# Entanglement entropy, conformal invariance, and the critical behavior of the anisotropic spin-s Heisenberg chains: DMRG study

#### J. C. Xavier

Instituto de Física, Universidade Federal de Uberlândia, Caixa Postal 593, 38400-902 Uberlândia, MG, Brazil (Received 2 February 2010; revised manuscript received 16 April 2010; published 1 June 2010)

Using the density-matrix renormalization group, we investigate the critical behavior of the anisotropic Heisenberg chains with spins up to s=9/2. We show that through the relations arising from the conformal invariance and the DMRG technique it is possible to obtain accurate finite-size estimates of the conformal anomaly c, the sound velocity  $v_s$ , the anomalous dimension  $x_{bulk}$ , and the surface exponent  $x_s$  of the anisotropic spin-s Heisenberg chains with relatively good accuracy without fitting parameters. Our results indicate that the entanglement entropy  $S(L, l_A, s)$  of the spin-s Heisenberg chains satisfies the relation  $S(L, l_A, s) - S(L, l_A, s) - (L, l_A, s) - (L, l_A, s)$  in the thermodynamic limit.

## DOI: 10.1103/PhysRevB.81.224404 PACS number(s): 75.10.Jm, 03.67.Mn, 05.70.Jk

#### I. INTRODUCTION

Conformal invariance plays an important role in the study of critical one-dimensional quantum systems. Several constraints appear if we assume that the critical systems are conformal invariant. In particular, the possible classes of critical behavior of the one-dimensional quantum systems are indexed by the conformal anomaly (or central charge) c as well as the values the anomalous dimensions  $x_{bulk}^{\alpha}$  of the primary scaling operators  $O^{\alpha}$ . In the study of the primary scaling operators  $O^{\alpha}$ .

In the mid eighties of last century, it was shown that the conformal anomaly c can be extracted from the large-L behavior of the ground-state energy  $E_0(L)$ . The ground-state energy of a system of size L behaves as<sup>4,5</sup>

$$\frac{E_0}{L} = e_\infty + \frac{f_\infty}{L} - \frac{v_s \pi c}{\delta 6L^2},\tag{1}$$

where the constant  $\delta$ =1(4) for the systems under periodic (open/fixed) boundary conditions (PBC),  $v_s$  is the sound velocity,  $e_\infty$  is the bulk ground-state energy per site, and  $f_\infty$  is the surface free energy, which vanishes for the systems under PBC. The structure of the higher energy states, for a system with periodic (open) boundary conditions, are related with the anomalous dimensions  $x_{bulk}^\alpha$  (surface exponents  $x_s^\alpha$ ). There are a tower of states in the spectrum of the Hamiltonian with energies  $E_{m,m'}^\alpha(L)$  given by<sup>6,7</sup>

$$E_{m,m'}^{\alpha}(L) - E_0(L) = \frac{2\pi v_s}{\eta L}(x + m + m'), \qquad (2)$$

where m, m' = 0, 1, 2, ..., the constant  $\eta = 1(2)$ , and  $x = x_{bulk}^{\alpha}(x_s^{\alpha})$  for the systems with periodic (open) boundary conditions.

The critical behavior of several models were studied using the conformal invariance relations above. In particular, the spin-1/2 XXZ chain is exactly soluble. For this reason, in this case, it is possible to obtain the spectrum of the energies of very large system sizes (solving the Bethe ansatz equations). Due to this fact, very accurate estimates of c,  $v_s$ ,  $x_{bulk}^{\alpha}$ , and  $x_s^{\alpha}$  were obtained for the spin-1/2 XXZ chain.<sup>8,9</sup> How-

ever, very few models are exactly soluble. And, in general, it is possible obtain the eigenspectrum only by exact numerical diagonalizations.

The Lanczos method of exact diagonalization (ED) can be used to extract the ground-state energies of the Hamiltonians. However, with ED it is possible to consider small system sizes, since the Hilbert space grows exponentially with the system size. Even though, relative good estimates of conformal anomaly c and the anomalous dimensions  $x_{bulk}^{\alpha}$  can be obtained with ED (see, for example, Refs. 10 and 11).

The density-matrix renormalization group (DMRG) (Ref. 12) is a powerful numerical technique that can be used to study very large one-dimensional systems. In principle, we can use the DMRG technique and the conformal invariance relations to obtain high-accuracy estimates of c,  $x_{bulk}^{\alpha}$ , and  $x_{s}^{\alpha}$ . Since with the DMRG it is possible to obtain the ground-states energies of large system sizes in a controlled way. However, it is not easy to estimate the sound velocity  $v_{s}$  with the DMRG technique, differently of the ED (it is possible to estimate  $v_{s}$  with the ED by the behavior of the energies in different momentum sectors). This is the major reason why the conformal invariance relations above were not explored in the studies of critical systems by the DMRG technique. <sup>13</sup>

In recent years, this has changed because Calabrese and Cardy related the entanglement entropy of one-dimensional critical systems with the conformal anomaly c (Ref. 14) (see also Refs. 15–17). As we will see, due to this new relation between the conformal anomaly and the entanglement entropy, it is now possible to obtain the *finite-size estimates of* c,  $v_s$ ,  $x_{bulk}$ , and  $x_s$  in a systematic way with the DMRG technique. The entanglement entropy can be defined as following. Consider a one-dimensional system with size L and composed by two subsystems A and B of sizes  $l_A$  and  $l_B = L - l_A$ , respectively. The entanglement entropy is defined as the von Neumann entropy  $S(L, l_A) = -\text{Tr } \rho_A \ln(\rho_A)$ , associated with the reduced density matrix  $\rho_A$ . For the critical one-dimensional systems the entanglement entropy behaves as  $l_A$ 

$$S(L, l_A) = \frac{c}{3\eta} \ln \left[ \frac{\eta L}{\pi} \sin \left( \frac{\pi l_A}{L} \right) \right] + c_1 - (1 - \eta) s_b, \quad (3)$$

where  $s_b$  is the boundary entropy, <sup>17</sup>  $c_1$  is a nonuniversal constant, and  $\eta$ =1(2) for the systems under periodic (open/fixed) boundary conditions.

Note that we can estimate the conformal anomaly c using Eq. (3) without the knowledge of the sound velocity  $v_s$ . Indeed, some authors have plotted  $S(L,l_A)$  as function of  $\ln[\frac{L}{\pi}\sin(\frac{\pi l_A}{L})]$  in order to estimate c by a numerical fit. Here, we use basically the same route that Zhao et al. used in Ref. 19 to extract c in an investigation of the XXZ Heisenberg chains with defects. We will estimate c by measuring the entanglement entropy of two systems with different sizes. With this procedure, we can obtain a finite-size estimate of c without a numerical fit. We have observed that this procedure gives errors smaller than the ones obtained by the fitting procedure (in same cases, the error is one order of magnitude smaller).

It is important to point out that some authors have used the DMRG to obtain the *critical exponents* of several models<sup>20</sup> through the asymptotic behavior of static correlation functions. This numerical procedure, use more CPU time and, usually, provides only rough estimates of the critical exponents. Thus, we see that a procedure to obtain accurate estimates of the critical exponents (based in the energies behavior) with the DMRG is also highly desirable.

The main aim of this paper is to show that if we explore all the *three conformal invariance relations* above [Eqs. (1)–(3)] with the DMRG technique, then it is possible to obtain accurate *finite-size estimates of c*,  $v_s$ ,  $x_{bulk}$ , and  $x_s$  in a systematic way with the DMRG technique *without any fitting parameter*. Several authors have explored some of these relations with the DMRG. However, they did not make use of all the three relations (with the exception of Ref. 21). We would like to point out here that with the multiscale entanglement renormalization ansatz it is also possible to extract these quantities with a good accuracy<sup>22</sup> (see also Ref. 23).

In order to illustrate the procedure that we use to extract c,  $v_s$ ,  $x_{bulk}^{\alpha}$ , and  $x_s^{\alpha}$ , we consider the anisotropic spin-s Heisenberg chains defined as

$$H = \sum_{j} (s_{j}^{x} s_{j+1}^{x} + s_{j}^{y} s_{j+1}^{y} + \Delta s_{j}^{z} s_{j+1}^{z}), \tag{4}$$

where  $\Delta = \cos(\gamma)$  is the anisotropy. It is well known that this model at the isotropic point  $\Delta = 1$  is gapless (gapful) for half-integer (integer) spins.<sup>24</sup> For this reason, we will consider only the half-integer spin cases. Although even the models with integer spins become gapless at some critical anisotropy.<sup>10</sup>

We investigate the model defined above using the DMRG (Ref. 12) method under open boundary conditions (OBC) and PBC, keeping up to m=4000 states per block in the final sweep. We have done  $\sim$ 6–9 sweeps, and the discarded weight was typically  $10^{-9}$ – $10^{-12}$  at that final sweep. The dimension of the superblock in the last sweep can reach up to 80 millions. In our DMRG procedure the center blocks are composed of (2s+1) states.

#### II. RESULTS

## A. s = 1/2

We will focus, first, in the anisotropic spin-1/2 Heisenberg chain, which is exactly soluble (for a review see Ref. 8). For

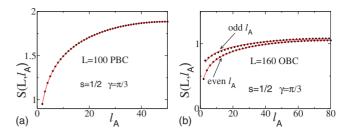


FIG. 1. (Color online) The entanglement entropy  $S(L, l_A)$  vs  $l_A$  for the anisotropic spin-1/2 Heisenberg with  $\gamma = \pi/3$ . The circles are numerical data and the red solid lines are fits to our data using Eq. (3) (see text). (a)  $S(L, l_A)$  vs  $l_A$  for a chain of size L = 100 and PBC. (b)  $S(L, l_A)$  vs  $l_A$  for a chain of size L = 160 and OBC.

this case, we be able to compare our numerical estimates of c,  $v_s$ ,  $x_{bulk}^{\alpha}$ , and  $x_s^{\alpha}$  with the exact results. In order to avoid the logarithmic corrections (due to the marginally irrelevant operator) which makes the finite-size analysis more complicated, we decided to investigate the model at the anisotropic point  $\gamma = \pi/3$  (which corresponds to  $\Delta = 1/2$ ). Few results for other values of  $\gamma$  were also explored in this work.

Before presenting the numerical results for the spin-1/2 chain, let us describe some known results based on analytical approaches. 8.25-28 The anisotropic spin-1/2 chain is critical for  $-1 < \Delta \le 1$  with central charge c=1, the anomalous dimension (surface exponent) associated to the lowest eigenenergy in the sector with total spin z component  $S_z=1$  is given by  $x_{bulk} = \frac{\pi-\gamma}{2\pi}(x_s = \frac{\pi-\gamma}{\pi})$  and the sound velocity is  $v_s = \frac{\pi \sin(\gamma)}{2\gamma}$ . Very interesting to note that for  $\gamma = \pi/3$  the anisotropic spin-1/2 Heisenberg chain presents a very peculiar ground state. For this reason, some analytical expressions for the two-point correlation functions<sup>29</sup> and for the reduced density matrix were obtained. Some exact results for the reduced density matrix with arbitrary  $\gamma$  were also obtained by Alba et al. in Ref. 31.

In Fig. 1(a), we present the entanglement entropy  $S(L, l_A)$ as function of the length  $l_A$  for the anisotropic spin-1/2 Heisenberg chain with PBC for a system of size L=100 and  $\gamma = \pi/3.32$  The red solid line in this figure is a fit to our data using Eq. (3). We show  $S(L, l_A)$  only for  $l_A \le L/2$  since  $S(L, L-l_A) = S(L, l_A)$ . The conformal anomaly obtained through this fit is c=1.005, which is very close to the exact value  $c_{exact}$ =1. Estimates of the conformal anomaly can also be acquired if we consider the system with OBC instead of PBC. In Fig. 1(b), we show  $S(L, l_A)$  as function of  $l_A$  for the model with OBC,  $\gamma = \pi/3$  and L = 160. Observe that for the OBC case,  $S(L, l_A)$  exhibits even-odd oscillations as function of  $l_A$ . In this case, for  $l_A$  even (odd) the fit to our data using Eq. (3) is c=1.09 (c=0.77). These even-odd oscillations have been reported in several works, 33-36 and it is expected to decay away from the boundary with a power law.<sup>33</sup> Very interesting to note that even for systems under PBC, the Rényi entropy also shows even-odd oscillations, which have been proposed to have an universal scaling law.<sup>37</sup>

The above route have been used by some authors to estimate the conformal anomaly of some critical models such as the transverse Ising chain, $^{36}$  the isotropic/anisotropic spin-1/2 Heisenberg chain, $^{21,36}$  the SU(N) chains, $^{21}$  and as well as a spin-3/2 fermionic cold atoms with attractive interactions. $^{35}$ 

TABLE I. Finite-size estimates of the conformal anomaly  $c^{\text{PBC}}$ , the sound velocity  $v_s$ , and the anomalous dimension  $x_{bulk}$  for the spin-1/2 anisotropic Heisenberg chain with PBC and  $\gamma = \pi/3$ . We use L' = L + 16 in Eq. (5).

L	$c^{\mathrm{PBC}}$	$v_s$	$x_{bulk}$
16	0.99596	1.30675	0.33314
32	0.99879	1.30103	0.33324
48	0.99942	1.29994	0.33328
64	0.99966	1.29955	0.33330
80	0.99977	1.29937	0.33331
96		1.29927	0.33332
Exact	1	1.29903	0.33333

In order to obtain good estimates of c with this procedure we need to consider large system sizes, mainly for the OBC case, which can demand large computational effort in general. Here, we use a slightly different route to obtain the finite-size estimates of the conformal anomaly c, as mentioned before. In particular, for the OBC case, we will see that with an extrapolation of the finite-size data, we are able to obtain estimates of c and  $x_s$  with good accuracy. Even considering relatively small system sizes, which requires a reasonably small computational effort.

A simply way to extract the conformal anomaly from Eq. (3), without any fitting parameter, is considering two systems with sizes L and L'. Let us assume that these two systems are composed of two subsystems of sizes  $l_A = L/2$  and  $l_A' = L'/2$ , respectively. Thus, from Eq. (3), we see that we can estimate c by

$$c(L,L') = 3\eta \frac{S(L,L/2) - S(L',L'/2)}{\ln(L/L')} = \frac{3\eta \Delta S}{\ln(L/L')}.$$
 (5)

Note that previously works<sup>19,38</sup> also use the increment of the entropy,  $\Delta S$ , to extract the conformal anomaly of the spin-1/2 XXZ Heisenberg model with defects/impurities. Läuchli and Kollath<sup>39</sup> also used the increment of entropy in order to locate the quantum critical point of the Bose-Hubbard chain.

In Table I, we show the finite-size estimates of the conformal anomaly, obtained by Eq. (5), for the anisotropic spin-1/2 Heisenberg chain with PBC and  $\gamma = \pi/3$ . Similar results were also found for  $\gamma = \pi/6$  and  $\gamma = \pi/8$ . For comparison purpose, we also present in this table the exact values of the conformal anomaly c, the sound velocity  $v_s$ , and the anomalous dimension  $x_{bulk}$ . Note that by using relatively small system sizes, we are able to estimate c with a small error ( $\sim 2 \times 10^{-4}$ ) without any fitting parameter.

Once the conformal anomaly c is obtained, we can use Eq. (1) to extract the sound velocity  $v_s$ . In particular, for the PBC case the finite-size estimate of the sound velocity is obtained by<sup>40</sup>

$$v_s(L) = \frac{6L}{\pi c} [Le_{\infty} - E_0(L)]. \tag{6}$$

Note that in this equation, we also need the bulk ground-state energy per site  $e_{\infty}$ . However, this is not a problem since with

TABLE II. Extrapolated and finite-size estimates of the conformal anomaly  $c^{\rm OBC}$  and the surface exponent  $x_s$  for the anisotropic spin-1/2 Heisenberg chain with OBC and  $\gamma = \pi/3$ . We use L' = L + 20 in Eq. (5). The extrapolated values were obtained by a numerical fit (see text).

	$c^{\mathrm{OBC}}$	$X_{S}$	
60	1.0859	0.64298	
80	1.0727	0.64809	
100	1.0633	0.65131	
120	1.0568	0.65353	
140	1.0518	0.65517	
160	1.0470	0.65642	
∞	1.004	0.66658	
Exact	1	0.66666	

the DMRG technique it is possible to obtain  $e_{\infty}$  with a high accuracy.

The finite-size estimates of  $v_s$  obtained using Eq. (6) are also presented in Table I. As observed in this table, accurate results are also acquired for  $v_s$ . As we already mentioned in the introduction, until very recently, it was not possible to extract the sound velocity  $v_s$ , based only in the large-L behavior of the ground-state energy with the DMRG technique. But, as we have observed, with the use of Eqs. (1) and (3) we can estimate  $v_s$ , with good accuracy, considering relatively small system sizes.

Finally, using Eq. (2), we extract the finite-size estimates of the anomalous dimension/surface exponent by

$$x(L) = \frac{\eta L[E_1(L) - E_0(L)]}{2\pi v_s},$$
(7)

where  $E_1(L)$  is the ground-state energy in the sector with total spin z component  $S_z=1$ . In Table I, we also show the finite-size estimates of  $x_{bulk}$  for the anisotropic spin-1/2 Heisenberg chain under PBC and  $\gamma=\pi/3$ . Note again that accurate results are obtained.

From the above results, we learn that it is possible to obtain good estimates of c,  $v_s$ , and  $x_{bulk}$ , without any fitting parameters (or extrapolations), considering relatively small system sizes under PBC. On the other hand, for the OBC case is necessary to extrapolate the finite-size estimates in order to obtain accurate results, as shown below.

Let us now estimate the conformal anomaly considering the model with OBC [Eq. (5) with  $\eta$ =2]. In Table II, we present the finite-size estimates of the conformal anomaly c for the anisotropic spin-1/2 Heisenberg chain with OBC and  $\gamma$ = $\pi$ /3. As we observed in this table, the finite-size estimates of  $c^{\rm OBC}$  are less accurate than the ones found for the model with PBC, even considering larger systems for the OBC case. We can improve the estimate of  $c^{\rm OBC}$  extrapolating the finite-size data to the infinite lattice value. We assume that conformal anomaly behaves as

$$c^{\text{OBC}}(L) = c + a/L + b/L^2$$
. (8)

The extrapolated values in Table II, were obtained from a fit to our data with this equation (we use only the last four

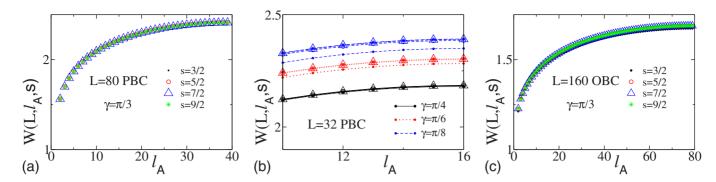


FIG. 2. (Color online) The rescaled entanglement entropy  $W(L, l_A, s)$  vs  $l_A$  for the anisotropic spin-s Heisenberg for some values of s (see legend). (a)  $W(L, l_A, s)$  vs  $l_A$  for chains of size L=80,  $\gamma=\pi/3$ , and PBC. (b)  $W(L, l_A, s)$  vs  $l_A$  for chains of size L=32, PBC, and some values of  $\gamma$  (see legend). The symbols refer to the values of the spins [we used the same symbols of figure (a)]. (c)  $W(L, l_A, s)$  vs  $l_A$  for chains of size L=160 and OBC.

points of our data in the numerical fit). Note that the extrapolated estimate is quite close to the exact value. As we see in this table, the estimate of  $c^{\rm OBC}$  obtained with this procedure gives an absolute error of about  $10^{-3}$ , which is quite good.

In a similar way, we also use Eq. (7) to obtain the surface exponent  $x_s$ . In Table II, we also present the finite-size estimates of  $x_s$  for the anisotropic spin-1/2 Heisenberg chain with OBC and  $\gamma = \pi/3$ . The extrapolated value of surface exponent  $x_s$  was obtained by a numerical fit, as we did for the conformal anomaly. We assume that the surface exponent behaves as

$$x_s(L) = x_s + a/L + b/L^2$$
. (9)

As observed in the table, the extrapolated value of  $x_s$  is also very close to the exact one.

B. 
$$s > 1/2$$

The results obtained above for the spin-1/2 chain are all known, and we studied the spin-1/2 case for the purpose of comparison/benchmark. However, that study was highly important, because it established that the procedure used by us provides accurate results. Now, let us consider the cases where s > 1/2.

Before presenting the estimates of c,  $x_{bulk}$ , and  $x_s$ , we will present an interesting behavior of the entanglement entropy  $S(L, l_A, s)$  for the spin-s Heisenberg chains with spin s > 1/2. We observed what appears to be an universal behavior of  $S(L, l_A, s)$  for s > 1/2. Our numerical data indicate that the entanglement entropy of two systems with spins s and s-1 respectively, with s > 3/2 are related by following the relation:

$$S(L, l_A, s) - S(L, l_A, s - 1) = \frac{1}{(2s - 1)} + a_1,$$
 (10)

where  $a_1$  is a very small term. Note that this is equivalent to, say, that the nonuniversal constant  $c_1(s)$  [see Eq. (3)] satisfies the relation  $c_1(s) - c_1(s-1) = \frac{1}{(2s-1)} + a_1$ .

We have observed that constant  $a_1$  decreases with the size of the systems. We were not able to proof that  $a_1$  is zero in the thermodynamic limit, although our numerical results suggest that, in particular, for a system with PBC (OBC),  $\gamma$ 

=  $\pi/3$ , and size L=80 (L=160) we found that  $a_1 \sim 10^{-3} (a_1 \sim 10^{-2})$ . In the discussion below we neglect this term. Due to Eq. (10), we can express the entanglement entropy  $S(L, l_A, s)$  of a systems with spin s>3/2, in terms of  $S(L, l_A, 3/2)$  by the equation

$$S(L, l_A, s) = S(L, l_A, 3/2) + \sum_{j=0}^{(s-5/2)} \frac{1}{2(s-j) - 1}.$$
 (11)

In order to check the validity of Eq. (11), we investigate the following function:

$$W(L, l_A, s) = S_{\text{DMRG}}(L, l_A, s) - \sum_{j=0}^{(s-5/2)} \frac{1}{2(s-j) - 1}, \quad (12)$$

and we set  $W(L, l_A, 3/2) = S_{DMRG}(L, l_A, 3/2)$ .

Let us focus, first, in the PBC case. In Fig. 2(a), we present the rescaled entanglement entropy  $W(L, l_A, s)$  as function of  $l_A$  for some values of spins for systems with PBC, L=80, and  $\gamma=\pi/3$ . As observed in this figure, all curves collapse onto a single universal scaling curve. Actually, there is a small difference around  $10^{-3}$  between these curves [see Fig. 2(b)]. Similar results are also observed for other values of  $\gamma$  for systems of size L=32, as shown in Fig. 2(b). Note that as  $\gamma$  decreases the differences between the curves increase. This is expected since finite-size effects become stronger as  $\gamma \rightarrow 0$  (or  $\Delta \rightarrow 1$ ). These results strongly indicate that Eq. (11) is valid for any values of spin s > 3/2 and  $\gamma$ . Our numerical data (not shown) support also that  $S_{\text{DMRG}}(L, l_A, 3/2) = S_{\text{DMRG}}(L, l_A, 1/2) + 11/18$  for the PBC case. We will see below that if we consider the systems with OBC, Eq. (11) still holds true for s > 3/2.

Now, let us consider the OBC case. In Fig. 3(a) we show  $S(L, l_A)$  for the anisotropic spin-s Heisenberg with OBC, L = 160,  $\gamma = \pi/3$ , and some values of spins s. Note that differently of the spin-1/2 case with OBC, for spins s > 1/2 the entanglement entropy  $S(L, l_A)$ , does not present the strong odd-even oscillations. Laflorencie *et al.* in Ref. 33 argued that the oscillating term in  $S(L, l_A)$  is universal and is connected with the antiferromagnetic nature of the Hamiltonian (however, at the present moment, there is no analytical deri-

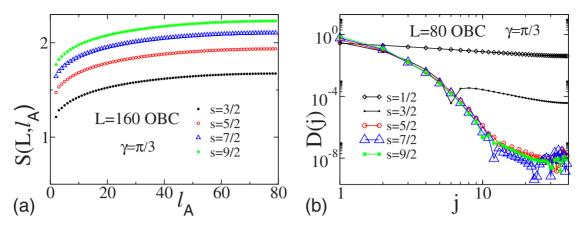


FIG. 3. (Color online) Some results for the anisotropic spin-s Heisenberg with OBC,  $\gamma = \pi/3$ , and some values of s (see legend). (a) The entanglement entropy  $S(L, l_A)$  vs  $l_A$  for chains of size L = 160. (b) The dimer parameter D(j) vs j for chains of size L = 80. We present D(j) only for distances j < 40.

vation of this statement). In particular, the alternating term in  $S(L,l_A)$  appears to be proportional to the alternating term in the energy density<sup>33</sup>

$$h(j) = \langle (s_i^x s_{i+1}^x + s_i^y s_{i+1}^y + \Delta s_i^z s_{i+1}^z) \rangle.$$
 (13)

In order to understand the absence of the strong odd-even oscillations in entanglement entropy  $S(L,l_A)$  for s>1/2, we study the behavior of the "dimer parameter" D(j)=h(j+1)-h(j). It is expected that D(j) decays with a power law.<sup>33</sup> In Fig. 3(b), we present the dimer parameter D(j) for chains of size  $L=80.^{41}$  We roughly estimate the errors of D(j) around  $\sim 10^{-6}$ , since we find numerically that  $[E_0-\Sigma_j h(j)]\sim 10^{-6}$ . As observed in this figure, the magnitude of the oscillations of h(i) for s>1/2 is very small. These results indeed corroborate that the alternating terms in  $S(L,l_A)$  and  $h(l_A)$  are connected. However, due to the fact that the values of D(i) is so small for s>1/2, we were not able to check that the alternate parts of  $S(L,l_A)$  and  $h(l_A)$  decay with the same exponent, as expected by Laflorencie  $et\ al.^{33}$ 

As in the PBC case, we also observed that the curves of the rescaled entanglement entropies  $W(L, l_A, s)$  of chains with  $s \ge 3/2$  and OBC collapse onto a single universal scaling curve, as we can see in Fig. 2(c).

Finally, let us present our estimates of  $c^{PBC}$ ,  $x_{bulk}$ , and  $x_s$  for several values of spins s. In Table III, a summary of our results is provided (acquired following the procedure ex-

plained in Sec. II A). The finite-size estimates of  $c^{\text{PBC}}$  and  $x_{bulk}$  were obtained considering systems of sizes L=80 or L=96 with PBC, while the extrapolated values of  $c^{\text{OBC}}$  and  $x_s$  were obtained considering the model with OBC and sizes up to L=180. We also show in this table the ratios of the dimensions  $x_s/x_{bulk}$ . Based in our benchmark results of the spin-1/2 case, we believe the errors of the quantities presented in Table III are smaller than  $10^{-3}$ .

Note that it is expected that the critical behavior of the Heisenberg chains with half-integer spins belongs to the same class of the Gaussian model.  $^{8,10,42}$  In particular, numerical  $^{8,10,43}$  and analytical  $^{25,28,42}$  techniques show that c=1 for the Heisenberg chains with half-integer spins. Moreover, it is expected that anomalous dimension of the anisotropic Heisenberg chains depends on the anisotropy and on the value of the spin s.  $^{8,10,28,44}$ 

As observed in Table III, our estimates of c are in agreement with the expected value of c=1. Moreover, our results for s=3/2 are in perfect agreement with the ones found by Alcaraz and Moreo. In particular, for  $\gamma=\pi/3$  they found the following extrapolated values: c=1.08,  $x_{bulk}=0.098$ , and  $x_s=0.198$ . Our results are also consistent with the Alcaraz-Moreo's conjecture  $x_s=2x_{bulk}$ . This conjecture was proposed based in the exact-diagonalization calculations of small system sizes. Besides that, Alcaraz and Moreo t=00 reported results only for spins up to t=01. For the antiferromagnetic region t=02. The expectation of t=03. The expectation of t=04. The expectation of t=04 and t=04 are expectation of t=04. The expectation of t=04 and t=04 are expectation of t=04. The expectation of t=04 are expectation of t=04 and t=04. The expectation of t=04 are expectation of t=04 and t=04. The expectation of t=04 are expectation of t=04. The expectation of t=04 are expectation of t=04 and t=04. The expectation of t=04 are expectation of t=04 are expectation of t=04. The expectation of t=04 are expectation of t=04 are expectation of t=04. The expectation of t=04 are expectation of t=04 are expectation of t=04. The expectation of t=04 are expectation of t=04 are expectation of t=04. The expectation of t=04 are expectation of t=04 are expectation of t=04. The expectation of t=04 are expectation of t=04 are expectation of t=04. The expectation of t=04 are expectation of t=04 are expectation of t=04. The expectation of t=04 are expectation of t=04 are expectation of t=04. The expectation of t=04 are expectation of t=04 are expectation of t=04. The expectation of t=04 are expectation of t=04 are expectation of t=04. The expectation of t=04 are expectation of t=04 are expectation of t=04 are expe

TABLE III. Finite-size estimates of the conformal anomaly  $c^{\text{PBC}}$  and the anomalous dimension  $x_{bulk}$  for the anisotropic spin-s Heisenberg chain with PBC and  $\gamma = \pi/3$  obtained with L = 80 - 96. The extrapolated values of the conformal anomaly  $c^{\text{OBC}}$  and the surface exponent  $x_s$  are also presented for the same model/coupling with OBC.

S	$c^{\mathrm{PBC}}$	$c^{\mathrm{OBC}}$	$x_{bulk}$	$x_s$	$x_s/x_{bulk}$
1/2	0.9997	1.004	0.3333	0.6665	1.999
3/2	0.9995	1.002	0.09918	0.1984	2.000
5/2	0.9993	0.999	0.0572	0.1143	1.998
7/2	0.9989	1.002	0.0403	0.0806	2.000
9/2	0.9995	1.001	0.0311	0.0623	2.003

ter estimates) and larger values of spins we show that this conjecture holds.

### III. CONCLUSION

In this paper, we present a simply procedure to obtain accurate estimates of the conformal anomaly c, sound velocity  $v_s$ , anomalous dimension  $x_{bulk}$ , and the surface exponent  $x_s$  using the conformal invariance relations and the density-matrix renormalization-group technique. In order to illustrate the procedure we use to get these quantities, we investigate the anisotropic spin-s Heisenberg chains with periodic/open boundary conditions.

Our results for the model with spin s=1/2 were compared with the exact results. For the spin-1/2 case, we found that the procedure that we used to estimate c,  $v_s$ ,  $x_{bulk}$ , and  $x_s$  gives accurate estimates with errors smaller than  $10^{-3}$ . We also present accurate results for the model with spins s

=3/2, 5/2, 7/2, and 9/2, and we confirm the Alcaraz-Moreo's conjecture  $x_s = 2x_{bulk}$ .

Our numerical results also support that the entanglement entropy of the spin-s Heisenberg chains satisfies the relation  $S(L,l_A,s)-S(L,l_A,s-1)=1/(2s+1)$  for s>3/2 in the thermodynamic limit. We also verified that the alternate terms of  $S(L,l_A)$  and  $h(l_A)$  seem to actually be connected, as suggested by Laflorencie  $et\ al.^{33}$  However, we were unable to verify that both terms decay with the same universal exponent. In this vein, it is interesting to observe the universal oscillatory behavior of the Rényi entropy predicted by Calabrese  $et\ al.$  in Ref. 37. This study is in progress and the results will be present elsewhere.

## ACKNOWLEDGMENT

This Research was supported by the Brazilian agencies FAPEMIG and CNPq.

<sup>&</sup>lt;sup>1</sup>P. Ginsparg, Applied Conformal Field Theory, in Fields, Strings, and Critical Phenomena, Proceedings of the Les Houches Summer School of Theoretical Physics, edited by E. Brezin and J. Zinn-Justin (North-Holland, Amsterdam, 1990); arXiv:hep-th/9108028.

<sup>&</sup>lt;sup>2</sup>J. Cardy, Scaling and Renormalization in Statistical Physics (Cambridge University Press, Cambridge, 1996).

<sup>&</sup>lt;sup>3</sup>P. Di Francesco, P. Mathieu, and D. Senechal, *Conformal Field Theory* (Springer, New York, 1999).

<sup>&</sup>lt;sup>4</sup>H. W. J. Blöte, J. L. Cardy, and M. P. Nightingale, Phys. Rev. Lett. **56**, 742 (1986).

<sup>&</sup>lt;sup>5</sup>I. Affleck, Phys. Rev. Lett. **56**, 746 (1986).

<sup>&</sup>lt;sup>6</sup>J. Cardy, Nucl. Phys. B **270**, 186 (1986).

<sup>&</sup>lt;sup>7</sup>J. Cardy, J. Phys. A **17**, L385 (1984).

<sup>&</sup>lt;sup>8</sup>F. C. Alcaraz, M. N. Barber, and M. T. Batchelor, Ann. Phys. 182, 280 (1988).

<sup>&</sup>lt;sup>9</sup>F. C. Alcaraz, M. N. Barber, M. T. Batchelor, R. J. Baxter, and G. R. W. Quispel, J. Phys. A **20**, 6397 (1987).

<sup>&</sup>lt;sup>10</sup>F. C. Alcaraz and A. Moreo, Phys. Rev. B **46**, 2896 (1992).

<sup>&</sup>lt;sup>11</sup>G. von Gehlen and V. Rittenberg, J. Phys. A **19**, L631 (1986); J. C. Xavier, F. C. Alcaraz, D. Pena Lara, and J. A. Plascak, Phys. Rev. B **57**, 11575 (1998); F. C. Alcaraz and A. L. Malvezzi, J. Phys. A: Math. Gen. **30**, 767 (1997).

<sup>&</sup>lt;sup>12</sup>S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).

<sup>&</sup>lt;sup>13</sup> If appropriate target states are used in the DMRG, it is possible to estimate the sound velocity. See K. A. Hallberg, Phys. Rev. B 52, R9827 (1995), and Ref. 43.

<sup>&</sup>lt;sup>14</sup>P. Calabrese and J. Cardy, J. Stat. Mech.: Theory Exp. (2004), P06002; for a review see J. Phys. A **42**, 504005 (2009).

<sup>&</sup>lt;sup>15</sup>C. Holzhey, F. Larsen, and F. Wilczek, Nucl. Phys. B **424**, 443 (1994).

<sup>&</sup>lt;sup>16</sup>G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. 90, 227902 (2003).

<sup>&</sup>lt;sup>17</sup>I. Affleck and A. W. W. Ludwig, Phys. Rev. Lett. **67**, 161 (1991).

<sup>&</sup>lt;sup>18</sup>C. H. Bennett, H. J. Bernstein, S. Popescu, and B. Schumacher, Phys. Rev. A **53**, 2046 (1996).

<sup>&</sup>lt;sup>19</sup>J. Zhao, I. Peschel, and X. Wang, Phys. Rev. B **73**, 024417 (2006).

<sup>&</sup>lt;sup>20</sup>N. Shibata, A. Tsvelik, and K. Ueda, Phys. Rev. B **56**, 330 (1997); S. Daul and R. M. Noack, *ibid.* **58**, 2635 (1998); J. C. Xavier and E. Miranda, *ibid.* **70**, 075110 (2004); G. Fáth, O. Legeza, P. Lajkó, and F. Iglói, *ibid.* **73**, 214447 (2006); A. L. Malvezzi, T. Paiva, and R. R. dos Santos, *ibid.* **73**, 193407 (2006); S. Ejima, F. Gebhard, and S. Nishimoto, *ibid.* **74**, 245110 (2006).

<sup>&</sup>lt;sup>21</sup> M. Führinger, S. Rachel, R. Thomale, M. Greiter, and P. Schmitteckert, Ann. Phys. 17, 922 (2008).

<sup>&</sup>lt;sup>22</sup>R. N. C. Pfeifer, G. Evenbly, and G. Vidal, Phys. Rev. A 79, 040301(R) (2009).

<sup>&</sup>lt;sup>23</sup>L. Tagliacozzo, T. R. de Oliveira, S. Iblisdir, and J. I. Latorre, Phys. Rev. B **78**, 024410 (2008); G. Evenbly, R. Pfeifer, V. Pico, S. Iblisdir, L. Tagliacozzo, I. McCulloch, and G. Vidal, arXiv:0912.1642 (unpublished).

<sup>&</sup>lt;sup>24</sup> See, for example, E. Dagotto and T. M. Rice, Science **271**, 618 (1996), and references therein.

<sup>&</sup>lt;sup>25</sup> I. Affleck, D. Gepner, H. J. Schulz, and T. Ziman, J. Phys. A 22, 511 (1989).

<sup>&</sup>lt;sup>26</sup>C. J. Hamer, J. Phys. A **18**, L1133 (1985).

<sup>&</sup>lt;sup>27</sup>F. Woynarovich and H.-P. Eckle, J. Phys. A **20**, L97 (1987).

<sup>&</sup>lt;sup>28</sup> A. Luther and I. Peschel, Phys. Rev. B **12**, 3908 (1975).

<sup>&</sup>lt;sup>29</sup> Y. Stroganov, J. Phys. A **34**, L179 (2001); A. V. Razumov and Y. G. Stroganov, *ibid.* **34**, 5335 (2001); M. T. Batchelor, J. de Gier, and B. Nienhuis, *ibid.* **34**, L265 (2001); L. Banchi, F. Colomo, and P. Verrucchi, Phys. Rev. A **80**, 022341 (2009).

<sup>&</sup>lt;sup>30</sup>B. Nienhuis, M. Campostrini, and P. Calabrese, J. Stat. Mech.: Theory Exp. (2009), P02063.

<sup>&</sup>lt;sup>31</sup>V. Alba, M. Fagotti, and P. Calabrese, J. Stat. Mech.: Theory Exp. (2009), P10020.

<sup>&</sup>lt;sup>32</sup>In order to avoid metastable configurations, we start the first part of the DMRG algorithm with large values of m. See J. C. Xavier, Braz. J. Phys. **39**, 596 (2009).

<sup>&</sup>lt;sup>33</sup>N. Laflorencie, E. S. Sørensen, M. S. Chang, and I. Affleck, Phys. Rev. Lett. **96**, 100603 (2006); I. Affleck, N. Laflorencie, and E. S. Sørensen, J. Phys. A: Math. Theor. **42**, 504009 (2009).

<sup>&</sup>lt;sup>34</sup> A. B. Kallin, I. González, M. B. Hastings, and R. G. Melko, Phys. Rev. Lett. **103**, 117203 (2009); Ö. Legeza, J. Sólyom, L. Tincani, and R. M. Noack, *ibid.* **99**, 087203 (2007).

- <sup>35</sup>G. Roux, S. Capponi, P. Lecheminant, and P. Azaria, Eur. Phys. J. B **68**, 293 (2009).
- <sup>36</sup>H.-Q. Zhou, T. Barthel, J. O. Fjærestad, and U. Schollwöck, Phys. Rev. A **74**, 050305(R) (2006).
- <sup>37</sup>P. Calabrese, M. Campostrini, F. Essler, and B. Nienhuis, Phys. Rev. Lett. **104**, 095701 (2010).
- <sup>38</sup> J. Ren, S. Q. Zhu, and X. Hao, J. Phys. B **42**, 015504 (2009).
- <sup>39</sup> A. Läuchli and C. Kollath, J. Stat. Mech.: Theory Exp. (2008), P05018.
- $^{40}$ It is also possible to extract finite-size estimates of  $v_s$  from Eq. (1) considering the system with OBC. For this case it is necessary to consider two systems with different sizes.

- <sup>41</sup>We choose to present the results for small system sizes, since it is expected the oscillations are stronger for small system sizes.
- <sup>42</sup>F. D. M. Haldane, Phys. Rev. Lett. **45**, 1358 (1980); I. Affleck, *ibid.* **56**, 2763 (1986); I. Affleck and F. D. M. Haldane, Phys. Rev. B **36**, 5291 (1987).
- <sup>43</sup> K. Hallberg, X. Q. G. Wang, P. Horsch, and A. Moreo, Phys. Rev. Lett. **76**, 4955 (1996).
- <sup>44</sup>For the ferromagnetic region  $-1 < \Delta \le 0$  Alcaraz and Moreo were able to find an analytical expression for the dimensions of the Gaussian model (see Ref. 10).
- <sup>45</sup>For the ferromagnetic region Alcaraz and Moreo reported results for spins up to s=3.