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Universal behavior of the Shannon and Rényi mutual information of quantum critical chains

F. C. Alcaraz and M. A. Rajabpour
Instituto de Física de São Carlos, Universidade de São Paulo, Caixa Postal 369, 13560-970, São Carlos, SP, Brazil
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We study the Shannon and Rényi mutual information (MI) in the ground state (GS) of different critical quantum spin chains. Despite the apparent basis dependence of these quantities we show the existence of some particular basis (we will call them conformal basis) whose finite-size scaling function is related to the central charge c of the underlying conformal field theory of the model. In particular, we verified that for large index n, the MI of a subsystem of size ℓ in a periodic chain with L sites behaves as $\frac{c}{4}\frac{n}{n-1}\ln[\frac{L}{\pi}\sin(\frac{\pi\ell}{L})]$, when the ground-state wave function is expressed in these special conformal basis. This is in agreement with recent predictions. For generic local basis, we will show that, although in some cases $b_n \ln[\frac{L}{\pi}\sin(\frac{\pi\ell}{L})]$ is a good fit to our numerical data, in general, there is no direct relation between b_n and the central charge of the system. We will support our findings with detailed numerical calculations for the transverse field Ising model, $Q = 3,4$ quantum Potts chain, quantum Ashkin-Teller chain, and the XXZ quantum chain. We will also present some additional results of the Shannon mutual information ($n = 1$), for the parafermionic Z_Q quantum chains with $Q = 5,6,7$, and 8.

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I. INTRODUCTION

Quantum entanglement measures have been frequently used recently to detect quantum phase transition in many-body quantum systems. Measures like von Neumann and Rényi entanglement entropy, concurrence, and quantum discord are among the most frequently used ones, see, for example, Refs. [1,2]. One of the important reasons for the success of these measures in detecting quantum phase transition and ultimately identifying the universality class of quantum critical behavior of the system is the simplicity in their calculation by using numerical techniques such as the power method and the density matrix renormalization group (DMRG) [3]. Since at the critical point one can usually describe the system with a conformal field theory (CFT), it is natural to look for observables that can be related to the important quantities in CFT. This program has been carried out in one dimension with significant detail by relating the von Neumann and Rényi entanglement entropy of a bipartite system to the central charge of the underlying CFT, see for example Ref. [4]. Although these quantities can be calculated relatively easily by numerical calculations they have been out of reach from the experimental point of view. Recently, another measure, the Shannon entropy, which is based on specific measurements in the system [5], has been also introduced in the context of quantum critical chains.

The Shannon entropy of the system $\mathcal{X}$ is defined as

$$Sh(\mathcal{X}) = -\sum_x p_x \ln p_x, \tag{1}$$

where p_x is the probability of finding the system in a configuration x. These probabilities, in the case where $\mathcal{A}$ is a subsystem of a quantum chain with wave function $|\Psi_{\mathcal{A}\cup\mathcal{B}}\rangle = \sum_{n,m} c_{n,m}|\phi^n_{\mathcal{A}}\rangle \otimes |\phi^m_{\mathcal{B}}\rangle$, are given by the marginal probabilities $p_{|\phi^n_{\mathcal{A}}\rangle} = \sum_m |c_{n,m}|^2$ of the subsystem $\mathcal{A}$, where $\{|\phi^n_{\mathcal{A}}\rangle\}$ and $\{|\phi_{\mathcal{B}}\rangle^m\}$ are the vector basis in subspaces $\mathcal{A}$ and $\mathcal{B}$. In our study we will always take the whole system $\mathcal{X} = L$, which also indicates the size of the system then the subsystems $\mathcal{A}$ and $\mathcal{B}$ will be denoted by ℓ and $L-\ell$, respectively. We will call the Shannon entropy of a subsystem of size ℓ as the reduced Shannon entropy $Sh(\ell)$ [6]. Notice that the Shannon entropy is basis dependent in opposite to the von Neumann entanglement entropy that is a basis independent quantity. However, as we will see in this paper, it also contains universal aspects in a specific sense that we will clarify later.

As we will see in the next sections, the reduced Shannon entropy has an extensive part which is nonuniversal. In order to extract this nonuniversal harmless part, it is useful to define the so-called Shannon mutual information. It is defined as

$$I(\ell,L) = Sh(\ell) + Sh(L-\ell) - Sh(L), \tag{2}$$

where as before $Sh(\ell)$ and $Sh(L-\ell)$ are the reduced Shannon entropies of the subsystems and $Sh(L)$ is the Shannon entropy of the whole system. The Shannon mutual information has an information theoretic meaning. It is one of the measures used to quantify the amount of information shared among two subsystems. It tells us how much information one can get about the subsystem $L-\ell$ by doing measurements in the subsystem ℓ and vice versa. This quantity has been calculated numerically for the quantum Ising model in Refs. [7,8] and for many other critical quantum spin chains in Ref. [9]. It is worth mentioning that in Ref. [10], it was proved that the Shannon mutual information of classical systems, like the entanglement entropy, should also follow the area law. Recently, there has been also some developments in calculating the Shannon and Rényi entropy of two-dimensional quantum critical systems [11,12]. Note that by changing $Sh(\ell)$ with the von Neumann entanglement entropy in (2) one can define the von Neumann mutual information, which is a different quantity from the Shannon mutual information $I(\ell,L)$. For recent developments in this direction see Refs. [13,14].

One can also generalize the above definitions to the Rényi entropy as

$$Sh_n(\mathcal{X}) = \frac{1}{1-n}\ln\sum_x p_x^n. \tag{3}$$

The $n \to 1$ limit gives back the Shannon entropy. Similarly, one can also generalize the Shannon mutual information by using the above definition. We consider in this paper the simple

naive definition

$$I_n(\ell, L) = Sh_n(\ell) + Sh_n(L-\ell) - Sh_n(L). \quad (4)$$

Differently from the entanglement entropy the Shannon and Rényi entropies are both basis dependent, however, as we will study in this paper, in some particular basis these entropies show universal behavior at the critical point that can be connected with the underlying CFT governing the long-distance physics at the quantum critical point. It is worth mentioning that these entropies were first studied in the context of Rokhsar-Kilvelson wave functions [15,17] for two-dimensional quantum systems [5,18–20]. Based on the transfer matrix approach, one can map the 1D quantum chain into a 2D classical model. From this classical model, we can define a Rokhsar-Kivelson wave function. It is the wave function of a two-dimensional quantum system expressed on basis with one-to-one correspondence with the configurations of the 2D classical model and whose coefficients are the corresponding Boltzmann weights. It is shown in Ref. [5] that the Shannon entropy of the periodic quantum spin chain is equal to the entanglement entropy of the half of the cylinder in the 2D Rokhsar-Kivelson wave function.

In this paper, we will study the Shannon and Rényi mutual information in different quantum critical spin chains such as Ising model, Q-state Potts model, Askin-Teller model, and the XXZ quantum chain. We will restrict ourselves to the case where the quantum chains are in the pure state formed by their ground state (GS). We will also analyze, in all these critical quantum chains, the importance of the basis used to express the wave functions. We will clarify which are the bases that possibly can have a direct connection to the central charge of the system. In the conclusions we will also present the results for the Shannon mutual information of the Z_Q-parafermionic quantum chains, with $Q = 5,6,7$, and 8.

II. MUTUAL INFORMATION IN QUANTUM SPIN CHAINS

In this section, we study different aspects of the Shannon and Rényi entropies in the transverse field Ising chain, three and four-state Potts model, the Ashkin-Teller model, and the XXZ chain. As it was already discussed in Ref. [22], we should expect a significant difference between the first four cases and the last one. We will start by discussing the known conjectures about different cases and then we will present our numerical results and, based on them, some conjectures. We will largely emphasize in this paper the important role played by the basis used to calculate the different kinds of entropies. In our study, we will always confine ourselves to critical chains.

A. Mutual information in the transverse field Ising spin chain

The Hamiltonian of this model is given by

$$H = -\lambda \sum_{i=1}^{L} \sigma_i^z \sigma_{j+1}^z - \sum_{i=0}^{L} \sigma_i^x, \quad (5)$$

where (σ_i^z, σ_i^x) are spin-1/2 Pauli matrices localized at the sites $i = 1, \ldots, L$. The system is critical at $\lambda = 1$. The Shannon entropy of the periodic system at the critical point was studied numerically in Refs. [5,23]. The numerical results suggested the following form for the Rényi entropy of the GS of the whole chain:

$$Sh_n(L) = \mu_n L + \gamma_n, \quad (6)$$

where μ_n and γ_n are nonuniversal and universal constants, respectively. The numerical results for the universal constant term γ_n for the periodic chain with ground state wave function expressed in the σ^z basis are [23]

$$\gamma_n(\lambda = 1) = \begin{cases} 0, & n < 1 \\ 0.2543925(5), & n = 1 \\ \ln 2, & n > 1 \end{cases}. \quad (7)$$

The discontinuity with respect to n means that the replica trick is probably not suitable to calculate the standard Shannon entropy from the Rényi ones. The very interesting fact is the constant value of γ_n for $n > 1$. This indicates that it can probably be calculated by looking to the asymptotic behavior $n \to \infty$ of Sh_n in the σ^z basis. This observation has very interesting consequences when one considers the reduced Rényi entropy for the transverse field Ising model. Due to the ferromagnetic nature of the quantum chain, the configurations with the highest probability [21] in the Ising model are the ones with all the spins up or spins down, so in principle when one considers the reduced Rényi entropy, the most important configurations are those with all the spins in the subsystem up or down. The corresponding probability $\mathcal{P}$ is usually called emptiness formation probability (EFP) and it has been calculated for conformal field theories in Ref. [22] and references therein. Introducing the logarithmic emptiness formation probability (LEFP) as $\mathcal{E} = -\ln \mathcal{P}$ one can summarize the result for the periodic boundary condition as [22]

$$\mathcal{E}(\ell) = a\ell + \frac{c}{8} \ln \left[\frac{L}{\pi} \sin \left(\frac{\pi \ell}{L} \right) \right] + \ldots, \quad (8)$$

where here and hereafter we denote by "..." the subleading terms. The idea behind this calculation is as follows: the configuration with all spins up, in the σ^x basis, can be seen in the two-dimensional classical Ising model as a free boundary condition. This happens because the classical spins in the transfer matrix approach actually correspond to the eigenstates of the matrix σ^z. Considering a CFT with a free boundary condition on the slit one can extract the above formula for the LEFP in the σ^x basis [22]. The crucial point is that the free boundary conditions in the Euclidean approach is a conformal boundary condition [24] and so one can use CFT techniques. One can follow a similar argument in the σ^z basis: it is not difficult to show that fixing the spins in the σ^z basis is equivalent to fixing the spins in the two-dimensional classical counterpart. This boundary condition is also a conformal boundary condition and by following the arguments in Ref. [22] one can get the same formula as Eq. (8).

Using the LEFP and the fact that the behavior of the Rényi entropy for $n > 1$ is controlled by $n \to \infty$, it was conjectured [22] that the reduced Rényi entropy of the GS should have the following form:

$$Sh_n(\ell) = \frac{n}{n-1} a\ell + \frac{c}{8} \frac{n}{n-1} \ln \left[\frac{L}{\pi} \sin \left(\frac{\pi \ell}{L} \right) \right] + \gamma_n + \ldots, \quad (9)$$

where $c = \frac{1}{2}$ is the central charge of the Ising model. As it was already mentioned one can not get the result for $n = 1$ by analytical continuation of the above result. Based on the numerical results presented in our previous work [9], we conjectured that the result for $n = 1$ is

$$Sh(\ell) = a\ell + \frac{c}{8}\ln\left[\frac{L}{\pi}\sin\left(\frac{\pi\ell}{L}\right)\right] + \gamma_1 + \ldots. \quad (10)$$

Based on the above formulas, one can conjecture the following formula for the Rényi mutual information of spin chains in the above two bases that are related to boundary CFT (from now on we will call them conformal basis) [9]:

$$I_n(\ell, L) = \frac{c_n}{4}\ln\left[\frac{L}{\pi}\sin\left(\frac{\pi\ell}{L}\right)\right] + \ldots, \quad (11)$$

where

$$c_n = c\begin{cases} 1, & n = 1 \\ \frac{n}{n-1}, & n > 1 \end{cases}. \quad (12)$$

The above formula for $n = 1$ has already been checked for many different quantum spin chains in Ref. [9] and the results looked consistent with the coefficient being very close to the central charge. However, recently [25], this result has been questioned in the case of Ising model, where the numerical estimated value is 0.480 instead of the central charge value $c = \frac{1}{2}$. In Fig. 1, we show the results of c_n in the quantum Ising chain in the two different bases σ^z and σ^x. These results were obtained by considering the fitting of (11) considering the subsystem sizes $\ell = 4, \ldots, L/2$. The results confirm the validity of (12) nicely for values of n bigger than $n_c \sim 2$. Taking spin chains with bigger lattice sizes might lead to a better compatibility with the formula (12) in the region $1 < n < 2$, see for example Ref. [25]. Our results also indicate that

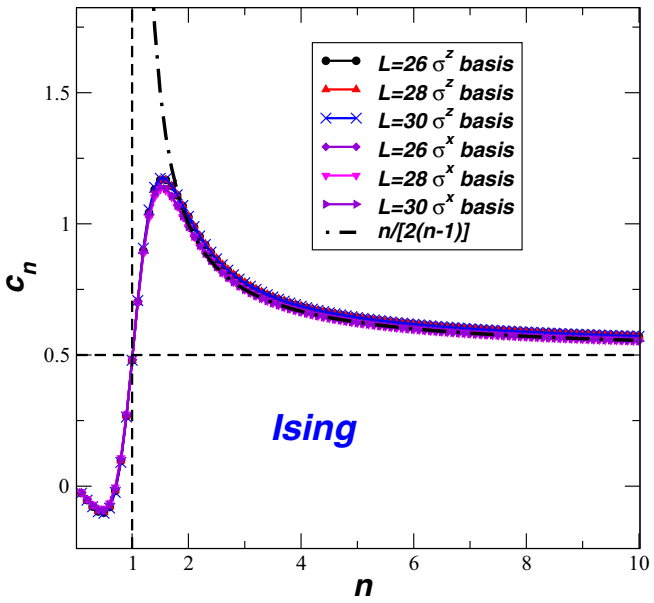

FIG. 1. (Color online) Coefficient of the logarithmic term of the Rényi MI in the Ising model in the σ^z and σ^x bases. The coefficients were found by restricting the fitting of (11) to the subsystem sizes $\ell = 4, 5, \ldots, L/2$. The dashed straight lines are guidelines for $n = 1$ and for the central charge $c = 0.5$.

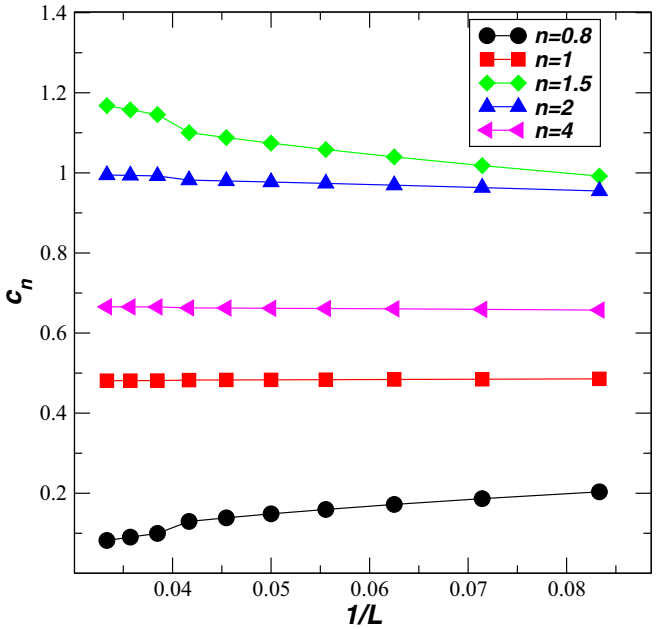

FIG. 2. (Color online) Finite-size data of $c_n(L)$, for $L = 12, 14, \ldots, 30$, for the GS Ising model in σ^x basis. The coefficients were calculated by conditioning the fitting to the subsystem sizes $\ell = 4, 5, \ldots, L/2$.

the formula (11) may also be valid for $0 < n < 1$ with the c_n values shown in Fig. 1 [26].

Let us make an important remark about the numerical results presented in Fig. 1, which will also be valid for all the subsequent numerical results presented in this paper. Although we obtained results for lattice sizes up to $L = 30$, it is difficult to obtain reliable results for c_n with precision smaller than a few percent by using extrapolating techniques. This is due to two reasons. The first one comes from the fact that the finite-size estimator $c_n(L)$, for a given lattice size L, is obtained from a fit of the data to (11), in which the effect of a given sublattice size ℓ is distinct for each lattice size L. In Fig. 2, we show the finite estimators $c_n(L)$, for $L = 12, 14, \ldots, 30$ obtained for the GS expressed in the σ^x basis. The second reason, which is more restrictive, comes from the fact that we do not know the functional dependence on L of the finite-size corrections of (11). These corrections may decay as powers of $\ln L$, which makes the precise evaluation quite difficult using lattice sizes $L \lesssim 100$.

It is interesting to stress at this point that all the above results are presumably correct if we work in the σ^x or σ^z basis, which corresponds to free and fixed conformal boundary conditions in the Euclidean approach. On the other hand, we know that in the Ising model we have just these two conformal boundary conditions [24]. Consequently, if one works with different bases, other than σ^x and σ^z, one might not get the same results as above because the corresponding boundary conditions are not conformal. In order to test this, we consider the general local basis,

$$\begin{bmatrix} |a\rangle \\ |b\rangle \end{bmatrix} = \begin{bmatrix} \cos\theta & \sin\theta e^{-i\alpha} \\ \sin\theta e^{-i\phi} & -\cos\theta e^{-i(\alpha+\phi)} \end{bmatrix}\begin{bmatrix} |\uparrow\rangle \\ |\downarrow\rangle \end{bmatrix}, \quad (13)$$

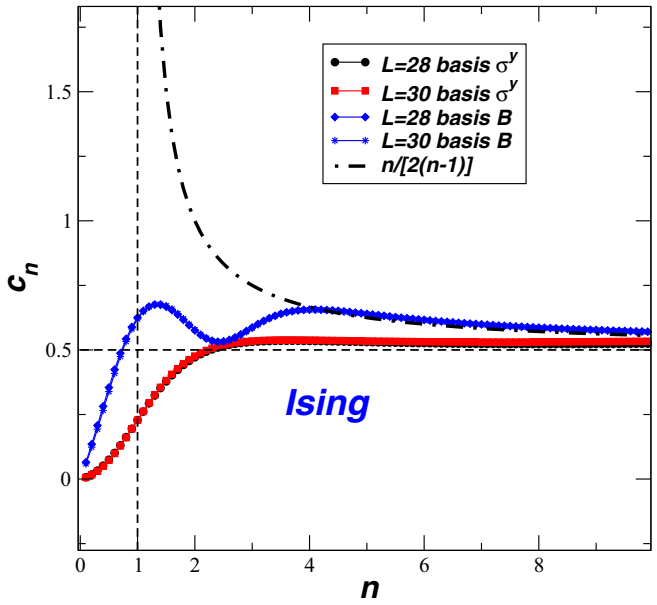

FIG. 3. (Color online) Coefficient of the logarithmic term of the Rényi MI in the Ising model in the σ^y basis $[(\theta,\phi,\alpha)=(\frac{\pi}{4},0,0)]$ and the B basis $[(\theta,\phi,\alpha)=(\frac{\pi}{3},\pi,\frac{\pi}{5})]$. The coefficients were found by conditioning the fitting to the subsystem sizes $\ell=4,5,\ldots,L/2$. The dashed straight lines are guidelines for $n=1$ and for the central charge $c=0.5$.

where $|\uparrow\rangle$ and $|\downarrow\rangle$ are the spin-up and -down components in the σ^z basis. We calculate the Shannon and Rényi entropies in different bases. The numerical results for the σ^y basis ($\theta=\pi/4,\alpha=\pi/2,\phi=0$) and for another arbitrary B basis, where $\theta=\pi/3$, $\alpha=\pi$, and $\phi=\pi/5$ are shown in the Fig. 3. We clearly see in this figure that the finite-size scaling function (11) looks valid even if we chose nonconformal basis, however, the n dependence of the coefficients is quite different from the one obtained in the two conformal bases.

B. Mutual information in the $Q=3$ and 4 state Potts quantum chain

The Q-state Potts model in a periodic lattice is defined by the Hamiltonian [28]

$$H_Q=-\sum_{i=1}^{L}\sum_{k=1}^{Q-1}\left(S_i^k S_{i+1}^{Q-k}+\lambda R_i^k\right), \tag{14}$$

where S_i and R_i are $Q\times Q$ matrices satisfying the following $Z(Q)$ algebra: $[R_i,R_j]=[S_i,S_j]=[S_i,R_j]=0$ for $i\neq j$ and $S_jR_j=e^{i\frac{2\pi}{Q}}R_jS_j$ and $R_i^Q=S_i^Q=1$. The system is critical at the self-dual point $\lambda=1$. The critical behavior is governed by a CFT with central charge $c=1-\frac{6}{m(m+1)}$, where $\sqrt{Q}=2\cos(\frac{\pi}{m+1})$. The $Q=2$ Potts chain is just the Ising model, which we already discussed in the previous section. In this section, we will discuss the mutual information of the GS in the $Q=3$ and 4 Potts chain, which follows a similar behavior as that of the Ising model. We first summarize our results regarding different basis in the $Q=3$ Potts model. In the basis where the S matrix is diagonal, the S and R matrices have the following forms:

$$S=\begin{bmatrix}1&0&0\\0&\omega&0\\0&0&\omega^2\end{bmatrix},\quad R=\begin{bmatrix}0&1&0\\0&0&1\\1&0&0\end{bmatrix}, \tag{15}$$

where $\omega=\exp(2\pi i/3)$. One can simply get the basis in which the R matrix is diagonal by just exchanging the two matrices $S\leftrightarrow R$.

Starting from the S diagonal or from the R diagonal basis $(|0\rangle,|1\rangle,|2\rangle)$, one can introduce another basis $(|\tilde{0}\rangle,|\tilde{1}\rangle,|\tilde{2}\rangle)$, by using the following transformations:

$$\begin{bmatrix}|\tilde{0}\rangle\\|\tilde{1}\rangle\\|\tilde{2}\rangle\end{bmatrix}=A_3\begin{bmatrix}|0\rangle\\|1\rangle\\|2\rangle\end{bmatrix}, \tag{16}$$

where

$$A_3(\theta,\phi)=\begin{bmatrix}\cos\theta&0&\sin\theta\\\sin\phi\sin\theta&\cos\phi&-\sin\phi\cos\theta\\-\sin\theta\cos\phi&\sin\phi&\cos\theta\cos\phi\end{bmatrix} \tag{17}$$

is characterized by the angles θ and ϕ. This is not the most general rotation that depends on the three Euler angles, but is enough for our purposes. Using this matrix, one can express the S and R matrices in a more general basis as

$$\tilde{S}=A_3^{-1}SA_3,\quad \tilde{R}=A_3^{-1}RA_3. \tag{18}$$

Having the full structure of the general basis in the three-state Potts model we calculated the Rényi mutual information in different bases. As one can see in Figs. 4 and 5, the n-behavior of the Rényi mutual information depends on the basis that one chooses. For the two bases, R or S diagonal (see Fig. 4), this

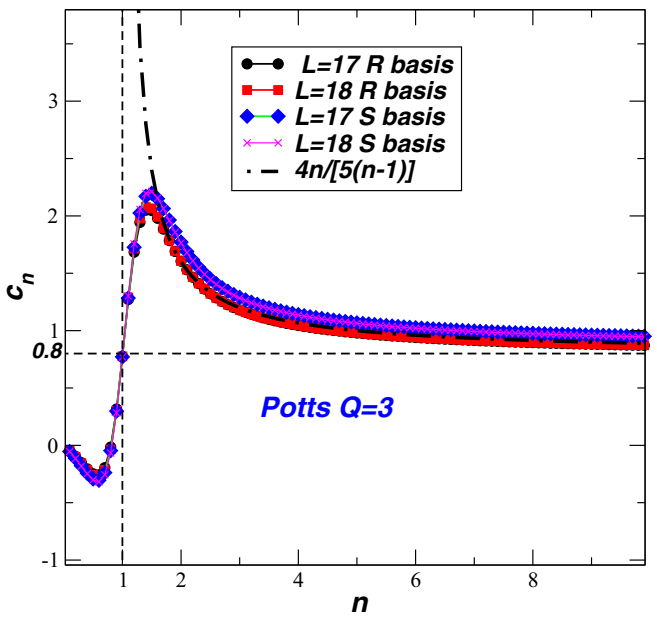

FIG. 4. (Color online) Coefficient of the logarithmic term of the Rényi MI in the $Q=3$ Potts model in the R and S basis [26]. The coefficients were found by restricting the fitting of (11) to the subsystem sizes $\ell=4,5,\ldots,\mathrm{Int}[L/2]$. The dashed straight lines are guidelines for $n=1$ and for the central charge $c=0.8$.

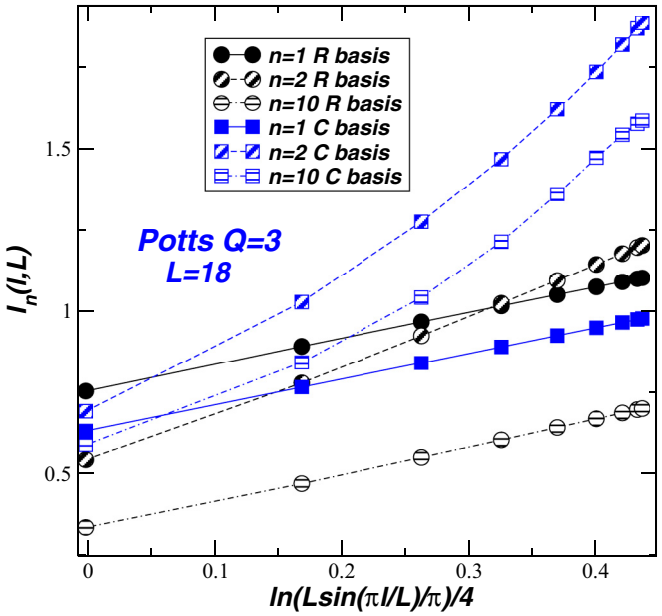

FIG. 5. (Color online) Rényi MI with respect to $\ln[\frac{L}{\pi}\sin(\frac{\pi\ell}{L})]$ in the $Q=3$ Potts model in the R and C basis $(\theta,\phi)=(\frac{\pi}{2},\frac{\pi}{4})$. In the R basis, the data show a good fit for all values of n. In the C basis (except at $n=1$), the fitting is reasonable only if we take just the last five or six points. Notice also that, in the large n limit, the linear coefficient of the fitting that give c_n, are very different in the two basis.

dependence is

$$I_n(\ell,L)=\frac{c_n}{4}\ln\left[\frac{L}{\pi}\sin\left(\frac{\pi\ell}{L}\right)\right]+\ldots, \tag{19}$$

with

$$c_n=c\begin{cases}1, & n=1\\ \frac{n}{n-1}, & n>1.5\end{cases}, \tag{20}$$

where $c=\frac{4}{5}$ is the central charge of the model. Based on our numerical calculation it is hard to conclude the existence or not of a discontinuity at $n=1$, however, if this is the case for the Ising model, it is likely to be true also in this model because they follow very similar behavior. Another important point is that although our results for $n=1$ are consistent with the $c_1=c$, it is very hard to exclude the possibility of this number being very close to the central charge and not the central charge itself, as claimed in Ref. [25] for the Ising model. Note that (19) is consistent with the picture that S and R bases lead to fixed and free boundary conditions, respectively, and so can be connected to the boundary CFT as we argued in the case of the Ising model.

As one can see in Fig. 5, the other basis [C basis means that starting from the S basis we choose $A_3(\frac{\pi}{2},\frac{\pi}{4})$ in (16)] does not follow a similar structure. Even if we try to fit the data to $\ln[\frac{L}{\pi}\sin(\frac{\pi\ell}{L})]$ by taking just the last four or five points, it is clear that the trend for large n is not compatible with $c_n=c\frac{n}{n-1}$. It is intriguing that even in this basis the results for $n=1$ are quite compatible with the results coming from the conformal basis. Although we checked few nontrivial basis and not found any other conformal basis, our study does not necessarily exclude some other possible complicated conformal bases. This is just simply because the boundary conformal field theory of the three-state Potts model is much richer than just the two cases (free and fixed) that we studied. Finding other possible conformal bases can be very interesting.

We now study the $Q=4$ Potts model, which has a very similar structure as the $Q=3$ Potts model. In the basis where the S matrix is diagonal, the S and R matrices are given by

$$S=\begin{bmatrix}1&0&0&0\\0&\omega&0&0\\0&0&\omega^2&0\\0&0&0&\omega^3\end{bmatrix},\quad R=\begin{bmatrix}0&1&0&0\\0&0&1&0\\0&0&0&1\\1&0&0&0\end{bmatrix}, \tag{21}$$

where $\omega=\exp(2\pi i/4)$. Like in the $Q=3$ case, one can get a basis that makes the R matrix diagonal by just exchanging the two matrices $S\leftrightarrow R$. The most general basis has a complicated form. Here, we work with a subset of the possible nontrivial basis, which are obtained by just using the transformation matrix A_3 of the $Q=3$ Potts chain. Starting with the basis $(|0\rangle,|1\rangle,|2\rangle,|3\rangle)$ where R or S is diagonal, we obtain the basis $(|\tilde{0}\rangle,|\tilde{1}\rangle,|\tilde{2}\rangle,|\tilde{3}\rangle)$:

$$\begin{bmatrix}|\tilde{0}\rangle\\|\tilde{1}\rangle\\|\tilde{2}\rangle\\|\tilde{3}\rangle\end{bmatrix}=\begin{bmatrix}\cos\theta&0&\sin\theta&0\\\sin\theta\sin\phi&\cos\phi&-\sin\phi\cos\theta&0\\-\sin\theta\cos\phi&\sin\phi&\cos\phi\cos\theta&0\\0&0&0&1\end{bmatrix}\begin{bmatrix}|0\rangle\\|1\rangle\\|2\rangle\\|3\rangle\end{bmatrix}. \tag{22}$$

We have calculated the Rényi mutual information in different basis. The structure is perfectly compatible with the results for the Ising and $Q=3$ Potts model. The Rényi mutual information, in the S and R bases, are shown in Fig. 6. They

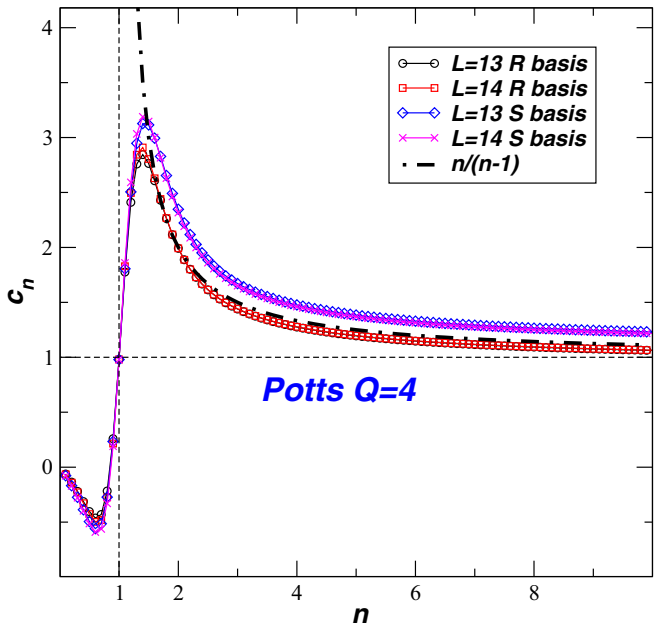

FIG. 6. (Color online) Coefficient of the logarithmic term of the Rényi MI in the $Q=4$ Potts model in the R and S bases [26]. The coefficients were found by conditioning the fitting to the subsystem sizes $\ell=4,5,\ldots,\mathrm{Int}[L/2]$. The dashed straight lines are guidelines for $n=1$ and for the central charge $c=1$.

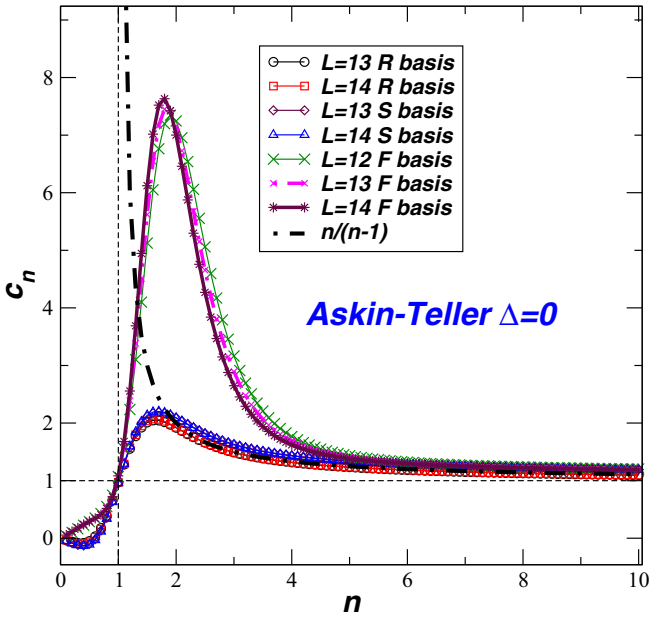

FIG. 7. (Color online) Coefficient of the logarithmic term of the Rényi MI in the Ashkin-Teller model with $\Delta = 0$ in the conformal R and S basis and in the F basis specified by the angles $(\theta,\phi) = (\frac{\pi}{4},\frac{\pi}{4})$ in (22). The coefficients [26] were found by conditioning the fitting to the subsystem sizes $\ell = 4,5,\ldots,\mathrm{Int}[L/2]$. The dashed straight lines are guidelines for $n = 1$ and for the central charge $c = 1$.

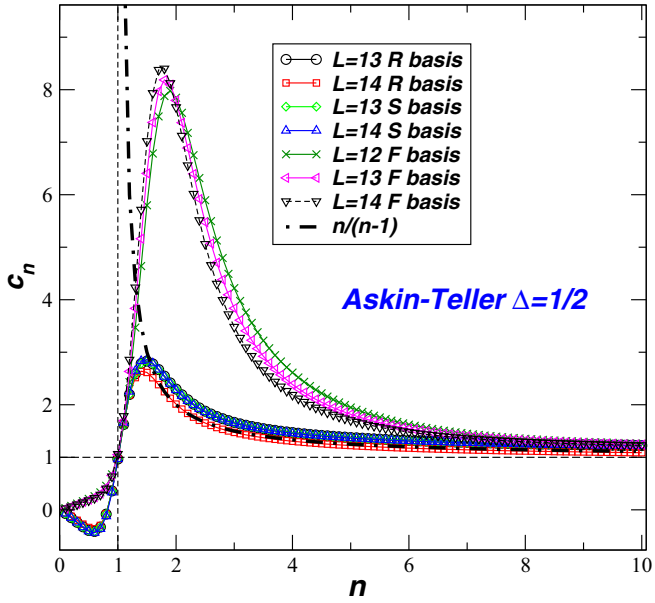

FIG. 8. (Color online) Coefficient of the logarithmic term of the Rényi MI in the Ashkin-Teller model with $\Delta = \frac{1}{2}$ in the conformal R and S bases and in the F basis specified by the angles $(\theta,\phi) = (\frac{\pi}{4},\frac{\pi}{4})$ in (22). The coefficients [26] were found by restricting the fitting to the subsystem sizes $\ell = 4,5,\ldots,\mathrm{Int}[L/2]$. The dashed straight lines are guidelines for $n = 1$ and for the central charge $c = 1$.

follow the Eqs. (19) and (20) with $c = 1$. The difference we see from the results of the two bases is probably due to the finite-size corrections since the largest lattice we considered is $L = 14$ for the $Q = 4$ Potts chain. In the other basis, we found a similar structure as we found in the case of the $Q = 3$ Potts model (see Fig. 5), indicating that even assuming the $c_n \ln[\frac{L}{\pi}\sin(\ell\pi/L)]$ behavior the coefficient c_n for n large is not given by (20). Here, we summarize the results for the Q-state Potts chain. (1) The mutual Rényi entropy follows the formulas (19) and (20) in the S and R bases. (2) In the region $1 < n < 1.5$, the c_n coefficient has a maximum. Our numerical calculation is consistent but nonconclusive with the possible presence of discontinuity at $n = 1$. (3) For arbitrary basis, the large n behavior of c_n is not given by (19).

C. Mutual information in the Ashkin-Teller quantum spin chain

The next model that we study is the Ashkin-Teller model which has a $Z(2)\otimes Z(2)$ symmetry and whose Hamiltonian is given by

$$H = -\sum_{i=1}^{L}\left[\left(S_i S_{i+1}^3 + S_i^3 S_{i+1} + \Delta S_i^2 S_{i+1}^2\right) + \left(R_i + R_i^3 + \Delta R_i^2\right)\right], \tag{23}$$

where S and R are the same matrices introduced in the $Q = 4$ Potts model. The model is critical and conformal invariant for $-1 < \Delta \leqslant 1$ with the central charge $c = 1$. It is worth mentioning that at $\Delta = 1$ we recover the $Q = 4$ Potts model and at $\Delta = 0$ the model is equivalent to two decoupled Ising models. We calculated the Rényi mutual information of the GS in different bases for $\Delta = 0$ and $\Delta = \frac{1}{2}$. The results are shown in Figs. 7 and 8. One can summarize the results as follows. (1) The mutual Shannon entropy follows the formula

$$I_n(\ell, L-\ell) = \frac{c}{4}\ln\left[\frac{L}{\pi}\sin\left(\frac{\pi\ell}{L}\right)\right] i + \cdots, \quad c = 1, \tag{24}$$

independent of Δ in the two conformal bases where S and R are diagonal.

(2) The mutual Rényi entropy is in general Δ dependent for $1 < n < 2$ even in the conformal basis (basis where S or R are diagonal), however, it follows the finite-size scaling function

$$I_n(\ell, L-\ell) = \frac{n}{4(n-1)}\ln\left[\frac{L}{\pi}\sin\left(\frac{\pi\ell}{L}\right)\right] \tag{25}$$

for $n > 2$, independent of the Δ, in the two bases where S or R are diagonal. Presumably, as we had in the $Q = 2$ and 3 cases, these two bases are also related to the fixed and free conformal boundary conditions. If we accept the picture that we had in the quantum Potts case, one might argue that the difference in the two cases $\Delta = 0$ and $\frac{1}{2}$ in the region $1 < n < 2$ is just a finite-size effect and, in the limit of large system sizes, the results are independent of Δ in the two conformal basis.

(3) For the nontrivial basis like the F basis, obtained by using in (22) $(\theta,\phi) = (\frac{\pi}{4},\frac{\pi}{4})$, we found that the logarithmic fit is reasonable for both values of $\Delta = 0, \frac{1}{2}$. However, the coefficients c_n could be very different from the conformal basis. See Figs. 7 and 8. Due to the large and uncontrolled finite-size corrections, it is difficult to predict a convergence towards the asymptotic behavior $n/(n-1)$.

D. Mutual information in the XXZ quantum spin chain

The Hamiltonian of the XXZ chain is defined as

$$H_{\rm XXZ} = -\sum_{i=1}^{L} \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z\right), \quad (26)$$

where σ^x, σ^y, and σ^z are spin-$\frac{1}{2}$ Pauli matrices and Δ is an anisotropy. The model is critical and conformal invariant for $-1 \leqslant \Delta < 1$. The long-distance critical fluctuations are ruled by a CFT with central charge $c = 1$ described by a compactified boson whose action is given by

$$S = \frac{1}{8\pi} \int d^2x (\nabla\phi)^2, \quad \phi \equiv \phi + 2\pi R, \quad (27)$$

where the compactification radius depends upon the values of Δ, namely,

$$R = \sqrt{\frac{2}{\pi} \arccos \Delta}. \quad (28)$$

The Shannon entropy of the system in the σ^z basis was already studied in many papers [5,19,20]. The analytical and numerical results, for the periodic case, indicate that

$$Sh(L) = \mu L + \ln R - \tfrac{1}{2}, \quad (29)$$

where R is given by (28). The extension of these results to the Rényi entropies is [5,20,27]

$$Sh_n(L) = \mu_n L + \begin{cases} \ln R - \frac{\ln n}{2(n-1)}, & n < n_c, \\ \frac{1}{n-1}(n \ln R - \ln d), & n \geqslant n_c, \end{cases}$$

where $n_c = \frac{d^2}{R^2}$ and the parameter d can be understood as the degeneracy of the configuration with the highest probability in the ground state. Since in this paper we will always fix the total magnetization in the σ^z basis to zero, we will always have $d = 2$.

In this section, we extend the above results to the reduced Shannon and the reduced Rényi entropies of the quantum chains on their GS. An important point to notice is that the techniques used in the previous section for the Ising model are not necessarily applicable in the present case because the configuration with the highest probability in the σ^z basis has antiferromagnetic nature (for $\Delta \leqslant 0$) rather than a simple ferromagnetic one [21]. The interesting point is that these kinds of spin alternating configurations are supposed to be renormalized to Dirichlet boundary conditions in the Luttinger liquid representation of the XXZ model [29] and one can hope that they might be connected to the underlying CFT [22,25] ruling the long-distance physics of the quantum chain. We conjecture, see also Ref. [25], that the reduced Rényi entropy for the subsystem size ℓ, in the σ^z basis, is given by

$$Sh_n(\ell) = b_n \ell + \frac{c_n}{8} \ln\left[\frac{L}{\pi} \sin\left(\frac{\pi \ell}{L}\right)\right] + \ldots, \quad (30)$$

which consequently leads to the following result for the mutual information:

$$I_n(\ell, L) = \frac{c_n}{4} \ln\left[\frac{L}{\pi} \sin\left(\frac{\pi \ell}{L}\right)\right] + \ldots, \quad (31)$$

where c_n is shown in Fig. 9. The coefficient of the logarithm in this case is dependent on n and Δ. In an interesting development, in Ref. [25], it was conjectured that the form of the c_n follows

$$c_n = \begin{cases} 1, & n < n_c \\ \frac{n}{n-1}, & n > n_c \end{cases}.$$

Based on Ref. [25], at $n = n_c$, the result has a discontinuity. The presence of the discontinuity at $n = n_c$ is attributed to the least irrelevant operator $V_d = \cos(\frac{d}{R}\phi)$. As far as $n < n_c$, it was argued in Ref. [25] that this operator is irrelevant and one can get $c_n = 1$ by simple Luttinger model arguments. However, when $n > n_c$, this operator is relevant and consequently the field gets locked into one of the minima of the potential $V_d = \cos(\frac{d}{R}\phi)$. This simply leads again to the $\frac{n}{n-1}$ behavior as we had in the Ising model case. Although our numerical results do not show any discontinuity, they are consistent with the general arguments in Ref. [25]. In Fig. 9, one can see the results of c_n for different values of Δ. Interestingly, all of them follow the behavior $\frac{n}{n-1}$ after a value of n close to $n_c = \frac{4}{R^2}$.

One can also do the same kind of analysis in the other two special basis where σ^x or σ^y are diagonal. Because of the symmetry one expect the same results for these two cases, and since the basis with fixed σ^x is connected to the Dirichlet boundary condition of the dual field in the Luttinger model representation [29], one can simply consider it as the Neumann boundary condition of the Luttinger field. This boundary condition is also a conformal boundary condition and consequently one might hope to be able to find the finite-size scaling behavior $\frac{c_n}{4} \ln[\frac{L}{\pi} \sin(\frac{\pi \ell}{L})]$ in the mutual information calculations. Interestingly, one can make the same kind of argument used in the σ^z basis and say that the field $V_d =$

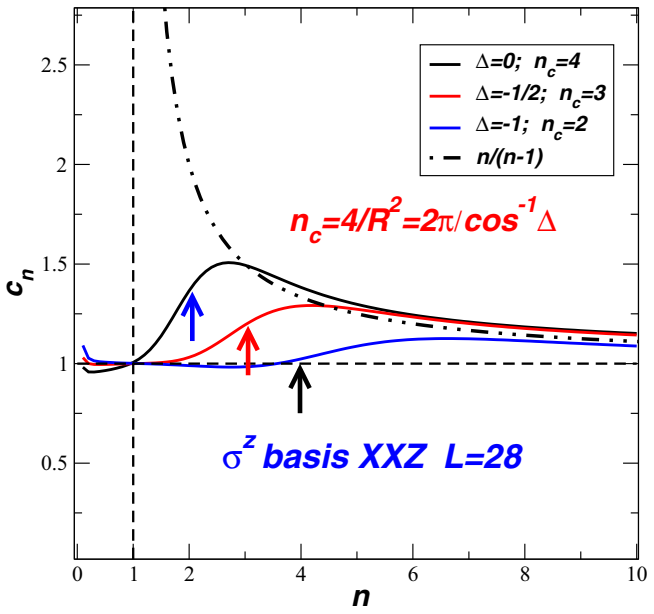

FIG. 9. (Color online) Coefficient of the logarithmic term of the Rényi MI in the XXZ model with $L = 28$ sites and with different anisotropy parameter Δ in the σ^z basis. The coefficients [26] were estimated by the average of the fittings obtained by restricting the subsystem sizes to $\ell = 4,5,\ldots,14$ and to $\ell = 5,6,\ldots,14$. The arrows indicate the predicted critical value n_c, where the asymptotic behavior begins. The dashed straight lines are guidelines for $n = 1$ and for the central charge $c = 1$.

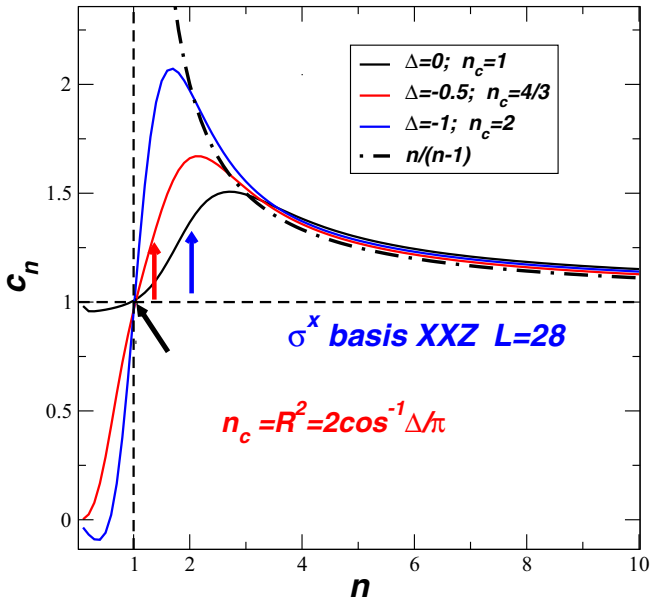

FIG. 10. (Color online) Coefficient of the logarithmic term of the Rényi MI in the XXZ with $L = 28$ sites and with different anisotropy parameter Δ in the σ^x basis. The coefficients [26] were estimated by the average of the fittings obtained by restricting the subsystem sizes to $\ell = 4,5,\ldots,14$ and to $\ell = 5,6,\ldots,14$. The coefficients were found by restricting the fitting to the subsystem sizes $\ell = 4,5,\ldots,L/2$. The arrows indicate the predicted critical value n_c, where the asymptotic behavior begins. The dashed straight lines are guidelines for $n = 1$ and for the central charge $c = 1$.

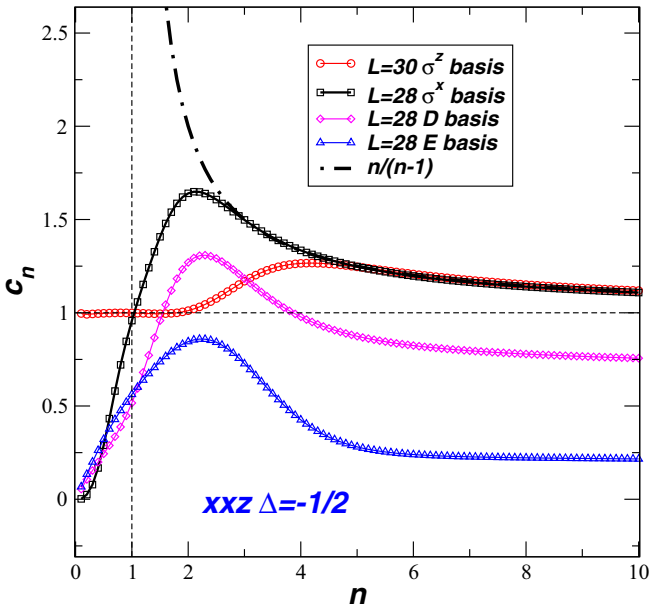

FIG. 11. (Color online) Coefficient of the logarithmic term of the Rényi MI in the XXZ model with $\Delta = -\frac{1}{2}$ in the σ^z, σ^x, D and E basis. The nonconformal bases D and E are obtained by setting in (13) $(\theta,\pi,\alpha) = (\frac{\pi}{3},\pi,\frac{\pi}{5})$ and $(\theta,\pi,\alpha) = (\frac{\pi}{2.3},\frac{\pi}{4.5},\frac{\pi}{8.2})$, respectively. The coefficients were found by conditioning the fitting to the subsystem sizes $\ell = 5,6,\ldots,L/2$. The dashed straight lines are guidelines for $n = 1$ and for the central charge $c = 1$.

$\cos(dR\tilde{\phi})$, with $\tilde{\phi} \equiv \tilde{\phi} + \frac{2\pi}{R}$ as the dual field, will be relevant at some value of $n_c = R^2$ and, consequently, one would expect the logarithmic behavior with coefficient $\frac{n}{n-1}$ for $n > n_c$. A very simple check for this guess comes from analyzing the point $\Delta = -1$, which is a point where all the bases should give the same result because of the U(1) symmetry. Indeed, one can simply see that this point has $R = \sqrt{2}$ and so both formulas for the critical n give the same answer.

The numerical results we obtained are consistent with the above argument. The prefactor c_n for different Δ's are shown in Fig. 10. It is important to stress here that the results for $n = 1$, apart from small deviations that we believe will disappear in the $L \to \infty$, are independent of Δ and equal to the result calculated in the σ^z basis. However, the results for $n \neq 1$ are in general different for distinct values of Δ, except when $n > n_c = R^2$, where we found the same behavior as we found in the Ising model (or also in the $Q = 3$ and 4 Potts models). In other words, the prefactor of the Rényi mutual information of XXZ model in the σ^x basis follows the following formula:

$$c_n = \begin{cases} 1, & n = 1 \\ \frac{n}{n-1}, & n > R^2 \end{cases}. \tag{32}$$

Our numerical calculations are not conclusive regarding the presence or absence of a discontinuity in the c_n at $n_c = R^2$. Further numerical calculations with much bigger sizes are needed to make a conclusive argument in this respect. In addition, based on our numerical results, it is not clear that in the regime $1 < n < R^2$, the prefactor is constant or not. Another intriguing point is that apart from $\Delta = -1$ case, in all the other cases, the mutual Rényi entropy for $n \to 0$ goes to zero. This behavior is different from what we had in the σ^z basis.

Finally, we should stress here that by considering some other basis, i.e., a nonconformal basis, will lead again to the finite-size scaling function $\frac{c_n}{4}\ln[\frac{L}{\pi}\sin(\frac{\pi\ell}{L})]$ for the mutual information. This is shown for some basis in Fig. 11. In this figure we choose in (13) the two nontrivial basis D and E, where $(\theta,\pi,\alpha) = (\frac{\pi}{3},\pi,\frac{\pi}{3})$ and $(\theta,\pi,\alpha) = (\frac{\pi}{2.3},\frac{\pi}{4.5},\frac{\pi}{8.2})$, respectively. However, as we might expect from the results of the previous sections, the pre factors are not even close to the central charge of the system, differently, as happens in the conformal basis where σ^z or σ^x are diagonal.

III. CONCLUSIONS

In this paper, we have studied different aspects of the mutual Shannon and mutual Rényi information of a bipartite system in different quantum critical spin chains such as the Ising model, Q-state Potts model, the Ashkin-Teller model, and the XXZ quantum chain. We showed that although the MI is in general basis dependent, there are some special bases, connected with the conformal boundary conditions of the underlying CFT, that are related to the central charge. We showed that the general behavior is the same for the four models: Ising model, $Q = 3$ and 4 Potts models, and Ashkin-Teller model. In all these four models, the MI calculations, in the conformal basis, show the behavior $c\frac{n}{4(n-1)}\ln[\frac{L}{\pi}\sin(\pi\ell/L)]$ for $n > 2$ with a possible extension of this regime also to $1 < n < 2$. At $n = 1$, we always get something very close to $\frac{c}{4}$ as the coefficient of

the logarithmic term. For nonconformal basis, the results for the coefficient of the logarithm are completely different and can not be simply related to the central charge of the system. In the case of the Ashkin-Teller model, we showed that in the conformal basis the results are independent of the anisotropy parameter. We also studied the same quantities in the XXZ model and showed that in the two conformal bases, where σ^x or σ^z are diagonal, the results are different. In general, one expects a special value of $n = n_c$ where beyond this value ($n > n_c$) the finite-size scaling behavior is $c\frac{n}{4(n-1)}\ln[\frac{L}{\pi}\sin(\ell\pi/L)]$. In more general basis, although one can fit the results with a logarithmic function, the coefficients do not follow the results obtained in the conformal basis.

Before closing this paper, let us consider again the possible relationship of the Shannon mutual information $I_1(\ell, L)$ with the central charge c of the critical chains. In Ref. [9], suggested by the analytical studies of coupled harmonic oscillators and by the numerical results of the quantum critical chains presented in earlier sections, and also for the spin-1 Fateev-Zamolodchikov quantum chain, we conjectured that the Shannon mutual information, like the von Neumann entanglement entropy, is exactly related to the central charge of the critical chain: $I_1(\ell, L) = \frac{c_1}{4}\ln[\frac{L}{\pi}\sin(\ell\pi/L)] + \gamma_n$, where $c_1 = c$. The numerical results obtained for all these models, in relative small system sizes, deviate from the predicted results, just a few percent. In Ref. [25], a numerical calculation for the quantum Ising model in σ^z basis, based on lattice sizes up to $L = 56$ indicates that the constant c_1 may not be exactly given by the central charge but by a close number (0.480 instead 0.5). If this disagreement is an effect or not of the unknown finite-size corrections is something that only further numerical results with larger lattices can decide. This makes the problem

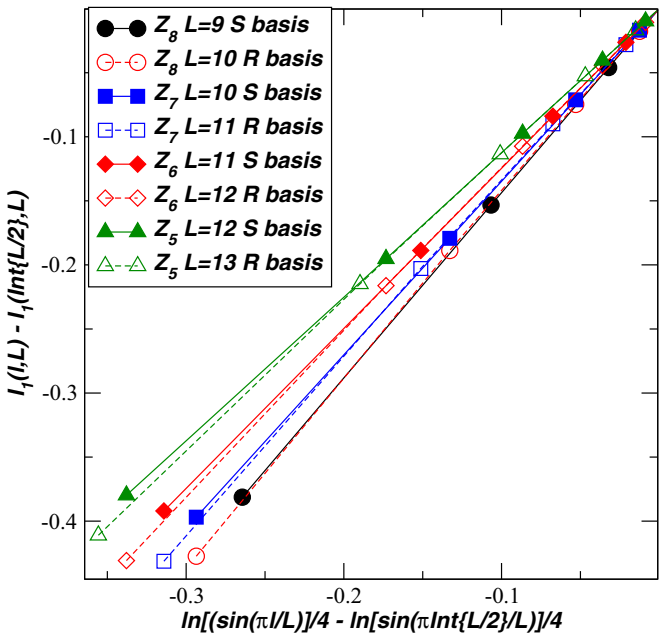

FIG. 12. (Color online) The Shannon mutual information $I_1(\ell, L)$ for the Z_5, Z_6, Z_7, and Z_8 parafermionic quantum chains with Hamiltonian given in (33). The results were obtained for lattice sizes L and in the basis where S or R is diagonal.

TABLE I. Numerical estimates for the constant c_1 for the Z_Q-parafermionic quantum chain given in (33). The results were obtained using all the subsystem sizes, with the ground-state wave function expressed either in S or R basis. The lattice sizes used as well the central charge $c = 2(Q-1)/(Q+2)$ are also shown.

Z_Q	Basis (L)	c_1	$c = 2(Q-1)/(Q+2)$
Z_5	S(12)	1.124	$\frac{8}{7} = 1.1427\cdots$
	R(13)	1.153	
Z_6	S(11)	1.250	$\frac{5}{4} = 1.25$
	R(12)	1.273	
Z_7	S(10)	1.352	$\frac{4}{3} = 1.3333\cdots$
	R(11)	1.372	
Z_8	S(9)	1.443	$\frac{7}{5} = 1.4$
	R(10)	1.456	

even more interesting, and gives rise to a natural question: if it is not the central charge, what should be this number that is quite close to the central charge for quite distinct critical quantum chains? In order to further illustrate this problem to other quantum chains, we also considered the parafermionic Z_Q-quantum spin chain [30], with a Hamiltonian given by [31,32]

$$H = -\sum_{i=1}^{L}\sum_{k=1}^{Q-1}\left(S_i^k S_{i+1}^{Q-k} + R_i^k\right)/\sin(\pi k/Q), \qquad (33)$$

where S_i and R_i are the $Q \times Q$ matrices that appeared in (14). This model is critical and conformal invariant with a central charge $c = 2(Q-1)/(Q+2)$. For the case where $Q = 2$ and 3, we recover the Ising and three-state Potts model, and for the case where $Q = 4$, we obtain the Ashkin-Teller model with the anisotropy value $\Delta = \frac{\sqrt{2}}{2}$.

In Fig. 12 and Table I, we plot the results obtained for the Z_5, Z_6, Z_7, and Z_8 spin models. We clearly see in Fig. 12 that in the basis where either S or R are diagonal, except for the first point (subsystem size $\ell = 2$), the finite-size scaling function is quite well represented by the function $\ln[\sin(\ell\pi/L)]$. In Table I, we show the results obtained for c_1 by considering in the numerical calculations the subsystem sizes ($\ell = 2, \ldots, \mathrm{Int}[\frac{L}{2}]$). These results show, like happened in the other models, an estimate of c_1, for both bases, that deviates a few percent from the central charge. It is remarkable that, although the lattice sizes are quite small, we were able to get values quite close to the predicted central charge. We hope that subsequent numerical and analytical studies of the Shannon mutual information, which certainly will come, will shed light to this interesting problem. Finally, we should emphasize that all the presented results are valid just for critical chains. In the gapped phases, we expect different behaviors.

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