Universal behavior of the Shannon mutual information in nonintegrable self-dual quantum chains

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An existing conjecture states that the Shannon mutual information contained in the ground-state wave function of conformally invariant quantum chains, on periodic lattices, has a leading finite-size scaling behavior that, similarly as the von Neumann entanglement entropy, depends on the value of the central charge of the underlying conformal field theory describing the physical properties. This conjecture applies whenever the ground-state wave function is expressed in some special basis (conformal basis). Its formulation comes mainly from numerical evidences on exactly integrable quantum chains. In this paper, the above conjecture was tested for several general nonintegrable quantum chains. We introduce new families of self-dual $Z(Q)$ symmetric quantum chains ($Q = 2,3,\ldots$). These quantum chains contain nearest-neighbor as well next-nearest-neighbor interactions (coupling constant p). In the cases $Q = 2$ and $Q = 3$, they are extensions of the standard quantum Ising and three-state Potts chains, respectively. For $Q = 4$ and $Q \geqslant 5$, they are extensions of the Ashkin-Teller and $Z(Q)$ parafermionic quantum chains. Our studies indicate that these models are interesting on their own. They are critical, conformally invariant, and share the same universality class in a continuous critical line. Moreover, our numerical analysis for $Q = 2$–8 indicate that the Shannon mutual information exhibits the conjectured behavior irrespective if the conformally invariant quantum chain is exactly integrable or not. For completeness we also calculated, for these new families of quantum chains, the two existing generalizations of the Shannon mutual information, which are based on the Rényi entropy and on the Rényi divergence.

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I. INTRODUCTION

The connection between the quantum correlations and the entanglement properties of quantum many-body systems provided us, in recent years, a powerful tool to detect [1] and classify quantum phase transitions (see Ref. [2] and references therein). Several measures of the entanglement were proposed along the years, like the von Neumann and Rényi entanglement entropies [2–4], the concurrence [5], the fidelity [6], etc. Among these measures the von Neumann and Rényi entanglement entropies are the most popular since in one dimension, where most of the critical chains are conformally invariant, they provide a way to calculate the central charge of the underlying conformal field theory (CFT), identifying the universality class of critical behavior. Although interesting proposals were presented [7–10], it is quite difficult to measure these quantities in the laboratory, and the central charge of a critical chain has never been measured experimentally.

An interesting measure that is also efficient in detecting quantum phase transitions is the Shannon mutual information. This quantity differently from the previous mentioned measures is based on the measurements of observables. It measures the shared information among parts of a quantum system. Consider a quantum chain with L sites that we split into two subsystems $\mathcal{A}$ and $\mathcal{B}$, formed by consecutive ℓ and $L-\ell$ sites, respectively. Suppose the quantum chain is in the quantum state given by the wave function $|\Psi_{\mathcal{A}U\mathcal{B}}\rangle = \sum_{n,m} c_{n,m}|\phi^n_{\mathcal{A}}\rangle \otimes |\phi^m_{\mathcal{B}}\rangle$, where $\{|\phi^n_{\mathcal{A}}\rangle\}$ and $\{|\phi^m_{\mathcal{B}}\rangle\}$ are the basis spanning the subsets $\mathcal{A}$ and $\mathcal{B}$. The Shannon mutual information of the subsets $\mathcal{A}$ and $\mathcal{B}$ is defined as

$$I(\mathcal{A},\mathcal{B}) = Sh(\mathcal{A}) + Sh(\mathcal{B}) - Sh(\mathcal{A}U\mathcal{B}), \tag{1}$$

where $Sh(\chi) = -\sum_x p_x \ln p_x$ is the standard Shannon entropy of the subsystem χ with probability p_x of being in the configuration x. The probability of the configurations in the subsets $\mathcal{A}$ and $\mathcal{B}$ are given by the marginal probabilities $p_{|\phi^n_{\mathcal{A}}\rangle} = \sum_m |c_{n,m}|^2$ and $p_{|\phi^m_{\mathcal{B}}\rangle} = \sum_n |c_{n,m}|^2$, respectively. It is important to notice that differently from the von Neumann entanglement entropy and the von Neumann mutual information, which are basis independent, the Shannon entropy Sh and the Shannon mutual information $I(\mathcal{A},\mathcal{B})$ are basis dependent quantities. In Ref. [11], it was conjectured that, for periodic critical quantum chains in their ground state, the Shannon mutual information shows universal features provided the ground state is expressed in some special bases, called *conformal basis*. A given basis of the Hilbert space of the quantum chain is related to a certain boundary condition in the time direction of the underlying (1+1)-Euclidean CFT. In general, these time-boundary conditions destroy the conformal invariance in the bulk. The conformal basis are related to the boundary conditions that do not destroy the conformal invariance, as happens in the case of Dirichlet and Neumann boundary conditions. It was conjectured [11] that whenever the ground-state wave function is expressed in the conformal basis, the leading finite-size scaling behavior of the Shannon mutual information for large systems and subsystem sizes is given by

$$I(\ell,L-\ell) = \frac{c}{4}\ln\left[\frac{L}{\pi}\sin\left(\frac{\ell\pi}{L}\right)\right] + \gamma, \tag{2}$$

where c is the central charge of the underlying CFT and γ is a nonuniversal constant. It is interesting to note that this leading behavior is the same as the Rényi entanglement entropy with Rényi index $n = 2$ [12].

The above conjecture was tested analytically and numerically for a large number of exactly integrable quantum chains [11,13,14], namely, a set of coupled harmonic oscillators (Klein Gordon theory), the XXZ quantum chain, the Ashkin-Teller, the spin-1 Fateev-Zamolodchikov, the Q-state Potts

models ($Q = 2,3,4$), and the $Z(Q)$ parafermionic models ($Q = 5$–8). Up to now, except for the chain of coupled harmonic oscillators, this conjecture was only tested numerically. Moreover, all the tests for this conjecture were done for exactly integrable models. Since there is no general analytical results supporting this conjecture it is import to check if the existing numerical agreement is not just a consequence of the exact integrability of all the quantum chains tested so far. All the agreements obtained are reasonable taking into account the lattice sizes of the considered quantum chains. However, there exist a controversy in the case of the Ising quantum chain. A numerical analysis due to Stéphan [15] on this quantum chain indicates that the prefactor in (2), instead of being the central charge ($c = 0.5$ in this case) is a close number $b \approx 0.4801$. In the conclusions of this paper, we present additional discussions about this point.

In this paper, we are going to check the universality feature of the conjecture (2) by considering critical chains belonging to several universality classes of critical behavior but being *not exactly integrable*. The ground-state eigenfunction can only be calculated numerically for quantum chains of relatively small lattice sizes. It will be then interesting to consider nonintegrable quantum chains whose critical points are exactly known. For this sake, we introduce in this paper a set of generalized self-dual nonintegrable quantum chains whose exact critical points are given by their self-dual points. Moreover, each of these quantum chains seems to share the same symmetries and long-distance physics of an exactly integrable conformally invariant chain whose central charge c is exactly known. The validity of the conjecture (2) will imply that the Shannon mutual information of these models share the same asymptotic behavior.

We should also mention some additional studies of the Shannon and Rényi entropies and mutual information in quantum systems [16,17], and also in two-dimensional spin systems [18]. The paper is organized as follows. In the next section, we introduce the several new quantum chains and show their self-dual properties. In Sec. III, we present our results for the models in the universality class of the Ising model and three-state Potts model. In Sec. IV, the results for the models in the universality class of the $Z(Q)$-parafermionic models, with $Q = 4$, 5, 6, 7, and 8 are presented. We also consider in this section a numerical analysis for a generalization of the $Z(Q)$ clock models with $Q = 5$, 6, 7 and 8. In Sec. V, we calculate for these new quantum chains the two existing extensions of the Shannon mutual information: the Rényi mutual information and the less known generalized mutual information [14,19]. Finally, in Sec. VI, we present our conclusions.

II. THE $Z(Q)$ GENERALIZED SELF-SUAL QUANTUM CHAINS

We introduce initially a special generalization of the nearest-neighbor Ising quantum chain that also contains next-nearest-neighbor interactions. The Hamiltonian is given by

$$H^{(2)}(\lambda,p) = -\sum_i \left[\sigma_i^z\sigma_{i+1}^z + \lambda\sigma_i^x - p\left(\sigma_i^z\sigma_{i+2}^z + \lambda\sigma_i^x\sigma_{i+1}^x\right)\right], \tag{3}$$

where σ_i^z and σ_i^x are spin-$\frac{1}{2}$ Pauli matrices attached to the lattice sites ($i = 1,2,\ldots$), and λ and p are the coupling constants. At $p = 0$, the Hamiltonian (3) reduces to the standard nearest-neighbor quantum Ising chain, which is exactly integrable and critical at $\lambda = 1$.

In order to show that $H^{(2)}(\lambda,p)$ is self-dual, for any value of p, let us define the new operators

$$\rho_{2i}^{(e)} = \sigma_i^z\sigma_{i+1}^z \quad \text{and} \quad \rho_{2i-1}^{(o)} = \sigma_i^x, \quad i = 1,2,\ldots, \tag{4}$$

that obey the following commuting and anticommuting relations:

$$\left(\rho_i^{(e)}\right)^2 = \left(\rho_i^{(o)}\right)^2 = 1, \quad \left[\rho_i^{(o)},\rho_j^{(o)}\right] = \left[\rho_i^{(e)},\rho_j^{(e)}\right] = 0,$$
$$\left[\rho_i^{(o)},\rho_j^{(e)}\right] = 0, \quad \text{unless } |i-j| = 1,$$
$$\left\{\rho_i^{(e)},\rho_j^{(o)}\right\} = 0, \quad \text{if } |i-j| = 1. \tag{5}$$

In terms of these new operators, the Hamiltonian (3) is given by

$$H^{(2)}(\lambda,p) = -\sum_i \left[\rho_{2i}^{(e)} + \lambda\rho_{2i-1}^{(o)} + p\left(\rho_{2i}^{(e)}\rho_{2i+2}^{(e)} + \lambda\rho_{2i-1}^{(o)}\rho_{2i+1}^{(o)}\right)\right]. \tag{6}$$

We now make a transformation by defining the new operators:

$$\tilde\rho_{2i}^{(e)} = \rho_{2i+1}^{(o)}, \quad \tilde\rho_{2i-1}^{(o)} = \rho_{2i}^{(e)}. \tag{7}$$

It is simple to see that these new operators obey the same commutation relations as the old ones, given in (5). In terms of these new operators, the Hamiltonian (3) is now given by

$$H^{(2)}(\lambda,p) = -\lambda\sum_i \left[\tilde\rho_{2i}^{(e)} + \frac{1}{\lambda}\tilde\rho_{2i-1}^{(o)} + p\left(\tilde\rho_{2i}^{(e)}\tilde\rho_{2i+2}^{(e)} + \frac{1}{\lambda}\tilde\rho_{2i-1}^{(o)}\tilde\rho_{2i+1}^{(o)}\right)\right]. \tag{8}$$

Consequently, apart from a boundary term[1] [20] that could be neglected as the lattice size increases, the model is self-dual:

$$H^{(2)}(\lambda,p) = \lambda H^{(2)}\left(\frac{1}{\lambda},p\right). \tag{9}$$

Implying that the low-lying eigenlevels in the eigenspectrum of both sides of (9) become identical as the lattice size increases. Since we have no reason to expect more than a single $Z(2)$ critical point for a fixed value of p, this model should be critical at $\lambda = 1$ and, *at least* for $p \leqslant p_c$ (with p_c finite), the model should share the same universality class as the standard quantum Ising chain $H^{(2)}(1,0)$. Actually, for $p \to \infty$, the model is $Z(2)\otimes Z(2)$ symmetric due to the commutations of $H^{(2)}(\lambda, p\to\infty)$ with the nonlocal $Z(2)$ operators $\mathcal{P}^{(e)} = \prod_i \sigma_{2i}^x$ and $\mathcal{P}^{(o)} = \prod_i \sigma_{2i-1}^x$, and therefore is not in the Ising universality class.

[1]This transformation for finite lattices will produce constraints among the operators $\{\rho_i^{(o)},\rho_i^{(e)}\}$ and the exact relation for finite chains only relate sectors of the associated Hilbert space.

Similarly as we did for the Ising quantum chain, we now introduce the self-dual generalized next-nearest-neighbor $Z(Q)$ models ($Q = 2,3,\ldots$). They describe the dynamics of the $Q \times Q$ matrices $\{S_i\}$, $\{R_i\}$, attached on the lattice sites $i = 1,2,\ldots$, and obey the algebraic relations

$$S_i^Q = R_i^Q = 1, \quad [S_i, S_j] = [R_i, R_j] = 0,$$
$$[S_i, R_j] = 0 \quad \text{if } i \neq j \quad \text{and} \quad S_i R_i = e^{i\frac{2\pi}{Q}} R_i S_i. \quad (10)$$

The Hamiltonian we introduce is given by

$$H^{(Q)}(\lambda,\{\alpha\}) = -\sum_i \left[\sum_{n=1}^{Q} \alpha_n \left(S_i^n S_{i+1}^{Q-n} + \lambda R_i^n\right) + p \sum_{n=1}^{Q} \alpha_n \left(S_i^n S_{i+2}^{Q-n} + \lambda R_i^n R_{i+1}^n\right)\right], \quad (11)$$

where λ and $\{\alpha_n\}$ ($n = 1,\ldots,Q$) are coupling constants. We chose real coupling constants and $\alpha_n = \alpha_{Q-n}$ to ensure the hermiticity of the Hamiltonian. This Hamiltonian reduces to (3) for $Q = 2$.

We now consider the $Z(Q)$ operators:

$$\rho_{2i}^{(e)} = S_i S_{i+1}^{Q-1} \quad \text{and} \quad \rho_{2i-1}^{(o)} = R_i, \quad i = 1,2,\ldots, \quad (12)$$

that obey the following algebraic relations:

$$\left(\rho_i^{(e)}\right)^Q = \left(\rho_i^{(o)}\right)^Q = 1, \quad \left[\rho_i^{(e)}, \rho_j^{(e)}\right] = \left[\rho_i^{(o)}, \rho_j^{(o)}\right] = 0,$$
$$\left[\rho_i^{(e)}, \rho_j^{(o)}\right] = 0 \text{ unless } |i-j| = 1,$$
$$\rho_i^{(e)} \rho_{i\pm1}^{(o)} = e^{\mp i\frac{2\pi}{Q}} \rho_{i\pm1}^{(o)} \rho_i^{(e)}. \quad (13)$$

In terms of these operators, we have

$$H^{(Q)}(\lambda,\{\alpha\}) = -\sum_i \left\{\sum_{n=1}^{Q-1} \alpha_n \left[\left(\rho_{2i}^{(e)}\right)^n + \lambda \left(\rho_{2i-1}^{(o)}\right)^n\right] + p \sum_{n=1}^{Q-1} \alpha_n \left[\left(\rho_{2i}^{(e)} \rho_{2i+2}^{(e)}\right)^n + \lambda \left(\rho_{2i-1}^{(o)} \rho_{2i+1}^{(o)}\right)^n\right]\right\}. \quad (14)$$

We now perform the same canonical transformation $\rho \to \tilde{\rho}$, given by (7). It is simple to verify that the transformation is canonical since the commutation's relations of the new operators are the same as the old ones. The Hamiltonian is now given by

$$H^{(Q)}(\lambda,\{\alpha\}) = -\lambda\left\{\sum_{n=1}^{Q-1} \alpha_n \left[\left(\tilde{\rho}_{2i}^{(e)}\right)^n + \frac{1}{\lambda}\left(\tilde{\rho}_{2i-1}^{(o)}\right)^n\right] + p \sum_{n=1}^{Q-1} \alpha_n \left[\left(\tilde{\rho}_{2i}^{(e)} \tilde{\rho}_{2i+2}^{(e)}\right)^n + \frac{1}{\lambda}\left(\tilde{\rho}_{2i-1}^{(o)} \tilde{\rho}_{2i+1}^{(o)}\right)^n\right]\right\}. \quad (15)$$

Comparing (14) and (15), we obtain, apart from a boundary term [18],

$$H^{(Q)}(\lambda,\{\alpha\}) = \lambda H^{(Q)}\left(\frac{1}{\lambda},\{\alpha\}\right). \quad (16)$$

The particular choice $\alpha_n = \frac{1}{\sin(\frac{\pi n}{Q})}$, $n = 1,2,\ldots,Q-1$ gives us an interesting family of quantum chains that we are going to study in the next sections. At their self-dual point ($\lambda = 1$), these Hamiltonians are given by

$$H^{(Q)}(p) = -\sum_i \left\{\sum_{n=1}^{Q-1} \frac{1}{\sin(\frac{\pi n}{Q})}\left[S_i^n S_{i+1}^{Q-n} + R_i^n + p\left(S_i^n S_{i+2}^{Q-n} + R_i^n R_{i+1}^n\right)\right]\right\}. \quad (17)$$

These Hamiltonians at $p = 0$ are critical, conformal invariant, and exactly integrable. They correspond for $Q = 2,3$ to the two-state and three-state Potts models, for $Q = 4$, it is the Ashkin-Teller model with a special value of its anisotropy, and for $Q > 4$, they correspond to the $Z(Q)$ parafermionic models [21]. For $p \neq 0$, the models lose their exact integrability but we do expect that, at least for small values of the parameter p, they stay critical and in the same universality class of the related $p = 0$ exactly integrable quantum chain. For large values of p, this may not be true since, as happened in the Ising case, for $p \to \infty$, the symmetry increases from a single $Z(Q)$ to a $Z(Q) \times Z(Q)$.

III. RESULTS FOR THE EXTENDED ISING AND THREE-STATE POTTS QUANTUM CHAINS

We present in this section our numerical results for the generalized self-dual Ising and three-state Potts quantum chains whose Hamiltonians $H^{(Q)}(p)$ are given by (17) with the values $Q = 2$ and $Q = 3$, respectively. At $p = 0$, these models are exactly integrable and conformally invariant, being ruled by a CFT with central charge $c = 1/2$ and $c = 4/5$, respectively. Our aim is to compute the Shannon mutual information for the values of the parameter ($p \neq 0$) where the models are still critical but not exactly integrable. Since we are testing a conjecture we should initially confirm the expectation that the models, for small values of the parameter p are still critical and in the same universality class as the $p = 0$ exactly integrable quantum chain.

A first test of the critical universality for the quantum chains can be done by comparing their central charge c calculated directly from the finite-size behavior of the ground-state energy and low-lying energy gaps. The ground-state energy $E_0(L)$ of a conformally invariant quantum chain with periodic boundary should have the asymptotic behavior [22]:

$$\frac{E_0}{L} = e_\infty - v_s \frac{\pi c}{6L^2} + o(L^{-2}), \quad (18)$$

where e_∞ is the energy per site in the bulk limit and v_s is the sound velocity. The sound velocity can be extracted from the leading finite-size behavior of the first energy gap related to a given primary operator of the underlying CFT [23]. For example, the lowest energies $E_1(p)$ in the eigensector with $Z(Q)$ charge $q = 1$ and momentum $P = 0, \frac{2\pi}{L}, \frac{4\pi}{L}, \ldots$ are associated to the $Z(Q)$-magnetic operators of these models. We have then the estimate $v_s(L)$ for the sound velocity [24]

$$v_s(L) = \frac{L[E_1(\frac{2\pi}{L}) - E_1(0)]}{2\pi} + o(L^{-1}),$$

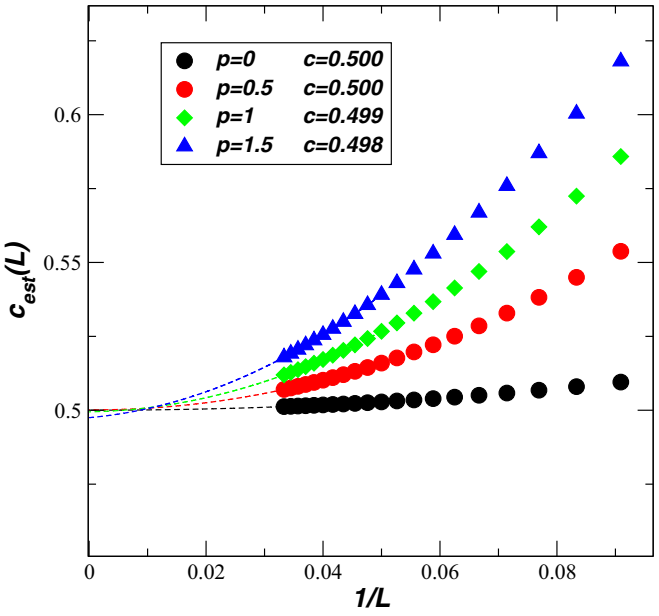

FIG. 1. The estimate $c_{\rm est}(L)$ given by (19) as a function of $1/L$ for the extended self-dual Ising model given by the Hamiltonian (3), and for the values of the parameter $p = 0$, 0.5, 1, and 1.5. The estimated values $c_{\rm est}(L \to \infty) = c$, shown in the figure, were obtained from a quadratic fit by considering the lattice sizes $20 \leqslant L \leqslant 30$.

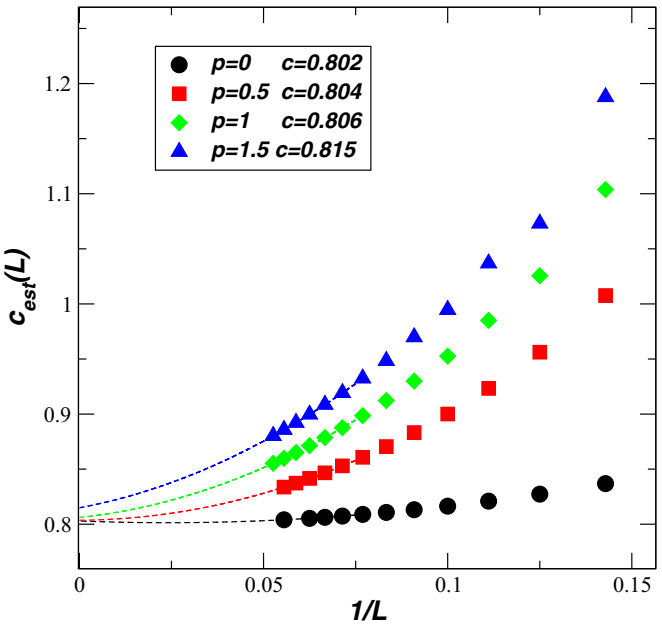

FIG. 2. The estimate $c_{\rm est}(L)$ given by (19), as a function of $1/L$, for the extended three-state Potts quantum chain by the Hamiltonian (17) and for the values of the parameter $p = 0$, 0.5, 1, and 1.5. The estimated values $c_{\rm est}(L \to \infty) = c$, shown in the figure, were obtained from a quadratic fit by considering the lattice sizes $14 \leqslant L \leqslant 19$.

that together with (18) give us an estimate for the central charge of the quantum chain:

$$c_{\rm est}(L) = -\frac{\frac{E_0(L)}{L} - \frac{E_0(L-1)}{L-1}}{\frac{1}{L^2} - \frac{1}{(L-1)^2}} \frac{12}{L\left(E_1\left(\frac{2\pi}{L}\right) - E_1(0)\right)} + o(L^{-1}). \tag{19}$$

In Figs. 1 and 2, we illustrate our results for the estimate $c_{\rm est}(L)$ in the extended self-dual Ising and three-state Potts models, respectively. We consider the models with the parameter $p =$ 0, 0.5, 1, and 1.5, and lattice sizes up to $L_{\rm max} = 30$ for the Ising case and $L_{\rm max} = 19$ for the three-state Potts case. We also show in the figures the estimated results $c_{\rm est}(L \to \infty)$ for the central charge c. They were obtained by considering a simple quadratic fit of $c_{\rm est}(L)$ for $30 \leqslant L \leqslant 20$ in the Ising case and $19 \leqslant L \leqslant 11$ in the three-state Potts case. The numerical results in these figures indicate that for the parameters $p \lesssim 1.5$, the extended models stay in the same universality class of the related $p = 0$ exactly integrable model, i.e., $c = 1/2$ ad $c = 8/10$ for the Ising and three-state Potts models, respectively.

A second test can be done by calculating the von Neumann entanglement entropy $S_{vN}(\ell, L)$ of subsystems with sizes ℓ and $(L - \ell)$ in the quantum chains. Its finite-size scaling behavior, for a periodic chain, is giving by [25–27]

$$S_{vN}(\ell, L-\ell) = \frac{c}{3} \ln\left[\frac{L}{\pi} \sin\left(\frac{\ell\pi}{L}\right)\right] + k, \tag{20}$$

where k is a constant. In order to calculate $S_{vN}(\ell, L)$, from a given ground-state wave function, we should fully diagonalize the reduced density matrix of the subsystems (dimension $Q^\ell \times Q^\ell$). This brings an extra numerical limitation since we can only handle the complete diagonalization of matrices with dimensions smaller than ∼6000. We are then restricted for the $Q = 2$ ($Q = 3$) model with sublattices sizes $\ell \leqslant 12$ ($\ell \leqslant 7$).

In Fig. 3 (Fig. 4), we show, for several values of p, $S_{vN}(\ell, L)$ as a function of $\sin(\frac{L}{\pi} \sin(\frac{\pi}{L}))/3$ for the $Q = 2$ ($Q = 3$)

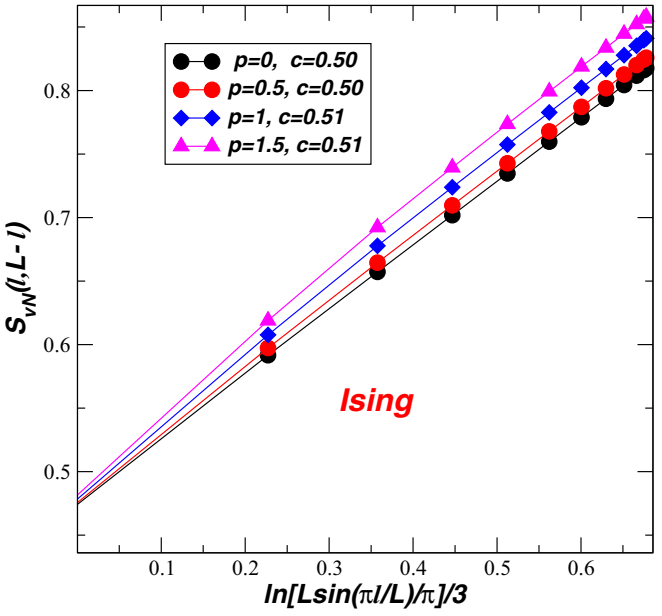

FIG. 3. The von Neumann entropy for the extended self-dual Ising model (3) with $L = 24$ sites and the parameter values $p =$ 0, 0.5, 1, and 1.5. The estimated values for the central charge are shown. They were obtained from a linear fit [see (20)], considering the sublattice sizes $\ell = 5$–12.

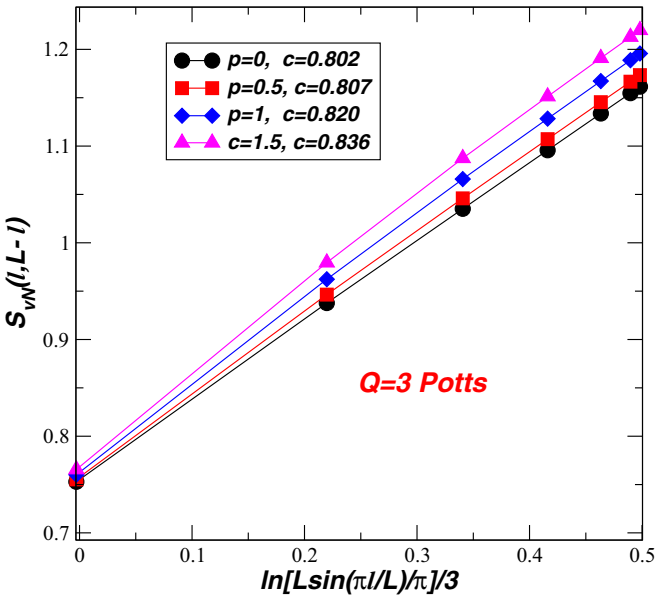

FIG. 4. The von Neumann entropy for the extended three-state Potts model (17) with $L = 14$ sites and the values of the parameter $p = 0$, 0.5, 1, and 1.5. The estimated values for the central charge are shown. They were obtained from a linear fit [see (19)], considering the sublattice sizes $\ell = 4$–7.

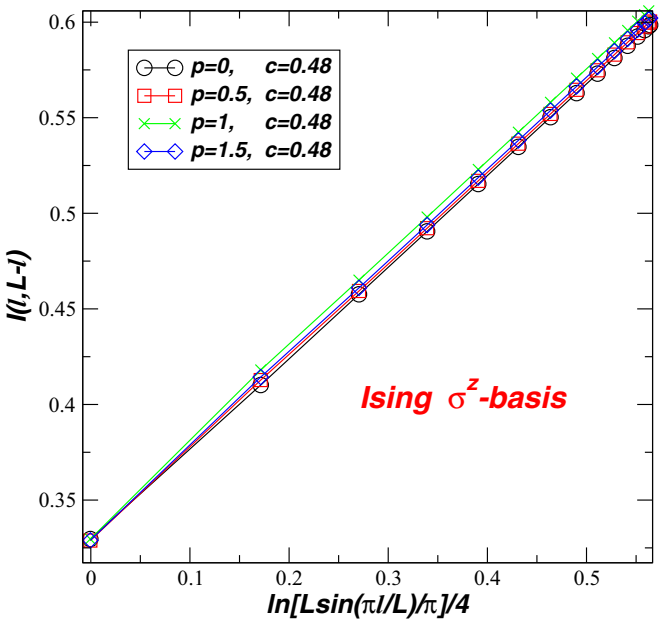

FIG. 5. The Shannon mutual information $I(\ell, L-\ell)$, as a function of $\ln[L\sin(\pi\ell/L)/\pi]/4$, for the extended self-dual Ising quantum chain (3), with the values of the parameter $p = 0$, 0.5, 1, and 1.5. The results are obtained for the ground-state wave function of the $L = 30$ sites quantum chain expressed in the basis where $\{\sigma_i^z\}$ are diagonal. The estimated results, based on the conjecture (2) are also shown. They were obtained from a linear fit by considering all the sublattices sizes.

extended quantum chains with $L = 24$ ($L = 14$) sites. We also show in these figures the estimated values of the central charge obtained from a linear fit. These results clearly indicate that these quantum chains are indeed critical, and share the same universality class of critical behavior as the exactly integrable quantum chain $p = 0$, whose central charge is $c = 0.5$.

Once we have convinced ourselves about the universal behavior of these nonintegrable quantum chains for $0 \leqslant p \lesssim 1.5$, we can now test the universal behavior (2) claimed for the Shannon mutual information $I(\ell, L-\ell)$ of periodic quantum chains in their ground states.

The Shannon mutual information depends on the particular basis we chose to express the ground-state wave function. The previous results [11,13], based on exactly integrable quantum chains, indicate that two good basis, where the universal behavior are shown, are the basis where either the "kinetic interactions" or the "static interactions" are diagonal. In the set of models, we are testing these basis are the ones where the operators $\{S_i\}$ or $\{R_i\}$ are diagonal.

In Figs. 5 and 6, the Shannon mutual information is shown for the extended Ising chain (3) with $L = 30$ sites and for values of the parameter $p = 0$, 0.5, 1, and 1.5. The results of Fig. 5 (Fig. 6) are obtained from the ground-state wave function given in the $\{\sigma^z\}$ basis ($\{\sigma^x\}$ basis). We clearly see in these figures a linear behavior indicating $\ln[L\sin(\pi\ell/L)]$ as the finite-size scaling function. The estimated values of the central charge $c = 0.48$–0.50, are also close to the expected value $c = 1/2$. These estimates were obtained from a linear fit by considering all the sublattice sizes.

In Figs. 7 and 8, we show the Shannon mutual information for the extended $Z(3)$ models with the values of the parameter $p = 0$, 0.5, 1, and 1.5. In Fig. 7 (Fig. 8), the quantum chain has $L = 18$ ($L = 19$) sites and is in the basis where the matrices $\{S_i\}$ ($\{R_i\}$) are diagonal, respectively. The linear fit obtained by using all the sublattice sizes predicts the value for the central charge $c \approx 0.77$–0.79. These values are close to the predicted value $c = 8/10$, indicating the validity of the conjecture (2) even for nonintegrable quantum chains. It is interesting to

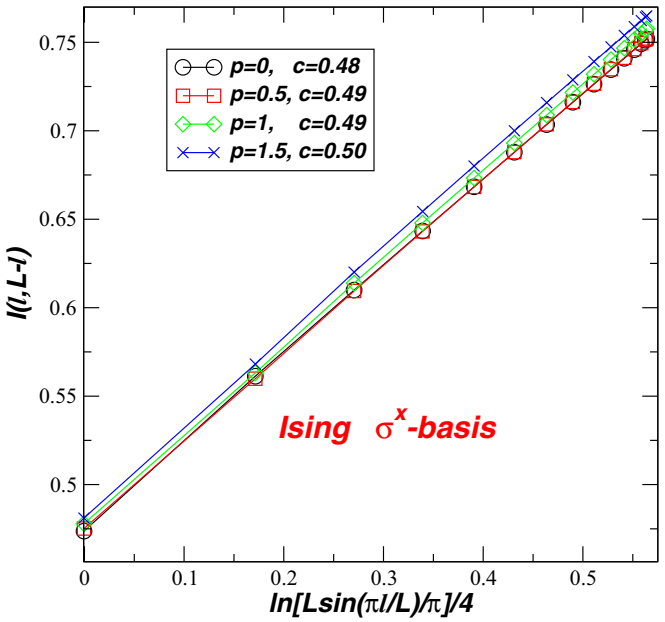

FIG. 6. Same as in Fig. 5 but with the ground-state wave function expressed in the basis where $\{\sigma_i^x\}$ are diagonal.

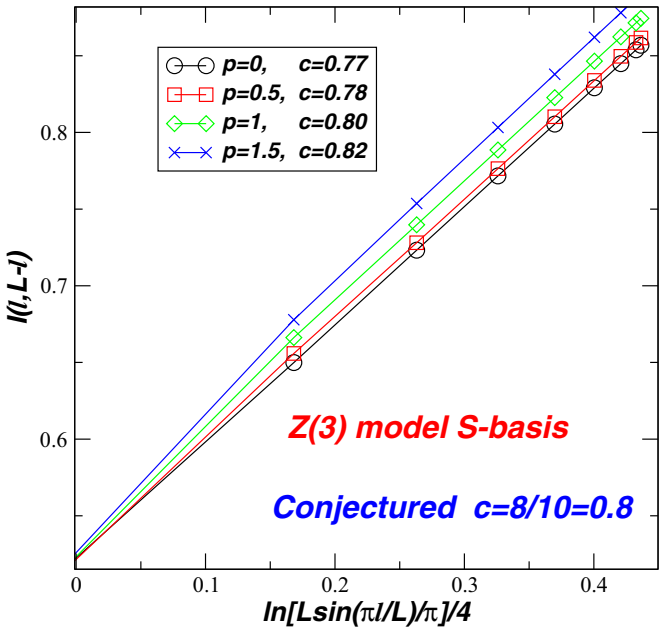

FIG. 7. The Shannon mutual information $I(\ell, L-\ell)$, as a function of $\ln[L\sin(\pi\ell/L)/\pi]/4$, for the extended $Q=3$ self-dual Potts quantum chain (17), with the values of the parameter $p=0$, 0.5, 1, and 1.5. The results are obtained for the ground-state wave function of the $L=18$ sites quantum chain, expressed in the basis where $\{S_i^z\}$ are diagonal. The estimated results, based on the conjecture (2) are also shown. They were obtained from a linear fit by considering all the sublattice sizes.

notice that differently from the calculation of $S_{vN}(\ell, L)$, it is not necessary to fully diagonalize reduced matrices and we could calculate $I(\ell, L-\ell)$ for larger lattice sizes, namely,

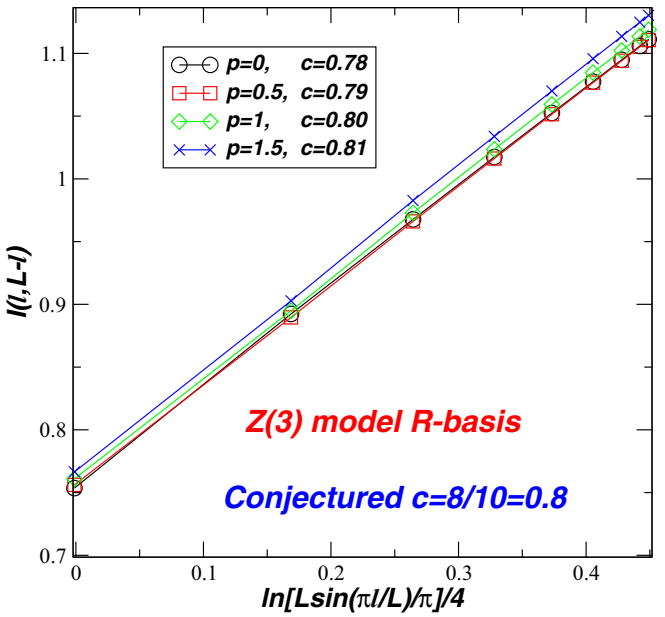

FIG. 8. Same as Fig. 7 but for lattice size $L=19$ and the results are obtained from the ground-state wave function expressed in the $\{R_i\}$ basis.

$L=30$ and 19 for the extended Ising and three-state Potts chains, respectively.

IV. RESULTS FOR THE EXTENDED Z(Q)-PARAFERMIONIC QUANTUM CHAINS

We consider in this section the numerical tests of the conjecture (2) for the extended nonintegrable $Z(Q)$-parafermionic models (17). The cases where the parameter $p=0$ reduces to the known exactly integrable $Z(Q)$-parafermionic quantum chains [21], which are critical and conformally invariant with conformal central charges:

$$c=\frac{2(Q-1)}{Q+2}, \quad Q=2,3,\ldots. \tag{21}$$

The cases $Q=2$ and 3 are the Ising and three-state Potts models considered in the last section. The quantum chain with $Q=4$ corresponds to a particular anisotropy of the $c=1$ critical line of the quantum Ashkin-Teller chain. The cases $Q>4$ are the $Z(Q)$-parafermionic quantum chains with central charge $c>1$. Actually, these last models are multicritical points and are expected to be endpoints [21, 28] of critical lines belonging to massless phases with central charge $c=1$ and belonging to the Berezinskii-Kosterlitz-Thouless universality class [28,29].

The Shannon mutual information for the extended $Q=4$ quantum chain with the values of $p=0$, 0.5, 1, and 1.5 is shown in Fig. 9. The calculations were done by expressing the ground-state wave function either in the S basis ($L=14$) or in the R basis ($L=13$). The linear fit, using all the sublattice sizes, gives the estimated values of the central charge shown in the figure $c\approx 0.97$–1.03, which within the numerical accuracy corroborates the conjecture (2).

Let us now consider the extended models with $Q>4$. Since the $p=0$ models are multicritical it is not clear if the nonintegrable quantum chains, although critical, will stay in the same universality class as the integrable model $p=0$. *Surprisingly*, this seems to be the case. In Figs. 10, 11, 12, and 13, we show for some values of p the Shannon mutual information for the quantum chains with $Q=5$, 6, 7, and 8, respectively. The calculation were done for the ground-state wave function expressed in the basis where either $\{S_i\}$ or $\{R_i\}$ are diagonal. The lattice sizes used are given in the figure captions. The estimated values for the central charge are give in the figure and were obtained from a linear fit, where all the sublattice sizes are considered. They are close to the predicted values: $c=8/7=1.14285\ldots$ ($Q=5$), $c=5/4=1.25$ ($Q=6$), $c=4/3=1.333\ldots$ ($Q=7$), and $c=7/5=1.4$ ($Q=8$). Taking into account the lattice sizes we could calculate, these results indicate that the models are still in the same universality class of the multicritical point ($p=0$), at least for the values of parameters $0<p\lesssim 1$. These results test the universal character of the conjecture (2), corroborating its validity for nonintegrable critical quantum chains.

Before closing this section let us do an additional test for the conjecture (2). For $Q\geqslant 5$, the $Z(Q)$ family of clock quantum chains (which is related to the time-continuum limit of the 2D classical clock models [30]) is known to have, besides a disordered and ordered phases, an intermediate massless phase

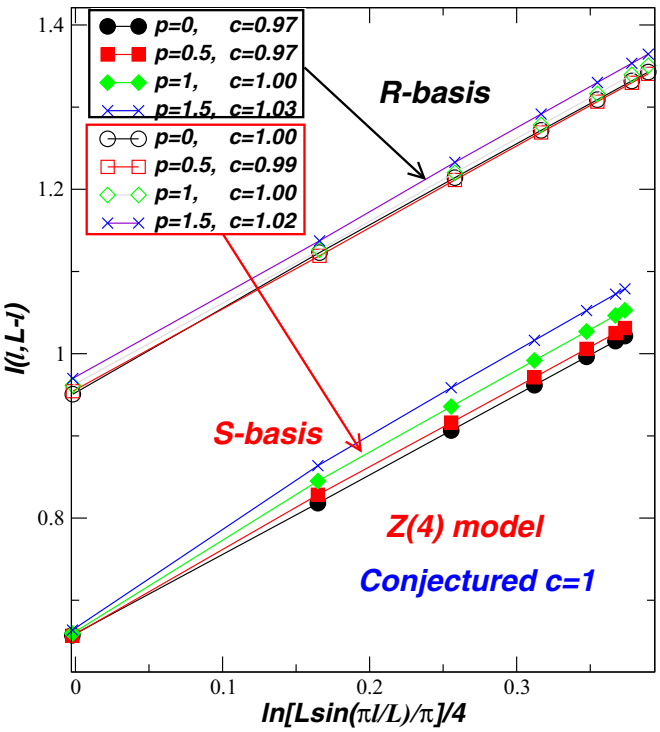

FIG. 9. The Shannon mutual information $I(\ell, L-\ell)$, as a function of $\ln[L\sin(\pi\ell/L)/\pi]/4$ for the extended $Q=4$ self-dual quantum chain (17), with the values of the parameters $p=0$, 0.5, 1, and 1.5. The results were obtained for the lattice size $L=15$ and 14, when the ground-state wave function spanned in the basis where $\{S_i\}$ and $\{R_i\}$ are diagonal, respectively. The estimated values shown in the figure were obtained from a linear fit by considering all the sublattice sizes.

belonging to the Berezinskii-Kosterlitz Thouless universality and are expected to be ruled by a CFT with central charge $c=1$ [28,29]. These models, although not exactly integrable, are self-dual. Their self-dual points belong to the intermediate $c=1$ CFT. Exploring the general results of Sec. II, similarly as we did for the $Z(Q)$-parafermionic models, we can extend the standard clock models by choosing in (11) $\alpha_n=\delta_{n,1}+\delta_{n,Q-1}$ for $(n=1,\ldots,Q-1)$. At its self-dual point, the extended clock models are given by

$$H_{\rm clock}(p)=-\sum_i[S_iS_{i+1}^{+}+S_i^{+}S_{i+1}+R_i+R_i^{+} + p(S_iS_{i+2}^{+}+S_i^{+}S_{i+2}+R_iR_{i+1}+R_i^{+}R_{i+1}^{+})], \tag{22}$$

where, as before, S_i and R_i are the $Z(Q)$ matrices with algebraic relations given by (10). At $p=0$, these Hamiltonians reduce to the standard $Z(Q)$ clock quantum chains. Our numerical results indicate that for arbitrary values of $0\leqslant p\leqslant 1$ the models share the same $c=1$ CFT. In Fig. 14, we show our tests for the Shannon mutual information $I(\ell, L-\ell)$ for the $Z(Q)$ clock model with $Q=5$, 6, 7, and 8. We only present the results in the case where the ground-state wave function is expressed in the $\{R_i\}$ basis. In this figure, for each value of Q, the data are for the values of the parameter $p=0$, 0.5, and 1. We clearly see the linear dependence with

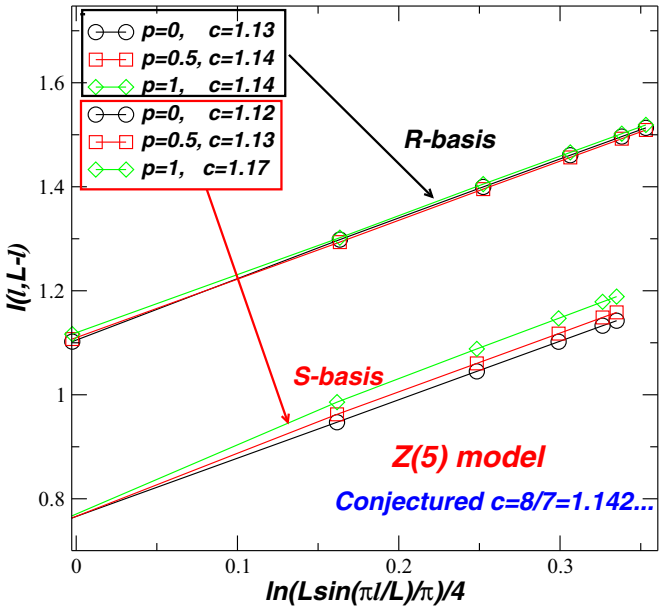

FIG. 10. The Shannon mutual information $I(\ell, L-\ell)$, as a function of $\ln[L\sin(\pi\ell/L)/\pi]/4$ for the extended $Q=5$ self-dual quantum chains (17), with the values of the parameters $p=0$, 0.5, and 1. The results were obtained for the lattice sizes $L=12$ and 13, when the ground-state wave function are in the basis where $\{S_i\}$ and $\{R_i\}$ are diagonal, respectively. The estimated values shown in the figure were obtained from a linear fit by considering all the sublattice sizes.

$\ln[L\sin(\pi\ell/L)]/4$. The linear fit, by considering all the values of p, and sublattice sizes for a given $Z(Q)$ model, give us estimates of the central charge in the range $c=1.03$–1.04, that

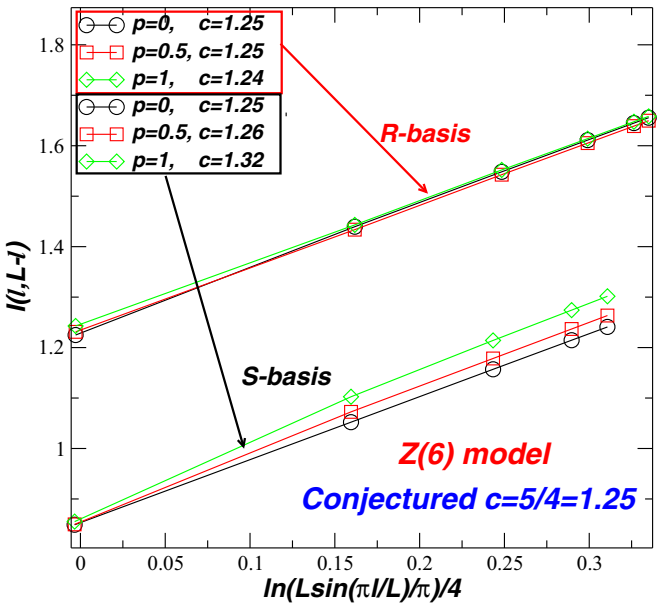

FIG. 11. Same as Fig. 10 for the extended $Z(6)$ sef dual quantum chain (17). The lattice sizes are $L=12$ and 13 for the basis where $\{S_i\}$ and $\{R_i\}$ are diagonal, respectively.

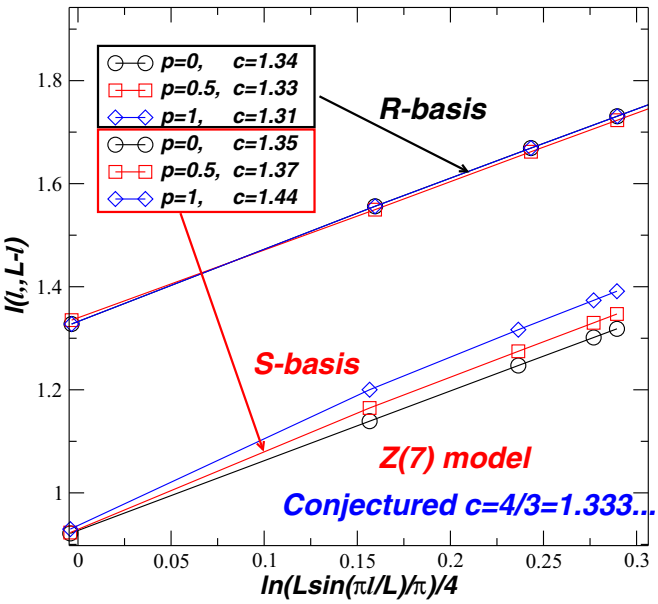

FIG. 12. Same as Fig. 10 for the extended $Z(7)$ self-dual quantum chain (17). The lattice sizes are $L = 11$ and 12 for the basis where $\{S_i\}$ and $\{R_i\}$ are diagonal, respectively.

are close to the expected value $c = 1$, indicating the validity of the conjecture (2).

V. GENERALIZED MUTUAL INFORMATIONS

A crucial step in deriving most of the analytical results (e.g., Refs. [27,31]) for the von Neumann entanglement entropy come from two facts. The Shannon entropy is obtained from the $n \to 1$ limit of the n-Rényi entanglement entropy, and at this limit the replica trick, used for the conformal

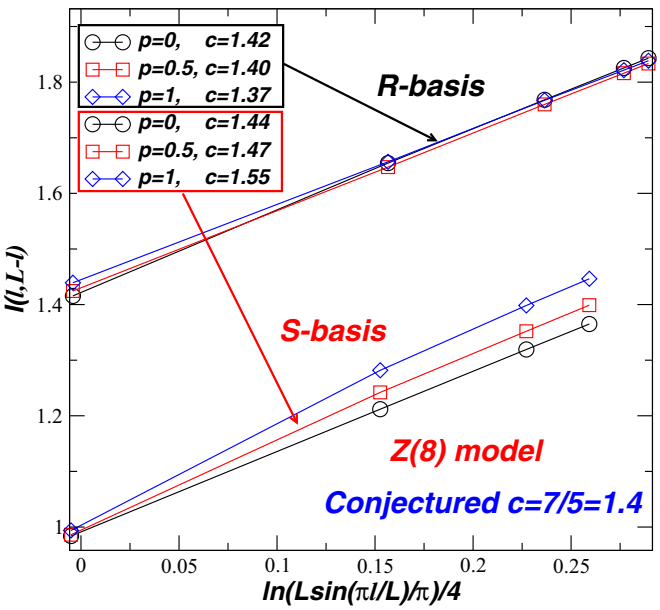

FIG. 13. Same as Fig. 10 for the extended $Q = 8$ self-dual quantum chain (17). The lattice sizes are $L = 10$ and 11 for the basis where $\{S_i\}$ and $\{R_i\}$ are diagonal, respectively.

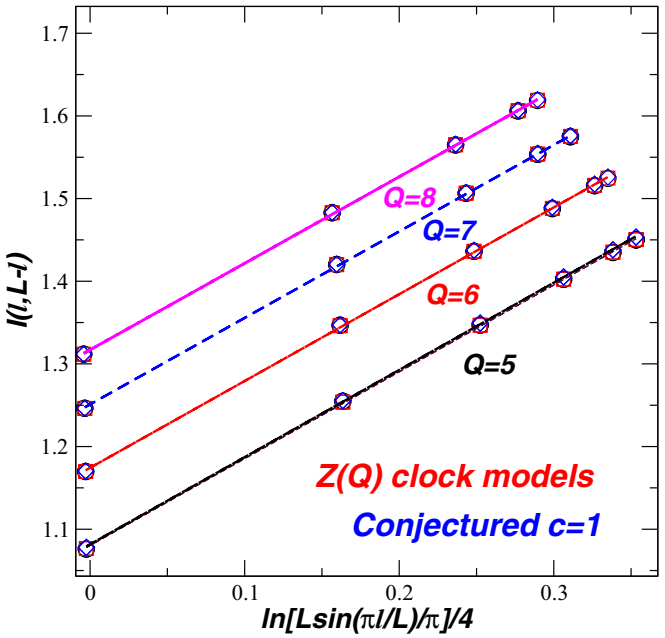

FIG. 14. The Shannon mutual information for the extended $Z(Q)$ clock models defined in (22), for the values of $Q = 5$, 6, 7, and 8, and lattice sizes $L = 13$, 12, 11, and 10, respectively. For each $Z(Q)$ model, the results are for the values of the parameter $p = 0$, 0.5, and 1. The calculations were done for the ground state spanned in the $\{R_i\}$ basis. The lines are the linear fit considering all the points for a given $Z(Q)$ model.

transformations, is regular. There exist two generalizations of the Shannon mutual information considered in the early sections. These extensions are based either on the Rényi entropy or on the Rényi divergence [19]. Previous numerical calculations on exactly integrable quantum chains [13,14] show numerical evidence that these quantities, when computed on the ground-state wave functions of critical chains expressed in a special basis (conformal basis), exhibit some universal features. It is then interesting to compute these generalized mutual information for the extended $Z(Q)$ models introduced in this paper and test the universal behavior for those critical nonintegrable quantum chains.

In order to define the generalized mutual information let us split, as before, the quantum chain $\mathcal{C}$ with L sites in the subsystems $\mathcal{A}$ and $\mathcal{B}$ formed by ℓ and $(L-\ell)$ consecutive sites, respectively. We now consider the quantum chain in the normalized ground state, with wave function $|\Psi_{\mathcal{C}}\rangle = \sum_{\{I_{\mathcal{A}},I_{\mathcal{B}}\}} a_{I_{\mathcal{A}},I_{\mathcal{B}}} |I_{\mathcal{A}}\rangle \otimes |I_{\mathcal{B}}\rangle$, where $|I_{\mathcal{A}}\rangle = |i_1, i_2, \ldots, i_\ell\rangle$ and $|I_{\mathcal{B}}\rangle = |i_{\ell+1}, \ldots, i_L\rangle$ are the local basis for the subsystems $\mathcal{A}$ and $\mathcal{B}$. The Rényi entropy for the entire system $\chi = \mathcal{C}$ and the subsystems $\chi = \mathcal{A}$ or $\chi = \mathcal{B}$ is given by

$$Sh_n(\chi) = \frac{1}{1-n} \sum_{\{I_\chi\}} \ln P^n_{I_\chi}, \quad \chi = \mathcal{A},\mathcal{B},\mathcal{C}, \tag{23}$$

where for the entire system $P_{I_{\mathcal{C}}} = |a_{I_{\mathcal{A}},I_{\mathcal{B}}}|^2$ and for the subsystems $\mathcal{A}$ and $\mathcal{B}$, $P_{I_{\mathcal{A}}} = \sum_{I_{\mathcal{B}}} |a_{I_{\mathcal{A}},I_{\mathcal{B}}}|^2$ and $P_{I_{\mathcal{B}}} = \sum_{I_{\mathcal{A}}} |a_{I_{\mathcal{A}},I_{\mathcal{B}}}|^2$, respectively. The Rényi mutual information is the shared information among the subsystems measured in terms of the

Rényi entropy (23), i.e.,

$$I_n(\ell, L-\ell) = Sh_n(\ell) + Sh_n(L-\ell) - Sh_n(L), \qquad (24)$$

where instead of denoting the subsystem, we denote their lattice sizes. At the limiting case $n \to 1$, the Rényi entropy and the Rényi mutual information reduces to the Shannon entropy and the Shannon mutual information, respectively.

Previous calculations of $I_n(\ell, L-\ell)$ for the ground-state wave functions of several exactly integrable chains show the same finite-size scaling function for arbitrary values of n:

$$I_n(\ell, L-\ell) = c_n \ln\left(\frac{L}{\pi}\sin\left(\frac{\ell\pi}{L}\right)\right) + k, \qquad (25)$$

where k is a $o(1)$ constant. As happens with the Shannon mutual information $I(\ell, L-\ell)$, this behavior is not general, it happens only when the ground-state wave function is expressed on the special basis (conformal basis). The coefficients c_n besides their n dependence also depend on the conformal basis considered. Under certain plausible assumptions, the large-n behavior of c_n is known analytically [32]. However, in the general case, the limiting case $n \to 1$ is singular, preventing a general analytical calculation of the Shannon mutual information $I_1(\ell, L-\ell) = I(\ell, L-\ell)$.

Our numerical analysis for the extended self-dual $Z(Q)$ models introduced in Sec. II indicates the same universal finite-size scaling behavior shown in (25). This confirmation was done for the values of the parameter p that we believe the model share the universality class of critical behavior of the corresponding exactly integrable model ($p = 0$). For brevity, we only show the results for the self-dual extended Ising models (3). In Figs. 15 and 16, the results are for the quantum chain with $L = 30$ sites and the ground-state wave function spanned in the conformal bases where $\{\sigma_i^z\}$ or $\{\sigma_i^x\}$ are diagonal. In theses figures we show the coefficient c_n obtained from the linear fit of (25), by using all the sublattice sizes. We can see that in both basis, apart from some small deviations, most probably due to the finite-size effects, the overall behavior of $I_n(\ell, L-\ell)$ is the same for different values of p, indicating the universal behavior of the models. It is clear from this figure that the singular behavior as $n \to 1$, already known [13] for the exactly integrable model ($p = 0$), also happens for the extended Ising quantum chains with $p \neq 0$.

Another interesting generalization of the Shannon mutual information, instead of being based in the Rényi entropy is based in the Rényi divergence [19]. Differently from the Rényi mutual information this generalized mutual information is always a positive function and is a more appropriate measure, from the point of view of information theory, of the shared information among subsystems. Using the notations in (23), this generalized mutual information is defined by

$$\tilde{I}_n(\ell, L-\ell) = \frac{1}{n-1}\ln\left(\sum_{\{I_A, I_B\}} \frac{P^n_{I_A, I_B}}{P^{n-1}_{I_A} P^{n-1}_{I_B}}\right). \qquad (26)$$

Like $I_n(\ell, L-\ell)$ this quantity, in the limiting case $n \to 1$, gives the Shannon mutual information. This quantity was measured for several exactly integrable quantum chains [14]. It shows the same universal finite-size scaling function given in (25) for $n \lesssim 2$ (we denote the linear coefficient as $\tilde{c}_n$).

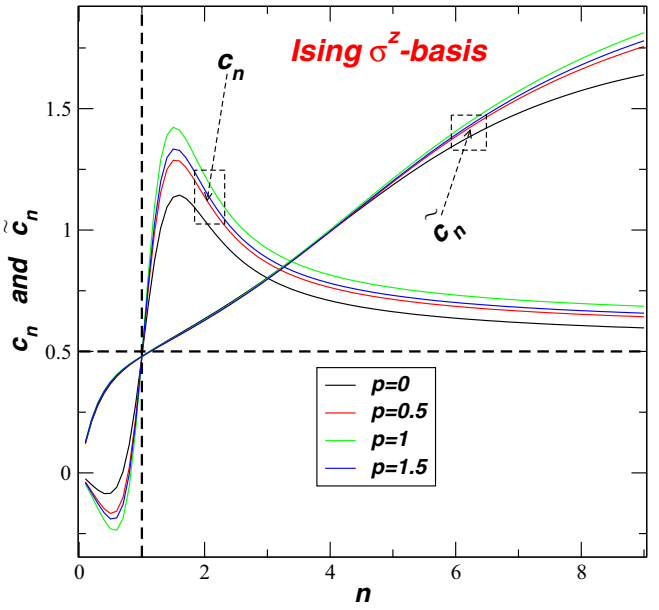

FIG. 15. The generalized mutual information for the ground-state wave function of the extended Ising chain (3), with $L = 30$ sites. The coefficients c_n and $\tilde{c}_n$ are obtained from the linear fit of (25) of the Rényi mutual information $I_n(\ell, L-\ell)$ (23) and (24) and from the generalized mutual information $\tilde{I}_n(\ell, L-\ell)$, given by (26), respectively. The ground sates of the quantum chains are expressed in the $\{\sigma^z\}$ basis and the values of the parameter $p = 0$, 0.5, 1, and 1.5.

We measured this quantity for the extended $Z(Q)$ models introduced in Sec. II. The results for the extended Ising quantum chain are shown in Figs. 15 and 16 for the ground-state wave function expressed in the $\{\sigma^z\}$ and $\{\sigma^x\}$ bases, respectively. Again, for $0 < n < 2$, we clearly see in both basis the independence of the curves with the parameter p of the

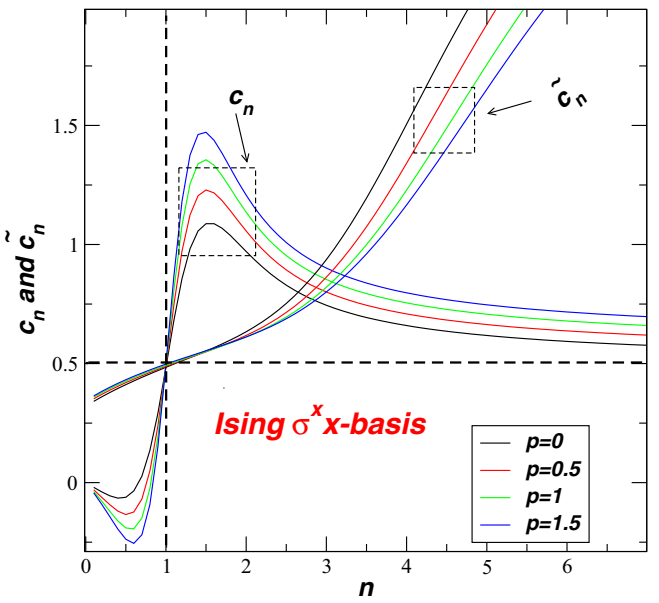

FIG. 16. Same as Fig. 15, but with the ground-state wave function spanned in the $\{\sigma^x\}$ basis.

nonintegrable quantum chain. Actually, the agreement of this behavior for several values of p is even better as compared with the case of the Rényi mutual information, this indicates that the finite-size scaling corrections in $\tilde{I}_n(\ell, L-\ell)$ are smaller than the ones in $I_n(\ell, L-\ell)$. It is also clearly shown that the limiting case $n \to 1$ is regular for all values of p, differently from the case of the Rényi mutual information. This imply that $\tilde{I}_n(\ell, L-\ell)$, as compared with $I_n(\ell, L-\ell)$ is a more suitable quantity for an analytical approach towards the proof of the conjecture (2).

VI. CONCLUSIONS

In this paper, we made an extensive test of the conjecture (2) for the Shannon mutual information $I(\ell, L-\ell)$ of conformally invariant quantum critical chains at their ground states. In general, the Shannon mutual information depends on the particular basis where the wave function is spanned. According to the conjecture (2), the finite-size scaling function of $I(\ell, L-\ell)$ give us an interesting tool for calculating the central charge c, if the ground state is spanned in the conformal basis. These basis corresponds, in the underlying Euclidean CFT, to the boundary condition in the time direction that do no destroy the conformal invariance of the CFT.

This paper provides us with the first extensive numerical check of the universal character of (2). The previous tests of (2) were done only for exactly integrable quantum chains, and since there is no analytical proof of (2) it is important to verify if its validity is not connected to the exact integrability of the critical quantum chains tested previously.

In order to produce tests for nonintegrable models, we introduced new families of self-dual quantum chains with nonlocal $Z(Q)$ symmetries. Due to their self-duality, their critical points are exactly known. All these nonintegrable quantum chains contains next-nearest-neighbor coupling constants p. Our numerical analysis concentrated in two special families of models. The first family is the generalization of the $Z(Q)$ parafermionic models ($Q = 2$–8), and the second one is the generalization of the $Z(Q)$ clock models ($Q = 5$–8). The first family at $p = 0$ reduces to the exactly integrable parafermionic quantum chains with central charge $c = \frac{1}{2}, \frac{4}{10}, 1, \frac{8}{7}, \frac{5}{4}, \frac{4}{3}, \frac{7}{5}$, for $Q = 2$–8, respectively. The second family reduces at $p = 0$ to nonintegrable quantum chains in the Beresinzkii-Kosterlitz Thouless universality, whose underlying CFT is expected to have a central charge $c = 1$ for $Q \geqslant 5$. Exploring the consequences of conformal invariance, our numerical studies of the low-lying energies of these quantum chains, at finite lattice sizes, indicate that at least for a finite range of the couplings $0 \leqslant p \leqslant p_c$ the models share the same universal critical behavior, and consequently are ruled by the same CFT.

The last observation makes these introduced quantum chains even more interesting, since as we change continuously the parameter p they give a critical line with a fixed value of the central charge. In particular, the extended parafermionic quantum chains for $Q \geqslant 5$ give us critical lines ruled by an underlying $Z(Q)$ parafermionic CFT with $c > 1$. The extensive calculations of the Shannon mutual information $I(\ell, L-\ell)$ of the ground-state wave functions of all these quantum chains indicate the validity of the conjecture (2) for general critical and conformally invariant quantum chains, irrespective of being exactly integrable or not.

It is important to mention that Stéphan [15] presented a contradictory prediction for the critical Ising quantum chain. In Ref. [15], by exploring the free-fermionic nature of the model, $I(\ell, L-\ell)$ was calculated numerically up to lattice sizes $L = 36$, and the results indicate that the pre-factor in (2) instead of being the central charge $c = 0.5$, is the close, but distinct number $c = 0.4801629(2)$. This would imply that the conjecture (2) is not valid and the prefactor is a universal unknown number whose value is close to the central charge, at least for the Ising case. All the numerical results we have obtained so far for several quantum chains do not have enough precision to discard the possibility that for all the critical chains the prefactor in the conjecture (2) could not be the central charge c, but a number close to it. The single exact analytical calculation we have is for the set of coupled harmonic oscillators that gives in this case the central charge value $c = 1$ [11]. The result in Ref. [15] was obtained by assuming that the finite-size corrections of $I(\ell, L-\ell)$ are given by the power series $\sum_{p=0}^{5} \alpha_p / \ell^p$, being the fitting quite stable indicating no presence of logarithmic corrections, like $\frac{\ln \ell}{\ell}$ terms.

As is well known in order to have a controlled prediction of quantities in the bulk limit, based on finite-size lattice estimators we should know the functional dependence of the finite-size corrections with the lattice size. Unfortunately, this is not the case for $I(\ell, L-\ell)$. This is an essential point. $I(\ell, L-\ell)$ is calculated by combining the probabilities $p_{\{x\}}$ of the configuration $\{x\}$ in the subsystem of size ℓ. The probabilities for special configurations of the Ising quantum chain can be calculated for quite large lattices $L \sim 1000$. The results for $\epsilon(\{x\}) = -\ln p_{\{x\}}$, also called the formation probabilities, show that for special commensurable configurations $\{x\}$, like the emptiness formation probability and generalizations (see Appendix of Ref. [17]), indicate that correction terms $\frac{\ln \ell}{\ell}$ are always present. If as a result of the combinations of the several probabilities in $I(\ell, L-\ell)$ these logarithmic corrections are canceled then the prediction of Stéphan [15] is correct and the conjecture has to be modified. On the other hand, if still these corrections are present in $I(\ell, L-\ell)$, then we should consider lattice sizes or order $L \sim 1000$ to discard or to confirm the conjecture (2). This is indeed a quite interesting point to be settled in the future. It is a challenge either to derive analytically $I(\ell, L-\ell)$ or at least to derive the behavior of the finite-size corrections.

There exist two extensions of the Shannon mutual information, namely The Rényi mutual information $I_n(\ell, L-\ell)$ and the generalized mutual information $\tilde{I}_n(\ell, L-\ell)$, based on the Rényi divergence. These quantities were calculated previously for several exactly integrable quantum chains in their ground state. As the Shannon mutual information they also show some universal features whenever the ground-state wave function is spanned in a conformal basis. We calculate the generalizations $I_n(\ell, L-\ell)$ and $\tilde{I}_n(\ell, L-\ell)$ for the nonintegrable models introduced in this paper. Our results indicate that the universal features previously observed [13,14] does not depend if the quantum chain is exactly integrable or not. It is important to mention that, as happens for the exactly integrable cases [14], $\tilde{I}_n(\ell, L-\ell)$ in general does not have a divergence as

$n \to 1$, differently from the generalization $I_n(\ell, L-\ell)$. Since this divergence destroys the analytical continuation $n \to 1$, the quantity $\tilde{I}(\ell, L-\ell)$ seems to be more appropriate for an analytical derivation for the conjecture (2) for the Shannon mutual information $\tilde{I}_1(\ell, L-\ell) = I(\ell, L-\ell)$.

ACKNOWLEDGMENTS

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