Generalized mutual information of quantum critical chains

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We study the generalized mutual information $\tilde{I}_n$ of the ground state of different critical quantum chains. The generalized mutual information definition that we use is based on the well established concept of the Rényi divergence. We calculate this quantity numerically for several distinct quantum chains having either discrete $Z(Q)$ symmetries (Q-state Potts model with $Q = 2,3,4$ and $Z(Q)$ parafermionic models with $Q = 5,6,7,8$ and also Ashkin-Teller model with different anisotropies) or the $U(1)$ continuous symmetries (Klein-Gordon field theory, XXZ and spin-1 Fateev-Zamolodchikov quantum chains with different anisotropies). For the spin chains these calculations were done by expressing the ground-state wave functions in two special bases. Our results indicate some general behavior for particular ranges of values of the parameter n that defines $\tilde{I}_n$. For a system, with total size L and subsystem sizes ℓ and $L - \ell$, the $\tilde{I}_n$ has a logarithmic leading behavior given by $\frac{\tilde{c}_n}{4} \log[\frac{L}{\pi} \sin(\frac{\pi \ell}{L})]$ where the coefficient $\tilde{c}_n$ is linearly dependent on the central charge c of the underlying conformal field theory describing the system's critical properties.

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I. INTRODUCTION

The entanglement entropy, as a tool to detect and classify quantum phase transitions, has been playing an important role in the last fifteen years (see Ref. [1] and references therein). In one dimension, where most of the critical quantum chains are conformal invariant, the entanglement entropy provides a powerful tool to detect, as well to calculate, the central charge c of the underlying conformal field theory (CFT). For example, for quantum chains, the ground-state entanglement entropy of a subsystem formed by contiguous ℓ sites of an infinite system, with respect to the complementary subsystem, has the leading behavior $S = \frac{c}{3} \ln \ell$ if the system is critical or $S = \frac{c}{3} \log \xi$, when the system is noncritical with correlation length ξ [2]. Although there are plenty of proposals to measure this quantity in the laboratory [3–5] the actual experiments were out of reach so far. Strictly speaking, the central charge of quantum spin chains has never been measured experimentally. Recently other quantities, which are also dependent of the central charge, have been proposed [6,7]. Among these proposals interesting measures that, from the numerical point of view, are also efficient in detecting the phase transitions as well as the universality class of critical behavior are the Shannon and Rényi mutual informations [8–11] (see also the related works [12–18]). The Rényi mutual information (the exact definition will be given in the next section) has a parameter n that recovers the Shannon mutual information at the value $n = 1$. The results derived in Refs. [8–11] indicate that the Shannon and Rényi mutual information of the ground state of quantum spin chains, when expressed in some special local bases, similarly as happens with the Shannon and Rényi entanglement entropy, show a logarithmic behavior with the subsystem's size whose coefficient depends on the central charge.

Recently additional new results concerning the Shannon and Rényi mutual information in quantum systems were obtained, see Refs. [19–23]. There are also studies of the mutual information in classical two-dimensional spin systems [18,24–28]. It is worth mentioning that the Shannon and Rényi mutual information studied in the above papers, as will be defined in the next section, are basis-dependent quantities. It is important to distinguish them from the more known basis-independent quantity, namely, the von Neumann mutual information. For recent developments on the calculation of the von Neumann mutual information in thermal equilibrium and nonequilibrium systems, see Refs. [29,30].

Most of the results regarding the Shannon and the Rényi mutual information, except for the case of harmonic chains, are based on numerical analysis, especially for systems with central charge not equal to one. One of the main problems in a possible analytical derivation comes from the presence of a discontinuity at $n = 1$ of the Rényi mutual information. This discontinuity prevents the use of the replica trick, which is normally a necessary step for the analytical derivation of the Shannon mutual information.

In this paper we will consider, for many different quantum chains, another version of the mutual information, which is also parametrized by a parameter n that reduces at $n = 1$ to the Shannon mutual information. The motivation for our calculations is twofold. First, this definition is more appropriate from the point of view of a measure of shared information among parts of a system, since it has the expected properties. This will be discussed in the Appendix.

Second, this quantity does not show any discontinuity at $n = 1$, so it might be a good starting point for the analytical calculation of the Shannon mutual information with some sort of analytical continuation of the parameter n. From now on we will call this new quantity generalized mutual information.

Having the above motivations in mind we first calculated numerically (using exact diagonalization) the generalized mutual information for several critical quantum spin chains. We considered models with $Z(Q)$ symmetries, such as the Q-state Potts models for $Q = 2,3$ and 4, the $Z(4)$ Ashkin-Teller model and the $Z(Q)$ parafermionic models with $Q = 5$–8. We then calculated the generalized mutual information for quantum critical harmonic chains (discrete version of Klein-Gordon field theory) and also for quantum spin chains with $U(1)$ symmetry, such as the XXZ and the spin-1 Fateev-Zamolodchikov quantum chains.

The structure of the paper is as follows: in the next section we will present the essential definitions of the Shannon and Rényi mutual information as well as generalized mutual information. In Sec. III we will present the numerical results of the generalized mutual information for many different critical quantum spin chains. Finally in the last section we present our conclusions.

II. GENERALIZED MUTUAL INFORMATION: DEFINITIONS

Consider the normalized ground-state eigenfunction of a quantum spin chain Hamiltonian $|\psi_G\rangle = \sum_I a_I |I\rangle$, expressed in a particular local basis $|I\rangle = |i_1, i_2, \ldots\rangle$, where $i_1, i_2, \ldots$ are the eigenvalues of some local operators defined on the lattice sites. The Rényi entropy is defined as

$$Sh_n(\mathcal{X}) = \frac{1}{1-n} \ln \sum_I p_I^n, \tag{1}$$

where $p_I = |a_I|^2$ is the probability of finding the system in the particular configuration given by $|I\rangle$. The limit $n \to 1$ gives us the Shannon entropy $Sh = -\sum_I p_I \ln p_I$. Since we are considering only local bases it is always possible to decompose the configurations as a combination of the configurations inside and outside of the subregions as $|I\rangle = |I_A I_{\bar{A}}\rangle$. One can define the marginal probabilities as $p_{I_A} = \sum_{I_{\bar{A}}} p_{I_A I_{\bar{A}}}$ and $p_{I_{\bar{A}}} = \sum_{I_A} p_{I_A I_{\bar{A}}}$.

In a previous paper [11] we studied the naive definition of the Rényi mutual information:

$$I_n(A, \bar{A}) = Sh_n(A) + Sh_n(\bar{A}) - Sh_n(A \cup \bar{A}). \tag{2}$$

From now on instead of using $p_{I_A I_{\bar{A}}}$ we will use just p_I. The known results of the Rényi mutual information of quantum critical chains are obtained by using the definition (2). For special bases, usually the ones where part of the Hamiltonian is diagonal (see Ref. [11]), the definition (2) for the Rényi mutual information gives us a logarithmic behavior with the subsystem size, for arbitrary values of n. However, as observed numerically for several quantum chains (see Refs. [10,11,13]), it shows a discontinuity at $n = 1$, that forbids the use of large-n analysis to obtain the most interesting case where $n = 1$, namely the standard Shannon mutual information. Although the definition (2) has its own uses it is not the one which normally has been considered in information sciences. For example I_n for $n \neq 1$ is not necessarily a positive function, a property that we naturally expect to be hold for the mutual information. In this paper we consider a definition that is common in information sciences [31]. The generalized mutual information with the desired properties, as a measure of shared information (see Appendix), is defined as [31]:

$$\tilde{I}_n(A, \bar{A}) = \frac{1}{n-1} \ln \sum_I \frac{p_I^n}{p_{I_{\bar{A}}}^{n-1} p_{I_A}^{n-1}}, \tag{3}$$

where p_{I_A} and $p_{I_{\bar{A}}}$, as before, are the probabilities that the subsystems are independently in the configurations $|I_A\rangle$ and $|I_{\bar{A}}\rangle$ that forms the configuration $|I\rangle$ that occurs with probability p_I.

Hereafter L will represent the size of the whole system and ℓ and $L - \ell$ the sizes of the subsystems. With this new notation one can write $\tilde{I}_n(A, \bar{A})$ as $\tilde{I}_n(\ell, L - \ell)$. This definition of the generalized mutual information comes from the natural extension of the relative entropy to the Rényi case and measures the distance of the full distribution from the product of two independent distributions. In the limit $n \to 1$ one easily recovers the Shannon mutual information $\tilde{I}_1(l, L - \ell) = Sh(\ell) + Sh(L - \ell) - Sh(L)$, where $Sh = -\sum_I p_I \ln p_I$ is the standard Shannon entropy. One of the important properties of $\tilde{I}_n$, that is not shared by I_n, is its nondecreasing behavior as a function of n (see Appendix). Our calculations for a set of distinct quantum spin chains will be done numerically, since up to our knowledge an analytical method to consider these quantum chains is still missing.

III. GENERALIZED MUTUAL INFORMATION IN QUANTUM CHAINS

In this section we will numerically calculate the ground-state generalized mutual information of two series of critical quantum spin chains with slightly different structure. In the first part we will calculate the generalized mutual information for systems with discrete symmetries such as the Q-state Potts models with $Q = 2,3$, and 4, the Ashkin-Teller model and the parafermionic $Z(Q)$-quantum spin chain [33] for the values of $Q = 5,6,7$, and 8. In the second part we will calculate the generalized mutual information for systems with $U(1)$ symmetry such as the Klein-Gordon field theory, the XXZ model and the Fateev-Zamolodchikov model with different values of their anisotropy parameters.

A. Generalized mutual information in quantum chains with discrete symmetries

In this subsection we will study the generalized mutual information of the ground state of different critical spin chains with $Z(Q)$ discrete symmetries. The results we present were obtained by expressing the ground-state wave function in two specific bases where the systems show some universal properties.

1. Generalized mutual information of the quantum Q-state Potts model and the quantum Ashkin-Teller model

Our results show that the Q-state Potts model and the Ashkin-Teller model share a similar behavior. For this reason we discuss them together. The critical Q-state Potts model in a periodic lattice is defined by the Hamiltonian [32]

$$H_Q = -\sum_{i=1}^{L} \sum_{k=1}^{Q-1} \left(S_i^k S_{i+1}^{Q-k} + R_i^k \right), \tag{4}$$

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 $S_j R_j = e^{i\frac{2\pi}{Q}} R_j S_j$ and $R_i^Q = S_i^Q = 1$. The model has its critical behavior 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 standard Ising quantum chain. The Ashkin-Teller model has a $Z(2) \otimes Z(2)$ symmetry and a Hamiltonian given

by:

$$H = -\sum_{i=1}^{L} \left(S_i S_{i+1}^3 + S_i^3 S_{i+1} + \Delta S_i^2 S_{i+1}^2 + R_i + R_i^3 + \Delta R_i^2\right), \quad (5)$$

where S_i and R_i 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.

In a previous paper [11] we already showed that the Shannon and Rényi mutual information, as defined in (2), are basis dependent. In other words one can get quite distinct different finite-size scaling behaviors by considering a different basis. Surprisingly in some particular bases, which we called conformal bases, the results show some universality. For example, the results for the Q-state Potts model and for the Ashkin-Teller model in the bases where the matrices R_i or the matrices S_i are diagonal are the same, and follow the asymptotic behavior

$$I_n(\ell, L-\ell) = \frac{c_n}{4} \ln\left[\frac{L}{\pi} \sin\left(\frac{\pi \ell}{L}\right)\right] + \cdots, \quad (6)$$

with

$$c_n = c \begin{cases} 1, & n = 1 \\ \frac{n}{n-1}, & n > 1.5 \end{cases}. \quad (7)$$

We should mention that in Ref. [10], based on numerical results, it was claimed that for $n = 1$ the coefficient c_1 might not be exactly equal to the central charge. As it was discussed in Refs. [10,11] it is quite likely that I_n is not a continuous function around $n = 1$ and so any attempt to do the replica trick using this definition of Rényi mutual information will be useless. This makes the analytical calculation a challenge. This is an additional reason to examine the behavior of $\tilde{I}_n$, besides being the correct extension, from the point of view of a measure of shared information. Having this in mind we calculated the $\tilde{I}_n$ for $Q = 2,3$, and $Q = 4$ Potts chains and for the Ashkin-Teller model in the R and the S bases. We found that in some regimes of variation of the parameter n one can fit the data nicely to

$$\tilde{I}_n(\ell, L-\ell) = \frac{\tilde{c}_n}{4} \log\left[\frac{L}{\pi} \sin\left(\frac{\pi \ell}{L}\right)\right] + \cdots, \quad (8)$$

being $\tilde{c}_n$ a monotonically nondecreasing function of n, consistent with what we expect for the mutual information, since it is a good measure of shared information (see the Appendix).

Here we summarize the results for the Q-state Potts and Ashkin-Teller quantum chains:

(i) The results in general depend on the basis we choose to express the ground-state wave function.

(ii) The generalized mutual information follows (8) in the S and R bases but with different coefficients for different bases. To illustrate the logarithmic behavior we show in Fig. 1 and Fig. 2 the mutual information $\tilde{I}_n$ for the Ising model ($Q = 2$) with $L = 28$ sites and ground-state eigenfunctions in the S and R basis, respectively. We see, from these figures, that for subsystem sizes $\ell \geqslant 3$ we have the logarithmic behavior given by (8) up to $n \approx 8$ in the S basis and $n \approx 4$ in the R basis. As we can see our results does not exclude the existence of some relevant ℓ-dependent terms in (8) for large values of n.

(iii) The coefficient of the logarithm $\tilde{c}_n$ in (8) is a continuous monotonically non-decreasing function of n and

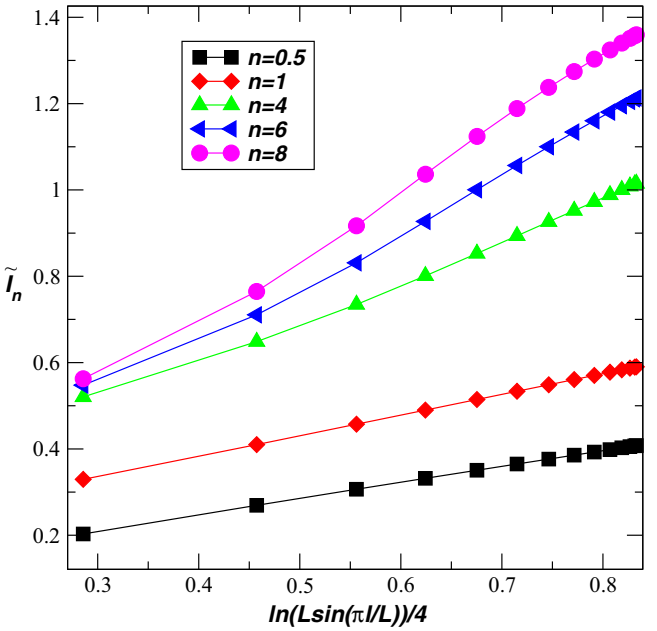

FIG. 1. (Color online) The generalized mutual information $\tilde{I}_n(\ell, L-\ell)$ of the $L = 28$ sites periodic Ising quantum chain, as a function of $\ln[L \sin(\frac{\pi \ell}{L})]/4$. The ground-state wave function is in the basis where the matrices S_i are diagonal (S bases).

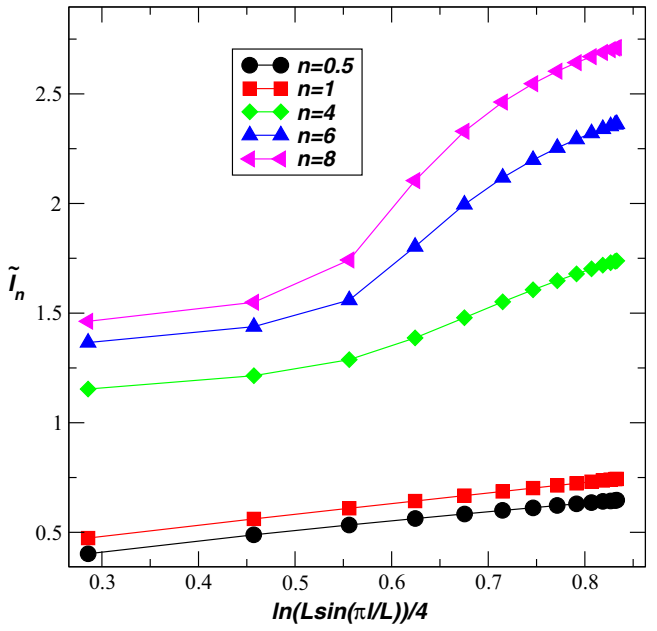

FIG. 2. (Color online) The generalized mutual information $\tilde{I}_n(\ell, L-\ell)$ of the $L = 28$ sites periodic Ising quantum chain, as a function of $\ln[L \sin(\frac{\pi \ell}{L})]/4$. The ground-state wave function is in the basis where the matrices R_i are diagonal (R bases).

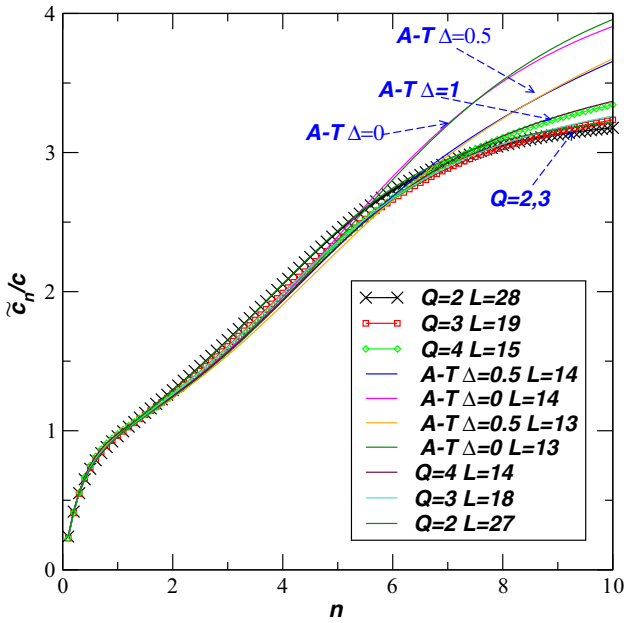

FIG. 3. (Color online) The ratio $\tilde{c}_n/c$ of the coefficient of the logarithm in Eq. (8) and the central charge c for the Q-state Potts model with $Q = 2,3$, and 4, and for the Ashkin-Teller model (A-T) with different anisotropies Δ. The Ashkin-Teller model at the isotropic point ($\Delta = 1$) is equivalent to the four-state Potts model. The ground-state wave functions are in the bases where the S_i matrices are diagonal. The lattice sizes of the models are shown and the coefficients $\tilde{c}_n$ were estimated by using the subsystem sizes $\ell = 3,5,\ldots,\mathrm{Int}[L/2]$.

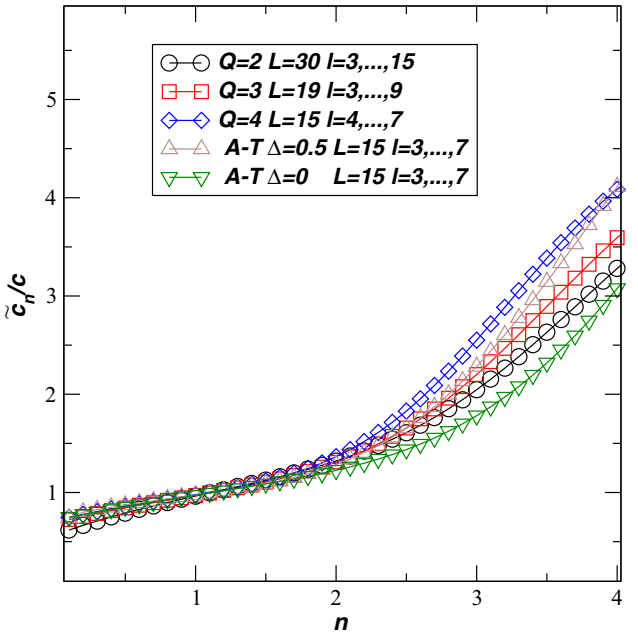

FIG. 4. (Color online) Same as Fig. 3, but with the ground-state wave functions of the quantum spin Hamiltonians expressed in the bases where the matrices R_i are diagonal. The lattice sizes of the models are shown in the figure, as well as the subsystems sizes ℓ used to estimate $\tilde{c}_n$.

it follows the following formula in the S basis:

$$\tilde{c}_n = cf(n), \quad \text{with} \quad f(1) = 1, \tag{9}$$

where c is the central charge and $f(n)$ seems to be a continuous universal function independent of the model, as we can see in Fig. 3. In the case of the Ashkin-Teller model the results start to deviate around $n = 6$ from the ones obtained for the Potts models. As we can see in Fig. 3, the deviation point is dependent on the anisotropy parameter Δ of the model.

(iv) In the case of the R basis, as one can see in Fig. 4, Eq. (9) is still valid for values of n up to $\sim$4. However the function $f(n)$ is distinct from the one obtained in the S basis. As shown in Fig. 4, up to $n = 2$ the form of the function $f(n)$ seems to be also independent of the model. This figure also shows that the Ashkin-Teller model has stronger deviations in this basis, as compared with the results obtained in the S basis. In order to better see the difference of the coefficients $\tilde{c}_n$ in the S and R basis, we present in Fig. 5 the data of Figs. 3 and 4 for the $Q = 2,3$ and four-state Potts models.

(v) The coefficient of the logarithm in the S basis always goes to zero as $n \to 0$, differently from the R basis where it approaches to a nontrivial number. This simply means that probably in the continuum limit all the probabilities in the S basis are positive but in the R basis some of them are zero. For the definition of the $n = 0$ case see the Appendix.

Our numerical results indicate that $\tilde{c}_n$ is a continuous function of n around $n = 1$. This means that $\tilde{I}_n$ should be a continuous function with respect to n and so it is a better candidate to be used in techniques exploring the analytical continuation of the value n, as happens, for example, in the replica trick. However, the appropriate technique that may be used is still unclear to us.

It is important to mention that the results obtained for the ratio $\tilde{c}_n/c$ in this section (Fig. 3) and in the subsequent ones (Figs. 8, 9, 11, and 13) are based on the linear fit with

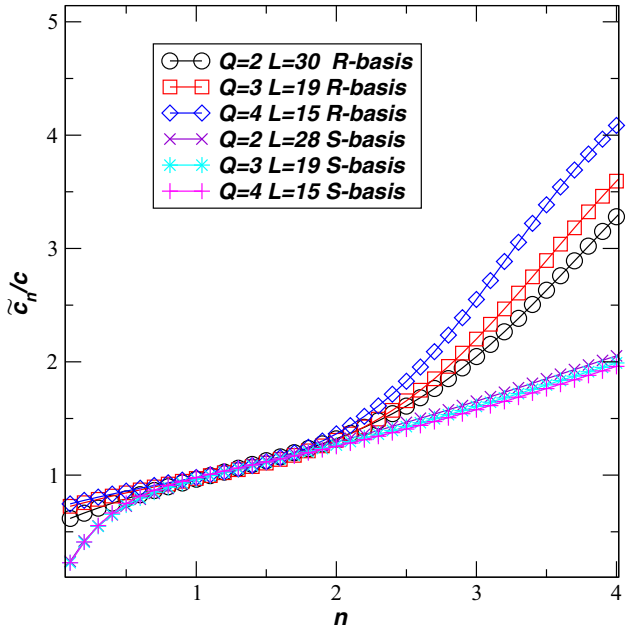

FIG. 5. (Color online) The values of the ratios $\tilde{c}_n/c$ of Figs. 3 and 4 for the $Q = 2,3$ and four-state Potts model are shown in the same figure, for comparison.

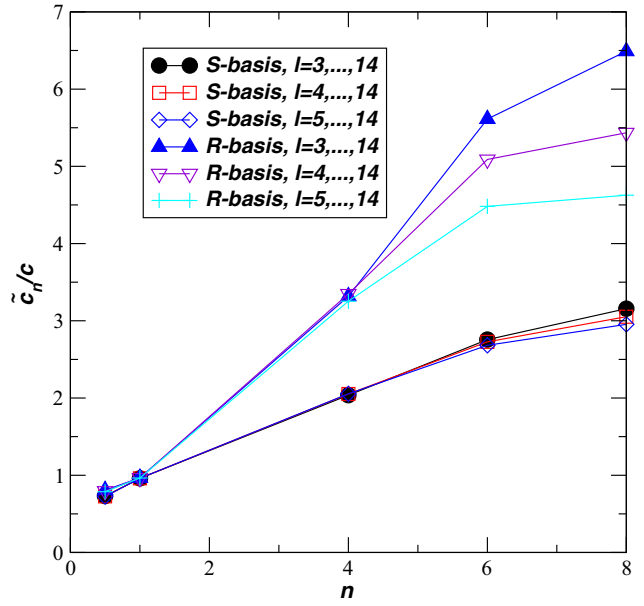

FIG. 6. (Color online) The values of $\tilde{c}_n/c$ obtained from the data of Figs. 1 and 2 for the Ising quantum chain with $L = 28$ sites and eigenfunction expressed in S and R basis.

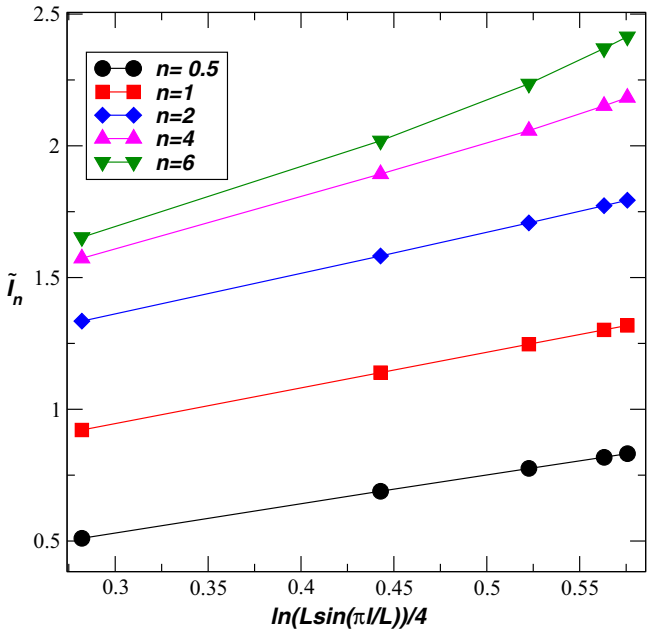

FIG. 7. (Color online) The generalized mutual information $\tilde{I}_n(\ell, L-\ell)$ of the $L = 10$ sites periodic $Z(7)$-parafermionic quantum chain, as a function of $\ln[L\sin(\frac{\pi\ell}{L})]/4$. The ground-state wave function is in the basis where the S_i matrices are diagonal (S bases).

the $\ln[L\sin(\ell\pi/L)]$ dependence. These fittings were done by choosing a set of subsystem sizes. In all the presented figures we only depict results where a small variation of the number of subsystem sizes gives us estimated values of $\tilde{c}_n$ that differs a few percent. As an example we consider the fittings obtained from the data of Figs. 1 and 2 for the Ising model with $L = 28$ sites and ground-state eigenfunction in the S and R basis, respectively. This is shown in Fig. 6. As we can see, while for the S basis the fitting is reasonable up to $n = 8$ in the R basis we do not have reliable results for $n > 4$.

2. *Generalized mutual information in the parafermionic $Z(Q)$-quantum spin chains*

In this subsection we consider the generalized mutual information for some critical spin chains with discrete $Z(Q)$ symmetry and central charge bigger than one. The quantum chains we consider are the parafermionic $Z(Q)$-quantum spin chains [33] with Hamiltonian given by [34,35]

$$H = -\sum_{i=1}^{L}\sum_{k=1}^{Q-1}\left(S_i^k S_{i+1}^{Q-k} + R_i^k\right)/\sin(\pi k/Q), \qquad (10)$$

where again S_i and R_i are the $Q \times Q$ matrices that appeared in (4). This model is critical and conformal invariant with a central charge $c = 2(Q-1)/(Q+2)$. For the case where $Q = 2$ and $Q = 3$ 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 $\Delta = \frac{\sqrt{2}}{2}$. We have considered the models with $Q = 5,6,7$, and 8 and the ground-state wave functions expressed in the S or R basis. The results for the several values of Q are shown in Figs. 7, 8, and 9. To illustrate the logarithmic dependence with the subsystem size ℓ we show in Fig. 7 $\tilde{I}_n(\ell, L-\ell)$, as a function of $\ln[L\sin(\pi\ell/L)]/4$ for the $Z(7)$ parafermionic quantum chain with $L = 10$ sites, with the ground-state wave function expressed in the S basis. In Figs. 8 and 9 we show the ratio $\tilde{c}_n/c$ of the logarithmic coefficient of (8) with the central charge c for the $Z(Q)$-parafermionic models with ground-state wave

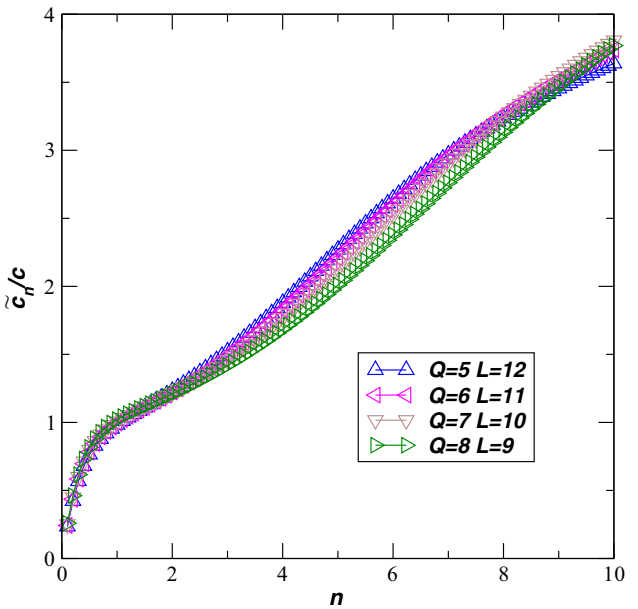

FIG. 8. (Color online) The ratio $\tilde{c}_n/c$ of the coefficient of the logarithm in Eq. (8) and the central charge c for the $Z(Q)$-parafermionic models with $Q = 5,6,7$, and 8. The ground states are in the bases where the S_i matrices are diagonal. The lattice sizes of the models are shown in the figure and the coefficients $\tilde{c}_n$ were estimated by using the subsystem sizes $\ell = 3,5,\ldots,\text{Int}[L/2]$.

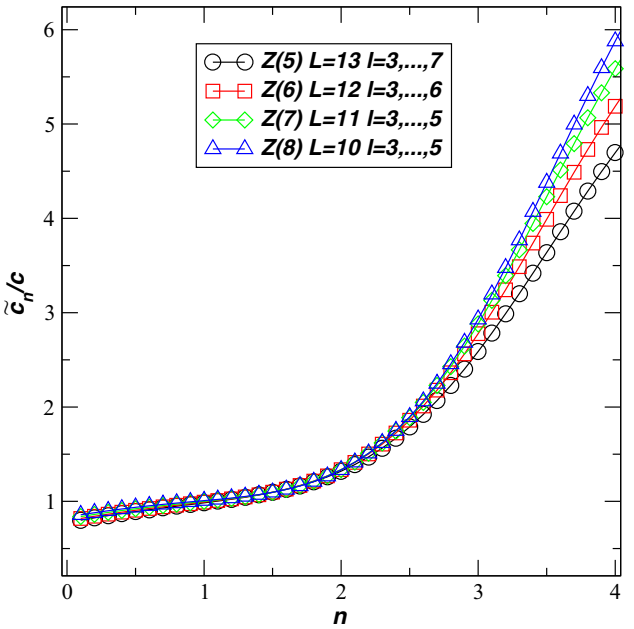

FIG. 9. (Color online) Same as Fig. 8, but with the ground-state wave function of the quantum spin Hamiltonians expressed in the bases where the matrices R_i are diagonal. The lattice sizes of the models, as well as the subsystems sizes ℓ used to estimate $\tilde{c}_n$ are shown.

function in the S and R basis, respectively. The maximum lattice sizes we used for the $Z(Q)$-parafermionic models are $L = 12,11,10$, and 9 for $Q = 5,6,7$, and 8, respectively. The results we obtained are very similar to the ones we already discussed in the previous case of the Q-state Potts models. All the five properties that we discussed in that subsection are equally valid also for the $Z(Q)$-parafermionic models. By comparing the results of Figs. 8 and 9 with Figs. 3 and 4 we observe that the function $f(n)$ in (9) are quite similar for the two set of models, at least for values of n up to $\sim$6. Probably the matching of these curves is not perfect due to the small system sizes we consider, specially for $Q > 4$.

B. Generalized mutual information of quantum chains with continuous symmetries

In this section we consider the generalized mutual information of critical chains having a continuous $U(1)$ symmetry. We studied a set of coupled harmonic oscillators which gives a discrete version of Klein-Gordon field theory as well as the spin-1/2 XXZ and the spin-1 Fateev-Zamolodchikov quantum chains. The last two models are interesting since, like the Ashkin-Teller model, they have an anisotropy that gives us a critical line of continuously varying critical exponents but with a fixed central charge.

1. Generalized mutual information in quantum harmonic chains

In this subsection we will first consider the generalized mutual information of the ground state of a system of generic coupled harmonic oscillators. Then at the very end we will confine ourselves to the simple case where we have only the nonzero couplings at the next-nearest sites, that in the continuum limit gives us the Klein-Gordon field theory.

Consider the Hamiltonian of L-coupled harmonic oscillators, with coordinates $\phi_1,\ldots,\phi_L$ and conjugated momenta $\pi_1,\ldots,\pi_L$:

$$\mathcal{H} = \frac{1}{2}\sum_{n=1}^{L}\pi_n^2 + \frac{1}{2}\sum_{n,n'=1}^{L}\phi_n K_{nn'}\phi_{n'}. \tag{11}$$

The ground state of the above Hamiltonian has the following form

$$\Psi_0 = \left(\frac{\det K^{1/2}}{\pi^L}\right)^{\frac{1}{4}} e^{-\frac{1}{2}<\phi|K^{1/2}|\phi>}. \tag{12}$$

For the general Hamiltonian (11), one can calculate the two point correlators $X_A = \mathrm{tr}(\rho_A\phi_i\phi_j)$ and $P_A = \mathrm{tr}(\rho_A\pi_i\pi_j)$ using the K matrix defined in (11). The squared root of this matrix, as well as its inverse, can be split up up into coordinates of the subsystems A (size ℓ) and $\bar{A}$ (size $L-\ell$), i.e.,

$$K^{-1/2} = \begin{pmatrix} X_A & X_{A\bar{A}} \\ X_{A\bar{A}}^T & X_{\bar{A}} \end{pmatrix}, \quad K^{1/2} = \begin{pmatrix} P_A & P_{A\bar{A}} \\ P_{A\bar{A}}^T & P_{\bar{A}} \end{pmatrix}.$$

Here we chose the couplings so that we always keep the equalities $P_{A\bar{A}}^T = P_{A\bar{A}}$ and $X_{A\bar{A}}^T = X_{A\bar{A}}$. The spectra of the matrix $2C = \sqrt{X_A P_A}$, can be used to calculate the Rényi entanglement entropy (see Ref. [37] and references therein) as

$$S_n(\ell, L-\ell) = \frac{1}{n-1}\mathrm{tr}\left\{\ln\left[\left(C+\frac{1}{2}\right)^n - \left(C-\frac{1}{2}\right)^n\right]\right\}.$$

In this formulation we only need the correlators inside the region A. Note that the above quantity is basis independent and is considered as an usual measure of the quantum entanglement. Here we need to introduce this quantity just for later use. To calculate the generalized mutual information for a system of coupled harmonic oscillators one first needs to fix the basis. Here we work in the position coordinate basis, however all the results are valid also in the momentum basis. One should notice that the same is not true if one works in a generic basis obtained through canonical transformations from the position or momentum basis. In order to calculate $\tilde{I}_n$ first we find $p(\Phi_A)$ and $p(\Phi_{\bar{A}})$ as

$$p(\Phi_A) = \sqrt{\frac{\det \tilde{P}_A}{\pi^\ell}} e^{-\Phi_A \tilde{P}_A \Phi_A}, \tag{13}$$

$$p(\Phi_{\bar{A}}) = \sqrt{\frac{\det \tilde{P}_{\bar{A}}}{\pi^{L-\ell}}} e^{-\Phi_{\bar{A}} \tilde{P}_{\bar{A}} \Phi_{\bar{A}}}, \tag{14}$$

where $\tilde{P}_A = P_A - P_{A\bar{A}}(P_{\bar{A}})^{-1}P_{A\bar{A}}^T$ and $\tilde{P}_{\bar{A}} = P_{\bar{A}} - P_{A\bar{A}}^T(P_A)^{-1}P_{\bar{A}A}$. Since ϕ takes continuum values one needs to consider the integral version of Eq. (3) as follows:

$$\tilde{I}_n = \frac{1}{n-1}\ln\int \mathcal{D}\Phi \frac{p^n(\Phi)}{p^{n-1}(\Phi_A)p^{n-1}(\Phi_{\bar{A}})}, \tag{15}$$

where $p(\Phi) = |\Psi_0|^2$. Plugging Eqs. (12), (13), (14) into Eq. (15) and performing the Gaussian integral one can derive

the generalized mutual information

$$\tilde{I}_n = \frac{1}{2}\ln\left(\frac{\det K^{\frac{1}{2}}}{\det\tilde{P}_A \det\tilde{P}_{\bar{A}}}\right) - \frac{1}{2(n-1)} \times \ln\left(\frac{\det\left[nK^{1/2} - (n-1)\begin{pmatrix}\tilde{P}_A & 0\\ 0 & \tilde{P}_{\bar{A}}\end{pmatrix}\right]}{\det K^{1/2}}\right).$$

The following determinant formulas

$$\det(\tilde{P}_A)\det P_{\bar{A}} = \det K^{1/2}, \quad (16)$$

$$\det(\tilde{P}_{\bar{A}})\det P_A = \det K^{1/2}, \quad (17)$$

$$\det P_{\bar{A}} \det K^{-1/2} = \det X_A, \quad (18)$$

$$\det P_A \det K^{-1/2} = \det X_{\bar{A}}, \quad (19)$$

allow us to write

$$\tilde{I}_n(\ell, L-\ell) = S_2(\ell, L-\ell) - \frac{1}{2(n-1)}\ln\det[n+(1-n)T], \quad (20)$$

where

$$T = \begin{pmatrix} X_A\tilde{P}_A & X_{A\bar{A}}\tilde{P}_{\bar{A}} \\ X^T_{A\bar{A}}\tilde{P}_A & X_{\bar{A}}\tilde{P}_{\bar{A}}\end{pmatrix} = \begin{pmatrix} 1 & X_{A\bar{A}}\tilde{P}_{\bar{A}} \\ X^T_{A\bar{A}}\tilde{P}_A & 1\end{pmatrix}. \quad (21)$$

There is an important remark that we should mention: in principle Eq. (20) makes sense only if $n+(1-n)T$ is a symmetric positive definite matrix. If we start with a symmetric positive definite matrix $K^{1/2}$ this is already warranted for $0 < n < 1$ but for $n > 1$ one needs to check its validity. This will be an important point when we study the short-range coupled harmonic oscillators. Finally one can write

$$\tilde{I}_n(\ell, L-\ell) = S_2(\ell, L-\ell) + \tilde{M}_n(\ell, L-\ell) = S_2(\ell, L-\ell) - \frac{1}{2(n-1)} \times \ln\det\left[1-(1-n)^2 X^T_{A\bar{A}}\tilde{P}_A X_{A\bar{A}}\tilde{P}_{\bar{A}}\right],$$

where $\tilde{M}_n(\ell, L-\ell)$ is the only n-dependent part. We notice here that by changing n to $2-n$ we just change the sign of the second term, i.e., $\tilde{M}_{2-n}(\ell, L-\ell) = -\tilde{M}_n(\ell, L-\ell)$.

When $n \to 1$ the second term vanishes and we recover the result of [8]

$$\tilde{I}_1(\ell, L-\ell) = S_2(\ell, L-\ell). \quad (22)$$

For massless Klein-Gordon theory the above result in one dimension gives, as a consequence the well known result for the Rényi entanglement entropy [36,37],

$$\tilde{I}_1(\ell, L-\ell) = \frac{1}{4}\ln\left[\frac{L}{\pi}\sin\left(\frac{\pi\ell}{L}\right)\right] + \cdots, \quad (23)$$

where the dots are the subleading terms. Our numerical analyses indicate that for short-range quantum harmonic oscillators the matrix $n+(1-n)T$ is symmetric positive definite up to just $n = n_c = 2$.[1] The numerical results show that for the values $0 < n < 2$ Eq. (8) is a very good approximation, as we can see for example in Fig. 10. The coefficient $\tilde{c}_n$ of the logarithmic term in (8) is obtained from the fitting of the model with $L = 120$ sites is shown in Fig. 11 and in the range $0.4 < n < 1.6$ surprisingly it follows the simple formula:

$$\tilde{c}_n = f(n) = 1 + 4\frac{n-1}{10}, \quad 0.4 < n < 1.6. \quad (24)$$

This is the red line in Fig. 11. At $n = 0$ we expect zero mutual information for our system, this means that based on the symmetry $n \to 2-n$ the coefficient for $n = 2$ should be $\tilde{c}_2 = 2$. Finally one can conclude that for integer values of $n = 0,1,2$ the coefficient of the logarithm is

$$\tilde{c}_n = f(n) = n, \quad n = 0,1,2. \quad (25)$$

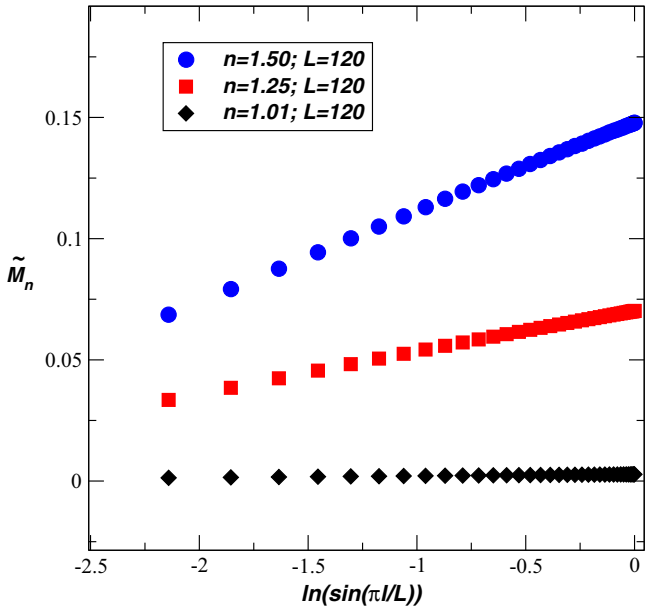

FIG. 10. (Color online) The second term in Eq. (22), $\tilde{M}_n(\ell, L-\ell)$, as a function of $\ln[L\sin(\frac{\pi\ell}{L})]$ for periodic quantum harmonic chain with $L = 120$ sites.

2. *Generalized mutual information of quantum spin chains with continuous symmetries*

The Hamiltonian of the XXZ chain is defined as

$$H_{\mathrm{XXZ}} = -\sum_{i=1}^{L}\left(\sigma^x_j\sigma^x_{j+1} + \sigma^y_j\sigma^y_{j+1} + \Delta\sigma^z_j\sigma^z_{j+1}\right), \quad (26)$$

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 $-1 \leqslant \Delta < 1$ with a constant central charge $c = 1$, giving us a good example to test the universality of our results with respect to the change of the anisotropy. The long-distance

[1] For a finite-size system n_c is not exactly equal to 2, however, by increasing the lattice size it approaches the value 2. We conjecture that $n_c = 2$ is exact in the thermodynamic limit.

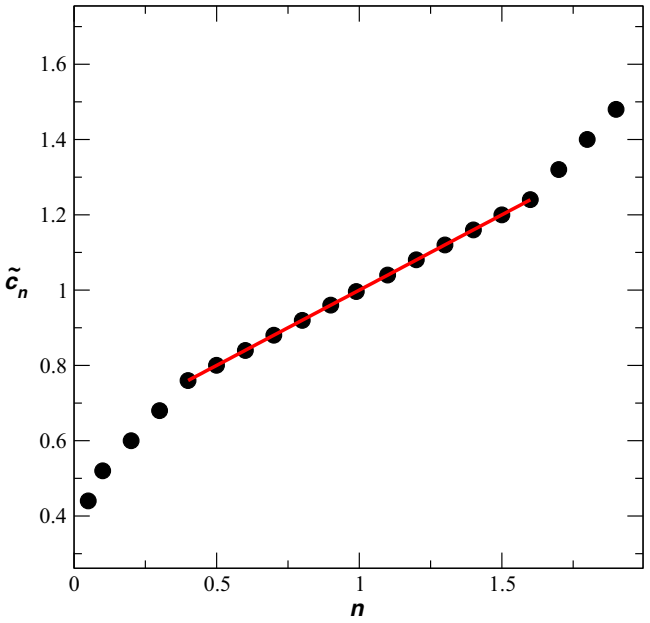

FIG. 11. (Color online) The coefficient of the logarithm $\tilde{c}_n$ in Eq. (8). The lattice size $L = 120$ and the coefficients $\tilde{c}_n$ were estimated by using the subsystem sizes $\ell = 3,5,\ldots \mathrm{Int}[L/2]$. The red line is given by Eq. (24).

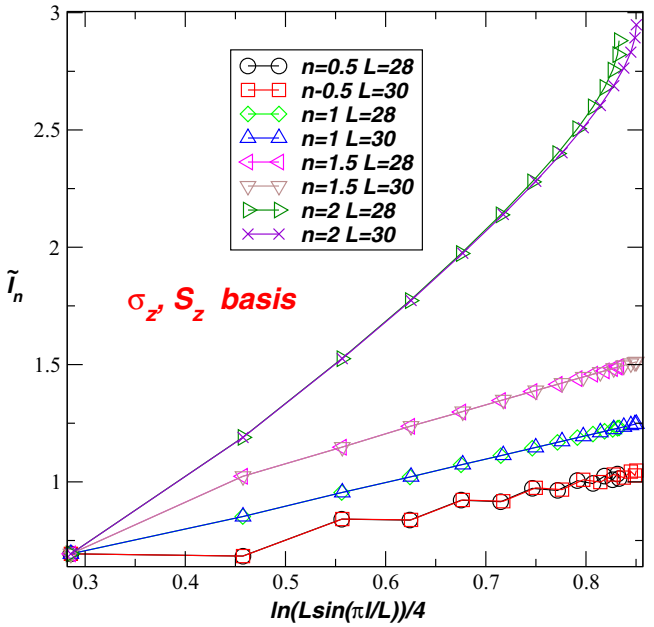

FIG. 12. (Color online) The generalized mutual information $\tilde{I}_n(\ell, L-\ell)$ of the periodic XXZ quantum chain with anisotropy $\Delta = -1/2$, as a function of $\ln[\sin(\frac{\pi\ell}{L})]/4$. The ground-state wave function is in the basis where the σ_i^z matrices are diagonal (σ^z basis). The results are for lattice sizes $L = 28$ and $L = 30$ and give an idea of the finite-size corrections.

critical fluctuations are ruled by a CFT with central charge $c = 1$ described by a compactified boson whose action is given by

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

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

$$R = \sqrt{\frac{2}{\pi}\arccos\Delta}. \tag{28}$$

As it is shown in Fig. 12, in the σ^z basis, the generalized mutual information $\tilde{I}_n(\ell, L-\ell)$ shows the logarithmic behavior given in (8) only for $n < 2$. This can be simply understood based on what we observed for the chain of harmonic oscillators. One can look to the Klein-Gordon field theory as a noncompactified version of the action (27). Since we showed that in that case the generalized mutual information is not defined beyond $n = 2$ we expect the same behavior also in the compactified version. Note that in our numerical calculations one can actually derive spurious big numbers for the generalized mutual information even for $n > 2$, but we expect all of them go to infinity in the thermodynamic limit. This behavior seems to be independent of the anisotropy parameter Δ.

The coefficient of the logarithm in (8) for $n < 2$ is again given by (9), as we can see in Fig. 13, with a function $f(n)$, which fits to the results of the harmonic chain perfectly. We also considered the results in the case where the ground-state wave function is expressed in the σ^x basis and, except around $n = 1$, Eq. (8) is not a good approximation. The second $U(1)$-symmetric model we considered is the spin-1 Fateev-Zamolodchikov quantum chain whose Hamiltonian is

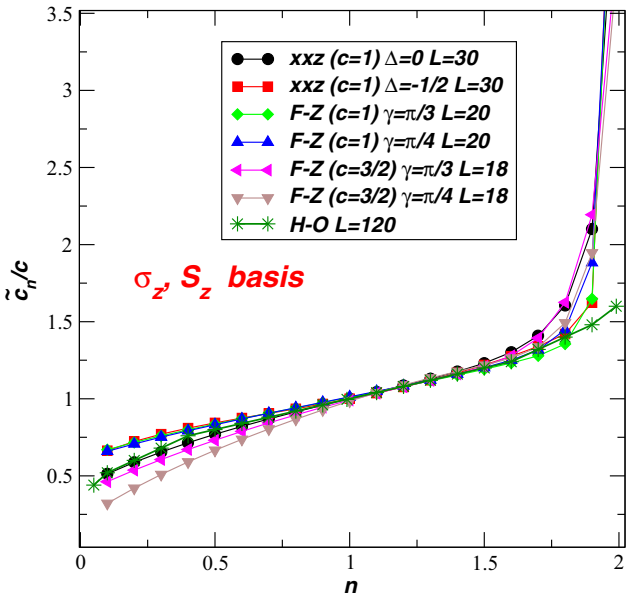

FIG. 13. (Color online) The ratio $\tilde{c}_n/c$ of the coefficient of the logarithm in Eq. (8) with the central charge c for the XXZ and for the spin-1 Fateev-Zamolodchikov quantum chains (F-Z). The XXZ (Fateev-Zamolodchikov) ground-state wave function are in the σ^z (S^z) basis. The results for the XXZ are for the anisotropies $\Delta = 0, -1/2$ and in the case of the Fateev-Zamolodchikov model their are for the couplings $\gamma = \pi/3, \pi/4$. The lattice sizes of the models are shown and the coefficients $\tilde{c}_n$ were estimated by using the subsystem sizes $\ell = 4,5,\ldots,L/2$.

given by [38]

$$H_{FZ} = \epsilon \sum_{i=1}^{L} \left[\sigma_i - \left(\sigma_i^z\right)^2 - 2(\cos\gamma - 1)\left(\sigma_i^{\perp}\sigma_i^z + \sigma_i^z\sigma_i^{\perp}\right) - 2\sin^2\gamma\left(\sigma_i^z - \left(\sigma_i^z\right)^2 + 2\left(S_i^2\right)^2\right)\right], \quad (29)$$

where $\vec{S} = (S^x, S^y, S^z)$ are spin-1 $SU(2)$ matrices, $\sigma_i^z = S_i^z S_{i+1}^z$ and $\vec{S}_i \vec{S}_{i+1} = \sigma_i^{\perp} + \sigma_i^z$. The model is antiferromagnetic for $\epsilon = +1$ and ferromagnetic for $\epsilon = -1$. It has a line of critical points ($0 \leqslant \gamma \leqslant \frac{\pi}{2}$) with a quite distinct behavior in the antiferromagnetic ($\epsilon = +1$) and ferromagnetic ($\epsilon = -1$) cases. The antiferromagnetic version of the model is governed by a CFT with central charge $c = \frac{3}{2}$ [39] while the ferromagnetic one is ruled by a $c = 1$ CFT [40]. We calculated $\tilde{I}_n(\ell, L-\ell)$ in both critical regimes where $c = 1$ and $c = \frac{3}{2}$, and for different values of the anisotropy. We found a very similar pattern as that of the XXZ quantum chain, as can be seen in Fig. 13. Equation (8) is valid for values of $n < 2$ and the coefficient of the logarithm follows (9) with a function $f(n)$, which is quite similar to the one we found for the quantum harmonic oscillators and the XXZ chain. This shows an interesting universal pattern for critical chains with continuous $U(1)$ symmetry.

IV. CONCLUSIONS

In this paper we calculated the generalized mutual information $\tilde{I}_n(\ell, L-\ell)$, as defined in (3), for quantum chains describing the dynamics of quantum systems with continuous or discrete degrees of freedom. Most of our analysis was purely numerical due to the absence, at the moment, of suitable analytical methods to treat this problem. We considered several integrable quantum spin chains. These quantum chains either have a $Z(Q)$ symmetry [such as the Q-state Potts model with $Q = 2,3$, and 4, the Ashkin-Teller model, and the $Z(Q)$-parafermionic model with $Q = 5,6,7$, and 8] or a $U(1)$ symmetry (XXZ quantum chain and the spin-1 Fateev-Zamolodchikov model). We also considered the discrete version of the Klein-Gordon field theory given by a set of coupled harmonic oscillators. In this case we have a continuum Hilbert space. We observed that by expressing the ground-state wave functions in general basis the obtained results are distinct. However, similarly as happens for the quantity I_n given in (2) (see Ref. [11]), our results on some special bases reveal some general features. These bases are the ones where the S or R operators are diagonal, for the models with $Z(Q)$ symmetry or the ones where σ^z or S^z are diagonal for the models with $U(1)$ symmetry. In a continuum field theory description of these quantum chains these bases are expected to be associated to the boundaries that do not destroy the conformal invariance of the bulk underlying Euclidean conformal field theory, and for this reason we call them conformal bases [11]. Our results indicate that in these special bases the mutual information $\tilde{I}_n$ has the same kind of leading behavior with the subsystem size ℓ as we have in the Rényi entanglement entropy, namely $\tilde{I}_n(\ell, L-\ell) \sim \frac{\tilde{c}_n}{4} \ln[\frac{L}{\pi}\sin(\frac{\pi\ell}{L})]$, with a function $\tilde{c}_n = cf(n)$, with $f(1) = 1$. Differently from the Rényi entanglement entropy where the equivalent function $f(n)$ is universal (for any model and any basis) in the case of $\tilde{I}_n$ our results indicate that the function $f(n)$ depends on the special basis chosen to express the ground-state eigenfunction of the particular model. For the set of $Z(Q)$-symmetric models we considered the function $f(n)$, for $n < 4$, although different for the S and R bases, are similar to the ones of the Q-state Potts chain ($Q = 2,3,4$) and the parafermionic $Z(Q)$ quantum chains ($Q = 5,6,7,8$). In the case of the Ashkin-Teller model our results indicate that $f(n)$, for $n > 2$, also depends on the anisotropy Δ of the model. On the other hand the models with continuum symmetry showed a similar behavior only for $n < 2$. For $n > 2$ we have strong evidence that most probably the generalized mutual information is not defined. It is quite interesting that in these cases one can understand most of the results by just studying simple short-range coupled harmonic oscillators.

In order to conclude we should mention that an analytical approach for the Shannon entropy or the Shannon mutual information [I_1 or $\tilde{I}_1$ in (2) and (3)] is a theoretical challenge. The analytical methods to treat this kind of problem normally use some sort of analytical continuation, in the parameter n, like the usual replica trick. The results we present showing the continuity of $\tilde{I}_n$ around $n = 1$, differently from what happens with I_n, indicate that $\tilde{I}_n$ is probably more appropriate for an analytical treatment.

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APPENDIX: RELATIVE ENTROPY AND RÉNYI DIVERGENCE

In this Appendix we review the definitions of the relative entropy and its generalization: the Rényi divergence. The relative entropy is defined as the expectation of the difference between the logarithm of the two distribution of probabilities p and q, from the point of view of the distribution p, i.e.,

$$D(p \parallel q) = \sum_i p_i \ln \frac{p_i}{q_i}. \quad (A1)$$

It can be considered as a measure of the difference between the two distributions p and q. Although it is not a symmetric quantity it helps us to define the mutual information of the subsets X and Y of the system as follows:

$$I(X,Y) = D[p(X,Y) \parallel p(X)p(Y)]. \quad (A2)$$

That is, the mutual information between two parts of a system is just the relative entropy between the distribution probability for the whole system and the product of the probability distributions of the different parts. It tells how much the different parts are correlated. The natural generalization of the relative entropy is the Rényi divergence and can be defined (see Ref. [31] for example), as

$$D_n(p \parallel q) = \frac{1}{n-1} \ln \sum_i p_i^n q_i^{1-n}. \quad (A3)$$

It has the following properties: for $n > 0$ we have $D_n(p \parallel q) \neq 0$ and if $p = q$ then we have $D_n(p \parallel q) = 0$. The especial case

$n \to 1$ gives the usual relative entropy. We also define the $n = 0$ case by:

$$D_0(p \parallel q) = -\ln q(i|p_i > 0). \tag{A4}$$

It is worth mentioning that using the above definition $D_0(p \parallel q)$ is not zero except when for all i's for which $q_i > 0$ also $p_i > 0$ holds.

Another important property is the following (see Ref. [41] and references therein):

Theorem. The Rényi divergence is a continuous and nondecreasing function of the parameter n.

Comparing (A3) with (A2) and (A1) the natural definition of the generalized mutual information is

$$\tilde{I}_n(X,Y) = D_n[p(X,Y) \parallel p(X)p(Y)]. \tag{A5}$$

The above definition is different from $I_n(\ell, L)$, as given by (2), and has been frequently used in different areas of information science.

[1] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. **80**, 517 (2008); K. Modi, A. Brodutch, H. Cable, T. Paterek, and V. Vedral, *ibid.* **84**, 1655 (2012); U. Schollwöck, *ibid.* **77**, 259 (2005).

[2] P. Calabrese and J. Cardy, J. Phys. A **42**, 504005 (2009).

[3] J. Cardy, Phys. Rev. Lett. **106**, 150404 (2011).

[4] D. A. Abanin and E. Demler, Phys. Rev. Lett. **109**, 020504 (2012).

[5] A. J. Daley, H. Pichler, J. Schachenmayer, and P. Zoller, Phys. Rev. Lett. **109**, 020505 (2012).

[6] J. Dubail and J-M. Stéphan, J. Stat. Mech. (2011) L03002.

[7] Y. Chen and G. Vidal, J. Stat. Mech. (2014) P10011.

[8] F. C. Alcaraz and M. A. Rajabpour, Phys. Rev. Lett. **111**, 017201 (2013).

[9] J-M. Stéphan, J. Stat. Mech. (2014) P05010.

[10] J-M. Stéphan, Phys. Rev. B **90**, 045424 (2014).

[11] F. C. Alcaraz and M. A. Rajabpour, Phys. Rev. B **90**, 075132 (2014).

[12] M. M. Wolf, F. Verstraete, M. B. Hastings, and J. I. Cirac, Phys. Rev. Lett. **100**, 070502 (2008).

[13] J-M. Stéphan, S. Furukawa, G. Misguich, and V. Pasquier, Phys. Rev. B **80**, 184421 (2009).

[14] J-M. Stéphan, G. Misguich, and V. Pasquier, Phys. Rev. B **82**, 125455 (2010).

[15] M. Oshikawa, arXiv:1007.3739.

[16] J-M. Stéphan, G. Misguich, and V. Pasquier, Phys. Rev. B **84**, 195128 (2011).

[17] J. Um, H. Park, and H. Hinrichsen, J. Stat. Mech. (2012) P10026.

[18] H. W. Lau and P. Grassberger, Phys. Rev. E **87**, 022128 (2013).

[19] M. Ghasemi Nezhadhaghighi and M. A. Rajabpour, Phys. Rev. B **88**, 045426 (2013).

[20] D. J. Luitz, F. Alet, and N. Laflorencie, Phys. Rev. Lett. **112**, 057203 (2014).

[21] D. J. Luitz, F. Alet, and N. Laflorencie, Phys. Rev. B **89**, 165106 (2014).

[22] D. J. Luitz, N. Laflorencie, and F. Alet, J. Stat. Mech. (2014) P08007.

[23] D. J. Luitz, X. Plat, N. Laflorencie, and F. Alet, Phys. Rev. B **90**, 125105 (2014)

[24] J. Wilms, M. Troyer, and F. Verstraete, J. Stat. Mech. (2011) P10011; J. Wilms, J. Vidal, F. Verstraete, and S. Dusuel, *ibid.* (2012) P01023.

[25] J. Iaconis, S. Inglis, A. B. Kallin, and R. G. Melko, Phys. Rev. B **87**, 195134 (2013).

[26] J-M. Stéphan, S. Inglis, P. Fendley, and R. G. Melko, Phys. Rev. Lett. **112**, 127204 (2014).

[27] A. Rahmani and G-W. Chern, Phys. Rev. B **88**, 054426 (2013).

[28] O. Cohen, V. Rittenberg, and T. Sadhu, J. Phys. A: Math. Theor. **48**, 055002 (2015).

[29] H. Bernigau, M. J. Kastoryano, and J. Eisert, J. Stat. Mech. (2015) P02008.

[30] V. Eisler and Z. Zimboras, Phys. Rev. A **89**, 032321 (2014).

[31] José C. Principe, *Information Theoretic Learning* (Springer, Berlin, 2010).

[32] F. Y. Wu, Rev. Mod. Phys. **54**, 235 (1982).

[33] V. A. Fateev and A. B. Zamolodchikov, Phys. Lett. A **92**, 37 (1982).

[34] F. C. Alcaraz and A. Lima Santos, Nucl. Phys. B **275**, 436 (1986).

[35] F. C. Alcaraz, J. Phys. A **20**, 2511 (1987).

[36] M. Cramer, J. Eisert, M. B. Plenio, and J. Dreissig, Phys. Rev. A **73**, 012309 (2006).

[37] H. Casini and M. Huerta, J. Phys. A **42**, 504007 (2009).

[38] A. B. Zamolodchikov and V. A. Fateev, Yad. Fiz. **32**, 581 (1980) [Sov. J. Nucl. Phys. **32**, 298 (1980)].

[39] F. C. Alcaraz and M. J. Martins, Phys. Rev. Lett. **61**, 1529 (1988); P. Di Francesco, H. Saleur, and J.-B. Zuber, Nucl. Phys. B **300**, 393 (1988).

[40] F. C. Alcaraz and M. J. Martins, Phys. Rev. Lett. **63**, 708 (1989).

[41] T. van Erven and P. Harremoës, in *Proceedings of the IEEE International Symposium on Information Theory (ISIT)* (IEEE, 2010), pp. 1335–1339.