chains with $s > 1/2$.

In order to estimate the exponents $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$ with some accuracy for quantum spin chains with $s > 1/2$, we need to find at least a region in the critical phase of the model where $x_p \sim 0.3$, as in the spin-1/2 case. As is well known,

TABLE II. The exponents $p_2^{(p)}$ and $p_3^{(o)}$ obtained through a fit of Eq. (2) for the spin-1/2 XXZ chains with PBC, $L = 96$, and some values of Δ and m. We considered $c = 1$ in the fitting to Eq. (2). We also discarded the first points of Rényi entropy S_α in the fitting procedure (up to 5). The values in the parentheses are the exact ones.

		$p_2^{(p)}$	$p_3^{(p)}$
$\Delta = \sqrt{2}/2$	$m = 0$	0.677	0.448
		(0.666)	(0.4444)
	$m = 1/6$	0.757	0.496
		(0.7498)	(0.4999)
	$m = 1/4$	0.811	0.553
		(0.8062)	(0.5375)
$\Delta = 0.9980$	$m = 0$	0.631	0.411
		(0.49)	(0.3267)
	$m = 1/6$	0.706	0.462
		(0.6946)	(0.4631)
	$m = 1/4$	0.771	0.528
		(0.7659)	(0.5106)
$\Delta = 2$	$m = 1/6$	0.587	0.390
		(0.5905)	(0.3937)
	$m = 1/4$	0.675	0.442
		(0.6895)	(0.4596)

at the isotropic point $\Delta = 1$ all spin-s Heisenberg chains have $x_p = 1/2$. However, at this isotropic point, the operator governing the finite-size corrections is marginal producing logarithmic corrections that make a slow convergence in the finite-size estimates. We then select an anisotropy close to the isotropic point. We choose $\Delta = \cos(\pi/50) = 0.9980$, although we should expect that even at this point the finite-size corrections are very large producing only rough estimates of x_p, $p_\alpha^{(p)}$, and $p_\alpha^{(o)}$.

In Table IV, we present the anomalous dimensions x_p for the spin-3/2 and spin-5/2 chains for $\Delta = 0.9980$ and some values of magnetization m. Note that $x_p < 0.15$, for the spin-5/2 quantum chains. This means that the evaluation of $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$ will be quite difficult even taking anisotropies close to the isotropic point. For this reason we concentrate in the $s = 3/2$ case at $\Delta = 0.9980$ and $m = 0$, where the estimate value is

TABLE III. Same as Table II but for chains with OBC. We fit the data with system sizes $L = 180$–196. We have discarded the first points (up to 12 points) in the fitting procedure.

		$p_2^{(o)}$	$p_3^{(o)}$
$\Delta = \sqrt{2}/2$	$m = 0$	0.300	0.221
		(0.3333)	(0.2222)
	$m = 1/6$	0.385	0.301
		(0.3749)	(0.2500)
	$m = 1/4$	0.378	0.240
		(0.4031)	(0.2687)
$\Delta = 1.2$	$m = 1/6$	0.315	0.251
		(0.3326)	(0.2217)
	$m = 1/4$	0.339	0.209
		(0.3722)	(0.248)

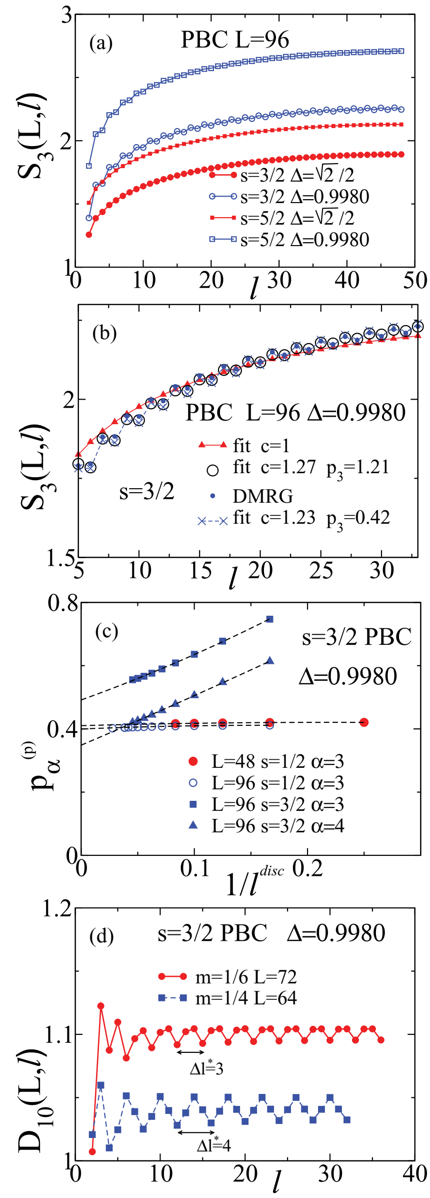

FIG. 3. (Color online) (a) The Rényi entropy $S_3(L,l)$ vs l for the spin-3/2 and spin-5/2 chains of size $L = 96$, and two values of Δ (see legend). (b) $S_3(L,l)$ vs l for the spin-3/2 chain of size $L = 96$ and $\Delta = 0.9980$. The solid circles are the DMRG data and the other symbols are fits (see legend). (c) Estimates of $p_\alpha^{(p)}$ as function of $1/l^{\text{disc}}$ for the spin-1/2 and spin-3/2 chains with PBC. The symbols are the numerical data and the dashed lines connect the fitted data (see text). (d) $D_{10}(L,l)$ vs l for the spin-3/2 chains at $\Delta = 0.9980$ and two values of the magnetization (see the legend).

$x_p = 0.39$. This value is close to the value $x_p = 0.375$ (see Table I) for the spin-1/2 with $\Delta = \sqrt{2}/2$. We then, naively, expect that the amplitudes $A_s^{(p)}$ and $A_s^{(o)}$ are of the same order in these two cases. However, to our surprise the amplitudes of the oscillations for $s = 3/2$ are quite smaller than those of the $s = 1/2$, as we can see in Figs. 3(a) and 3(b). Similar results were also observed for the $s = 3/2$ chains with OBC and $m \neq 0$ (for $\alpha = 1$ and $m = 0$, see also Ref. 22). These results

TABLE IV. The anomalous dimension x_p for the anisotropic spin-3/2 and spin-5/2 Heisenberg chains with PBC, with anisotropy $\Delta = 0.9980$ and some values of the magnetization m.

	$m=0$	$m=1/6$	$m=1/4$	$m=3/10$
$s=3/2$	0.39	0.1235	0.1177	0.1157
$s=5/2$	0.12	0.074	0.071	0.070

indicate that the nonuniversal constants $g_\alpha^{(p)}$ and $g_\alpha^{(o)}$ appearing in Eqs. (5) and (6) are very small for $s > 1/2$, as compared with the $s = 1/2$ case. This means that the evaluation of $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$ directly from the decaying of the Rényi entropy oscillation, for the $s > 1/2$ quantum chains, is quite a hard task.

Despite the above difficulties, we try to estimate $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$ for the spin-3/2 chain at the anisotropy $\Delta = 0.9980$ and magnetization $m = 0$. As already mentioned, we should expect rough estimates since we are close the the isotropic point. Like the $s = 1/2$ case the oscillations, although smaller, happens only for $\alpha > 1$. The central charge obtained by fitting Eq. (2) is, in the $\alpha = 1$ case, $c = 1.01$ at $\Delta = \sqrt{2}/2$, and $c = 1.2$ at $\Delta = 0.9980$. If we fix $c = 1$ the fitting is quite poor at $\Delta = 0.9980$. A nice fit, at this anisotropy, is obtained only by allowing c as a free parameter. Certainly the estimate of c, as we increase L, decreases toward the exact value $c = 1$. Let us now concentrate on the case of $\alpha = 3$ where the amplitudes are clearly present. We are going to fit the data with Eq. (2) in three distinct ways.

First, we try to fit the DMRG data to Eq. (2) by considering $c = 1$ fixed. In this case, the least-squares fitting give us $g_3^{(p)} = 0$ for the best fit with $\chi^2 = 0.0426$[53] [red triangles in Fig. 3(b)]. This means that through this procedure we get no oscillations[54] [see Fig. 3(b)] and we are not able to extract values of $p_3^{(p)}$.

In the second procedure we allow c and $p_3^{(p)}$ as free fit parameters. In this case we get $p_3 = 1.21$ and $c = 1.27$ with $\chi^2 = 0.0041$ for $L = 96$ [black circles in Fig. 3(b)]. Similar results were obtained for $L = 48$ where we get $p_3^{(p)} = 1.19$.

In the third procedure we fix the expected value of $p_3^{(p)} = \frac{1}{6x_p} = 1/(6 \times 0.39) = 0.427$. In this case the get $\chi^2 = 0.0087$ which is higher than previous procedure. In Fig. 3(b), the blue dashed line connects the fit to our data by considering the predicted exponent $p_3^{(p)} = 0.427$ fixed. Although the finite-size corrections are large, since we are close to the isotropic point, the results suggest that the oscillating term of the Rényi entropy decays as Eq. (5). We note that for the spin-3/2 chains, different from the spin-1/2 case, the estimates of $p_\alpha^{(p)}$ depend strongly on how many sites l of the subsystem A we discard. In Fig. 3(c), we present the estimates of the exponents $p_3^{(p)}$ and $p_4^{(p)}$ as function of $1/l^{\text{disc}}$, where l^{disc} is the number of sites we discard in the fit procedure (we discard the sites $l = 1,\ldots,l^{\text{disc}}$). As we can note in this figure, for the spin-1/2 case the estimates of $p_\alpha^{(p)}$ weakly depend on the values l^{disc} and L. The weak dependence with the lattice size L also happens for $s = 3/2$. However, contrarily to the spin-1/2 case, those estimates are very sensitive to the number of sites l^{disc} of the subsystem A we discard, as shown in Fig. 3(c). In order to take into account this effect, we assume that $p_\alpha^{(p)}(l^{\text{disc}})$ behaves as

$$p_\alpha^{(p)}(l_\alpha^{\text{disc}}) = p_\alpha^{(p)} + \frac{a_\alpha}{l^{\text{disc}}} + \frac{b_\alpha}{(l^{\text{disc}})^2}. \tag{13}$$

If we fit our data for the spin-3/2 case [presented in Fig. 3(c)] with this equation, we obtain $p_3^{(p)} = 0.49$ and $p_4^{(p)} = 0.34$. These values are quite close to the predicted ones [$p_3^{(p)} = 0.427$ and $p_4^{(p)} = 0.32$]. In the above fit procedure the central charge c is also a free fit parameter. We also observed, in this case, that the estimates of c are sensitive to the values of l^{disc}, and as we increase l^{disc} they get closer to the expected value $c = 1$. In Fig. 3(c), we present the fits for the spin-3/2 chains only for $l^{\text{disc}} < 20$, since for large values of l the amplitudes of the oscillations are of the same order of the numerical errors. Finding estimates of the exponent $p_\alpha^{(o)}$ for the spin-3/2 chains with OBC are even more difficult. In this case the estimates of p_α are very sensitive to l^{disc} *and also* to L. For this reason we are not able to find a simple procedure to estimate this exponent for the spin-3/2 chains with OBC.

We could naively expect that for $m > 0$, where logarithmic corrections are not expected, $p_\alpha^{(p)}$ would be better estimated. However, for $m > 0$ the anomalous dimension x_p is small (see Table IV) and, consequently, the amplitudes of the oscillations are also small, complicating our analysis, as discussed earlier. However, we can observe an important feature of Eq. (5) in the Rényi entropy of the spin-3/2 chains. To better see this feature, it is convenient to define the difference $D_\alpha(L,l) = S_\alpha - S_\alpha^{\text{CFT}}$. In Fig. 3(d), we present $D_{10}(L,l)$ as a function of l for the spin-3/2 chain for $\Delta = 0.9980$ and two values of the magnetization. We choose to present a large value of α since the amplitudes are bigger as we increase α. According to Eq. (5) the period of the oscillations is $\Delta l^* = \pi/k_F = 2/(2 - 2m)$. In fact, we have observed this periodicity, as shown in Fig. 3(d) for two values of the magnetization.

IV. DISCUSSION

In this paper, we investigate the Rényi entropies of the spin-s anisotropic Heisenberg chains in a magnetic field. These quantum chains are critical and conformal invariant in a wide region of values of the magnetic field h and anisotropy Δ. The long-distance physics of this critical region is described by a Luttinger liquid CFT, with central charge $c = 1$. For this reason, these models are very attractive for testing predictions for one-dimensional critical systems. In particular, it is expected that the α-Rényi entropies have a term that oscillates with the subsystem size, whose amplitudes show a power-law decay with universal exponents $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$. These exponents are expected to depend on the Luttinger parameter K, i.e., $p_\alpha^{(p)} = 2K/\alpha$ and $p_\alpha^{(o)} = K/\alpha$ for PBC and OBC, respectively. This universal behavior was obtained exactly for the spin-1/2 XXZ chains with a magnetic field with PBC and OBC for $\Delta = 0$ (XX chains).[12,24] Moreover, for $h = 0$, DMRG calculations of the spin-1/2 XXZ chain also indicate that the oscillating term indeed decays as predicted.[23] As part of this work, we made an extensive study of the spin-1/2 model but considered a much wider region of couplings than those considered earlier. Using the DMRG technique, we also investigate extensively the quantum spin-s chains (up to $s = 5/2$) with PBC/OBC for several values of anisotropy Δ and magnetic field. Using the CFT machinery we were able to get accurate estimates of the Luttinger parameter K. For the spin-1/2 chains with PBC and OBC, we extract the exponents $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$ through a fit of Eq. (2) and confirm the predicted universal behavior of the Rényi entropy for several values of magnetization m and anisotropy Δ. For spin $s = 3/2$ our estimates of the the exponent p_α are not so accurate due to the fact that the nonuniversal constants $g_\alpha^{(p)}$ and $g_\alpha^{(o)}$ are very small (typically one order of magnitude smaller than the ones of spin-1/2 chain), even though our results indicate that $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$ are related with the Luttinger parameter, as predicted. We also observe that the periodicity of the oscillating term changes with the magnetization, as conjectured. For $s > 3/2$ we were not able to extract the exponents $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$, mainly due to the fact that the $g_\alpha^{(p)}$ and $g_\alpha^{(o)}$ are so small, making the data difficult to analyze. In this case, the Luttinger parameter K is larger (compared with the ones of the spin-1/2) and also contributes to make the oscillating term $S^{\rm osc}$ almost imperceptible. We could even think that this term is null, as happens in the Ising model,[24,55] and that such small oscillations comes from numerical errors. However, we are convinced that those small oscillations are not related with the truncation errors in the DMRG. We have observed that those oscillations do not decrease as we increase the number states kept (up to $\tilde{m} = 4000$) in the DMRG procedure. These results strongly indicate that the nonuniversal amplitudes $g_\alpha^{(p)}$ and $g_\alpha^{(o)}$ decrease very fast as the spin s increases. This makes a huge challenge the determination of the exponents $p_\alpha^{(p)}$ and $p_\alpha^{(o)}$ with reasonable accuracy for $s > 1/2$.

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[1] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature **416**, 608 (2002).
[2] T. J. Osborne and M. A. Nielsen, Phys. Rev. A **66**, 032110 (2002).
[3] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003).
[4] A. Amico, R. Fazio, Osterloh, and V. Vedral, Rev. Mod. Phys. **80**, 517 (2008).
[5] V. E. Korepin, Phys. Rev. Lett. **92**, 096402 (2004).
[6] P. Calabrese and J. Cardy, J. Stat. Mech. (2004) P06002.
[7] F. C. Alcaraz and M. S. Sarandy, Phys. Rev. A **78**, 032319 (2008).
[8] J. I. Latorre and A. Riera, J. Phys. A: Math. Theor. **42**, 504002 (2009).
[9] C. Holzhey, F. Larsen, and F. Wilczek, Nucl. Phys. B **424**, 443 (1994).
[10] P. Calabrese and J. Cardy, J. Phys. A: Math. Theor. **42**, 504005 (2009).
[11] I. Affleck and A. W. W. Ludwig, Phys. Rev. Lett. **67**, 161 (1991).
[12] M. Fagotti and P. Calabrese, J. Stat. Mech. (2011) P01017.
[13] I. Affleck, N. Laflorencie, and E. S. Sørensen, J. Phys. A: Math. Theor. **42**, 504009 (2009).
[14] F. C. Alcaraz, M. I. Berganza, and G. Sierra, Phys. Rev. Lett. **106**, 201601 (2011).
[15] N. Laflorencie, E. S. Sørensen, M. S. Chang, and I. Affleck, Phys. Rev. Lett. **96**, 100603 (2006).
[16] H.-Q. Zhou, T. Barthel, J. O. Fjærestad, and U. Schollwöck, Phys. Rev. A **74**, 050305(R) (2006).
[17] M. Fuehringer, S. Rachel, R. Thomale, M. Greiter, and P. Schmitteckert, Ann. Phys. (Berlin) **17**, 922 (2008).
[18] A. M. Läuchli and C. Kollath, J. Stat. Mech. (2008) P05018.
[19] A. B. Kallin, I. González, M. B. Hastings, and R. G. Melko, Phys. Rev. Lett. **103**, 117203 (2009).
[20] G. Roux, S. Capponi, P. Lecheminant, and P. Azaria, Eur. Phys. J. B **68**, 293 (2009).
[21] J. I. Cirac and G. Sierra, Phys. Rev. B **81**, 104431 (2010).
[22] J. C. Xavier, Phys. Rev. B **81**, 224404 (2010).
[23] P. Calabrese, M. Campostrini, F. Essler, and B. Nienhuis, Phys. Rev. Lett. **104**, 095701 (2010).
[24] P. Calabrese and F. H. L. Essler, J. Stat. Mech. (2010) P08029.
[25] M. Fagotti, P. Calabrese, and J. E. Moore, Phys. Rev. B **83**, 045110 (2011).
[26] J. Cardy and P. Calabrese, J. Stat. Mech. (2010) P04023.
[27] I. Affleck, Phys. Rev. Lett. **56**, 746 (1986).
[28] H. W. J. Blöte, J. L. Cardy, and M. P. Nightingale, Phys. Rev. Lett. **56**, 742 (1986).
[29] J. Cardy, Nucl. Phys. B **270**, 186 (1986).
[30] J. Cardy, J. Phys. A: Math. Gen. **17**, L385 (1984).
[31] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[32] F. D. M. Haldane, Phys. Lett. A **93**, 464 (1983).
[33] F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983).
[34] H. J. Schulz, Phys. Rev. B **34**, 6372 (1986).
[35] I. Affleck, D. Gepner, H. J. Schulz, and T. Ziman, J. Phys. A: Math. Gen. **22**, 511 (1989).
[36] F. C. Alcaraz and A. Moreo, Phys. Rev. B **46**, 2896 (1992).
[37] K. Hallberg, X. Q. G. Wang, P. Horsch, and A. Moreo, Phys. Rev. Lett. **76**, 4955 (1996).
[38] F. C. Alcaraz, M. N. Barber, and M. T. Batchelor, Ann. Phys. **182**, 280 (1988).
[39] F. C. Alcaraz, M. N. Barber, M. T. Batchelor, R. J. Baxter, and G. R. W. Quispel, J. Phys. A: Math. Gen. **20**, 6397 (1987).
[40] C. J. Hamer, J. Phys. A: Math. Gen. **18**, L1133 (1985).
[41] F. Woynarovich and H.-P. Eckle, J. Phys. A: Math. Gen. **20**, L97 (1987).
[42] A. Luther and I. Peschel, Phys. Rev. B **12**, 3908 (1975).
[43] J. Sato, M. Shiroishi, and M. Takahashi, J. Stat. Mech. (2006) P12017.
[44] L. Banchi, F. Colomo, and P. Verrucchi, Phys. Rev. A **80**, 022341 (2009).
[45] J. Sato and M. Shiroishi, J. Phys. A: Math. Theor. **40**, 8739 (2007).

[46] V. Alba, M. Fagotti, and P. Calabrese, J. Stat. Mech. (2009) P10020.
[47] B. Nienhuis, M. Campostrini, and P. Calabrese, J. Stat. Mech. (2009) P02063.
[48] F. Woynarovich, H.-P. Eckle, and T. T. Truong, J. Phys. A: Math. Gen **22**, 4027 (1989).
[49] J. D. Johnson and B. M. McCoy, Phys. Rev. A **6**, 1613 (1972).
[50] M. Takahashi, Prog. Theor. Phys. **50**, 1519 (1973).
[51] V. L. Pokrovsky and A. L. Talapov, Sov. Phys. JETP **51**, 134 (1980).
[52] F. C. Alcaraz and A. L. Malvezzi, J. Phys. A: Math. Gen. **28**, 1521 (1995).
[53] For a set of N data $d_i (i = 1, \ldots N)$ whose fitted points are f_i the χ^2 is given by $[\sum_i^N (f_i - d_i)^2]^{1/2}$.
[54] If we discard the first sites, the oscillations are "recovered." However, if we consider c as a free parameter, we obtain a better fit.
[55] F. Iglói and R. Juhász, Europhys. Lett. **81**, 57003 (2008).