

Universal Behavior of the Shannon Mutual Information of Critical Quantum Chains

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We consider the Shannon mutual information of subsystems of critical quantum chains in their ground states. Our results indicate a universal leading behavior for large subsystem sizes. Moreover, as happens with the entanglement entropy, its finite-size behavior yields the conformal anomaly c of the underlying conformal field theory governing the long-distance physics of the quantum chain. We study analytically a chain of coupled harmonic oscillators and numerically the Q -state Potts models ($Q = 2, 3$, and 4), the XXZ quantum chain, and the spin-1 Fateev-Zamolodchikov model. The Shannon mutual information is a quantity easily computed, and our results indicate that for relatively small lattice sizes, its finite-size behavior already detects the universality class of quantum critical behavior.

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Entanglement measures have emerged nowadays as powerful tools for the study of quantum many body systems [1,2]. In one dimension, where most quantum critical systems have their long-distance physics ruled by a conformal field theory (CFT), the entanglement entropy has been proved the most important measure of entanglement. It allows one to identify the distinct universality classes of critical behaviors. Let us consider a periodic quantum chain with L sites and partition the system into subsystems \mathcal{A} and \mathcal{B} of length ℓ and $L - \ell$, respectively. The entanglement entropy is defined as the von Neumann entropy of the reduced density matrix $\rho_{\mathcal{A}}$ of the partition \mathcal{A} : $S_{\ell} = -\text{Tr}_{\mathcal{A}} \rho_{\mathcal{A}} \ln \rho_{\mathcal{A}}$. If the system is critical and in the ground state, in the regime where the subsystems are large compared with the lattice spacing, S_{ℓ} is given by [3,4]

$$S_{\ell} = \frac{c}{3} \ln \left[\frac{L}{\pi} \sin \left(\frac{\pi \ell}{L} \right) \right] + \gamma_s, \quad (1)$$

where c is the central charge of the underlying CFT and γ_s is a nonuniversal constant. A remarkable fact is that even in the case where the system is in a pure state formed by an excited state, the conformal anomaly dictates the overall behavior of the entanglement, similarly as in Eq. (1) [5]. It is worth mentioning that recently many interesting methods were proposed [6–8] to calculate the entanglement entropy and ultimately central charge; however, up to now they have not been implemented experimentally. A natural question concerns the possible existence of other measures of shared information that, similarly as the entanglement entropy, are also able to detect the several universality classes of critical behavior of quantum critical chains.

In this Letter, we present results that indicate that the Shannon mutual information of local observables is such a measure. The Shannon mutual information of the subsystems \mathcal{A} and \mathcal{B} , of sizes ℓ and $L - \ell$, is defined as

$$I(\mathcal{A}, \mathcal{B}) \equiv \text{Sh}(\mathcal{A}) + \text{Sh}(\mathcal{B}) - \text{Sh}(\mathcal{A} \cup \mathcal{B}), \quad (2)$$

where $\text{Sh}(\mathcal{X}) = -\sum_x p_x \ln p_x$ is the Shannon entropy of the subsystem \mathcal{X} with probabilities p_x of being in a configuration x . These probabilities, in the case where \mathcal{A} is a subsystem of a quantum chain with wave function $|\Psi_{\mathcal{A} \cup \mathcal{B}}\rangle = \sum_{n,m} c_{n,m} |\phi_{\mathcal{A}}^n\rangle \otimes |\phi_{\mathcal{B}}^m\rangle$, are given by the marginal probabilities $p_{|\phi_{\mathcal{A}}^n\rangle} = \sum_m |c_{n,m}|^2$ of the subsystem \mathcal{A} , where $\{|\phi_{\mathcal{A}}^n\rangle\}$ and $\{|\phi_{\mathcal{B}}^m\rangle\}$ are the vector bases in subspaces \mathcal{A} and \mathcal{B} .

It is important to notice that the Shannon entropy and the Shannon mutual information are basis dependent quantities, reflecting the several kinds of observables we can evaluate in the system and subsystems. Since we are interested in the evaluation of local observables that can be measured in any of the subsystems (sizes $\ell = 1, \dots, L$), we consider the only vector basis obtained from the tensor product $\{|\phi_1\rangle \otimes |\phi_2\rangle \otimes \dots\}$ of the local spin basis $\{|\phi_i\rangle\}$ spanning the Hilbert space associated to the site i . In Ref. [9], it was conjectured that the mutual information, like the entanglement entropy, should follow the area law; see also Ref. [10]. Many authors studied the Shannon entropy of the one-dimensional quantum spin chains [11–13] and found useful applications in classifying one- and two-dimensional quantum critical points. Several authors also studied different properties of the Shannon mutual information in two-dimensional classical systems [14,15]. They found that although the mutual information of two halves of a cylinder has its maximum value at a temperature higher than the critical temperature, its derivative diverges at the critical temperature. Most recently, Um *et al.* [16] studied the mutual information of a subregion with respect to the rest in the periodic transverse Ising model and surprisingly found that it has the same dependence $\ln[\sin(\pi\ell/L)]$ as Eq. (1) but with a distinct multiplicative constant. In this Letter, we study the Shannon mutual information of local observables in different critical spin chains and argue about their possible connections to the central charge of the underlying CFT. Our results based on the study of several quantum chains suggest that for

periodic chains in the ground state, the Shannon mutual information in the scaling regime ($\ell, L \gg 1$) is universal and has a dependence with the subsystem size ℓ similar to the one of the entanglement entropy, i.e.,

$$I(\ell, L) = \frac{c}{4} \ln \left[\frac{L}{\pi} \sin \left(\frac{\pi \ell}{L} \right) \right] + \gamma_I, \quad (3)$$

where c is the central charge of the underlying CFT and γ_I is a nonuniversal constant. Up to the moment, in contrast with the entanglement entropy, there is no simple general field theoretical method to calculate the Shannon entropy and consequently the Shannon mutual information. The difficulty comes from the evaluation of the summation over the amplitudes of the ground-state eigenfunction.

In order to justify our conjecture (3), we calculate the Shannon mutual information for quantum systems in finite geometries. We first present our analytical results for a system of coupled harmonic oscillators (Klein-Gordon field theory) and then our numerical analysis for several critical quantum spin chains: the Q -state Potts model ($Q = 2, 3$, and 4), the spin-1/2 XXZ spin chain, and the spin-1 Fateev-Zamolodchikov model in the antiferromagnetic and ferromagnetic regimes.

Harmonic oscillator.—The Hamiltonian of L coupled harmonic oscillators with coordinates Φ_1, \dots, Φ_L and conjugated momenta π_1, \dots, π_L is given by

$$\mathcal{H} = \frac{1}{2} \sum_{n=1}^L \pi_n^2 + \frac{1}{2} \sum_{n,n'=1}^L \phi_n K_{nn'} \phi_{n'}, \quad (4)$$

where in the case of nearest-neighbor couplings the interaction K matrix is just the discrete Laplacian. In the continuum limit, the above Hamiltonian is the one of a simple scalar free field theory (central charge $c = 1$). Let us now consider $\Phi_{\mathcal{A}} = (\phi_1, \phi_2, \dots, \phi_\ell)$ and $\Phi_{\mathcal{B}} = (\phi_{\ell+1}, \phi_{\ell+2}, \dots, \phi_L)$ as the position vectors of the subsystems \mathcal{A} and \mathcal{B} and $\Pi_{\mathcal{A}, \mathcal{B}}$ the respective momentum vectors. The Shannon mutual information $I(\mathcal{A}, \mathcal{B}) \equiv I(\ell, L)$ between two regions \mathcal{A} and \mathcal{B} is

$$I(\ell, L) = \int d^L \Phi p(\Phi_{\mathcal{A}}, \Phi_{\mathcal{B}}) \ln \frac{p(\Phi_{\mathcal{A}}, \Phi_{\mathcal{B}})}{p_1(\Phi_{\mathcal{A}}) p_2(\Phi_{\mathcal{B}})}, \quad (5)$$

where $p(\Phi_{\mathcal{A}}, \Phi_{\mathcal{B}}) = |\Psi_0|^2$ is the total, and $p_1(\Phi_{\mathcal{A}}) = \int [\prod_{m \in \mathcal{B}} d\phi_m] |\Psi_0|^2$ and $p_2(\Phi_{\mathcal{B}}) = \int [\prod_{m \in (\mathcal{A})} d\phi_m] |\Psi_0|^2$ are the reduced probability densities in position space [$\Psi_0(\phi_1, \dots, \phi_L)$ is the ground-state wave function]. Then, after simple integrations, one gets [17] $I(\ell, L) = \sum_{i=1}^{\ell} \ln(2\nu_i)$, where ν_i are the eigenvalues of the matrix $C = \sqrt{X_{\mathcal{A}} P_{\mathcal{A}}}$, and $X_{\mathcal{A}}$ and $P_{\mathcal{A}}$ are $\ell \times \ell$ matrices describing correlations of position and momentum within subsystem \mathcal{A} [18]. In other words, for $0 < i, j < \ell + 1$, we have $(X_{\mathcal{A}})_{ij} := \langle \phi_i \phi_j \rangle = (1/2)(K^{-1/2})_{ij}$ and $(P_{\mathcal{A}})_{ij} := \langle \pi_i \pi_j \rangle = (1/2)(K^{1/2})_{ij}$. We noticed that the above formula is exactly equal to the quantum Rényi entanglement entropy with $n = 2$ [18], and consequently, using the

CFT techniques [4], one can get the following result for a periodic system

$$I(\ell, L) = \frac{1}{4} \ln \left[\frac{L}{\pi} \sin \left(\frac{\pi \ell}{L} \right) \right] + \gamma_I \quad (6)$$

that agrees with the conjecture (3). It is worth mentioning that the mutual Shannon information $I(\mathcal{A}, \mathcal{B})$ obtained in a momentum basis also follows the same formula.

Quantum Q -state Potts model.—The model in a periodic lattice is defined by the Hamiltonian [19]

$$H_Q = - \sum_{i=1}^L \sum_{k=0}^{Q-1} (S_i^k S_{i+1}^{Q-k} + \lambda R_i^k), \quad (7)$$

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 $S_j R_j = e^{i(2\pi/Q)} R_j S_j$ and $R_i^Q = S_i^Q = 1$. The system is critical at the self dual point $\lambda = 1$. For $Q = 2, 3$, and 4, its critical behavior is governed by a CFT with central charge $c = 1 - [6/m(m+1)]$ where $\sqrt{Q} = 2 \cos(\pi/m + 1)$. We first calculate the ground state of the Hamiltonian (7) for $Q = 2, 3$, and 4 in a different local spin basis by exact diagonalization. We verified for the critical chains we studied that, as the lattice size increases, the Shannon mutual information exhibits a dominant behavior, as conjectured in Eq. (3). In order to illustrate this result, we show in Fig. 1 the difference $I(\ell, L) - I(L/2, L)$ obtained from the ground state at the critical point of the $Q = 2, 3$, and 4 Potts models. The calculations were done by expressing the ground state in the basis where either the matrices R_i or S_i are diagonal. Apart from the initial point $\ell = 1$, we already see for these lattice sizes a quite good agreement among the results in both basis. In order to show the dominant ℓ dependence of $I(\ell, L)$ and test Eq. (3),

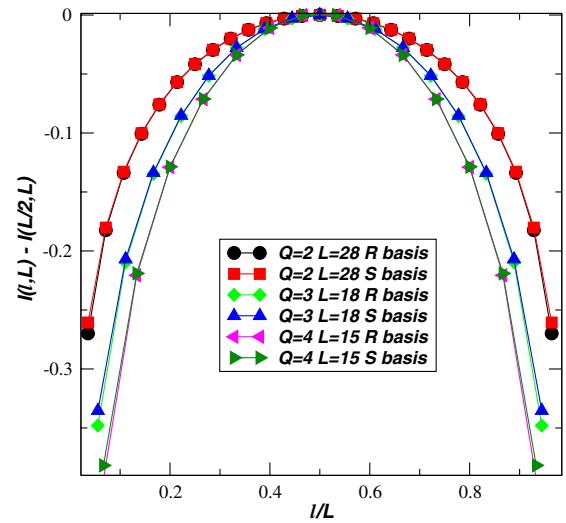


FIG. 1 (color online). $I(\ell, L) - I(L/2, L)$ as a function of the subsystem size for the $Q = 2, 3$, and 4 state Potts models in the R_i and S_i bases.

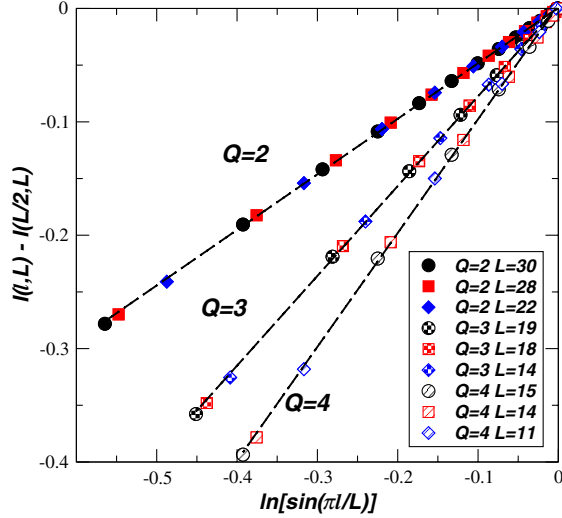


FIG. 2 (color online). Mutual information for the $Q = 2, 3,$ and 4 Potts models with different lattice sizes L . The dashed straight lines are obtained from the fitting by using the largest lattice size shown for each model. (The ground states were taken in the R_i basis.)

we consider the difference $I(\ell, L) - I(L/2, L)$, since in this case the nonuniversal constant γ_i is canceled. In Fig. 2, we plot this difference, as a function of $\ln[\sin(\pi\ell/L)/4]$, for some lattice sizes of the $Q = 2, 3,$ and 4 state Potts models. Clearly, the data of distinct lattice sizes collapse in a straight line in agreement with Eq. (3). The angular coefficient of these lines gives us the estimate $c(L)$, for lattice size L . In Table I, we give these estimates. The agreement with the predicted values is remarkable already for the lattice sizes we considered.

XXZ quantum chain.—The model describes the dynamics of spin-1/2 particles given by the Hamiltonian

$$H_{XXZ} = - \sum_{i=1}^L (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z), \quad (8)$$

where $\sigma^x, \sigma^y,$ and σ^z are spin-1/2 Pauli matrices and Δ an anisotropy. This model provides an interesting check for

TABLE I. Numerical values of the constant $c(L)$ for $Q = 2, 3, 4$ Potts models, the XXZ model (XXZ_Δ), and the Fateev-Zamolodchikov (FZ_γ^c) model. The expected values for the conformal anomalies together with the lattice sizes used in the numerical calculation are also shown.

	$Q = 2$	$Q = 3$	$Q = 4$	$XXZ_{-1/2}$	$XXZ_{1/2}$
c	1/2	4/5	1	1	1
$c(L)$	0.49	0.79	1.00	1.00	1.03
L	30	19	14	30	30
	XXZ_0	$FZ_{\pi/3}^1$	$FZ_{\pi/4}^1$	$FZ_{\pi/3}^{-1}$	$FZ_{\pi/3}^{-1}$
c	1	3/2	3/2	1	1
$c(L)$	1.02	1.53	1.47	1.03	1.06
L	30	20	20	20	20

the universal behavior of the Shannon mutual information. It has a continuous critical line $-1 \leq \Delta < 1$, whose CFT has a central charge $c = 1$. According to Eq. (3), we should expect a data collapse of $I(\ell, L) - I(L/2, L)$ for distinct lattice sizes and anisotropies.

In order to illustrate this fact, we plot in Fig. 3 the ratio $[I(\ell, L) - I(L/2, L)] / \{\ln[\sin(\pi\ell/L)/4]\}$ as a function of ℓ/L . We clearly see that for distinct anisotropies and lattice sizes, the ratio is close [20] to a constant value given by the conformal anomaly. Similarly as we did for the Potts models, the estimated values $c(L)$ for the anisotropies $\Delta = 0$ and $\Delta = \pm(1/2)$ are shown in Table I.

Fateev-Zamolodchikov model.—This is a spin-1 model whose Hamiltonian is given by [21]

$$H_{FZ} = \epsilon \sum_{i=1}^L \{ \sigma_i - (\sigma_i^z)^2 - 2(\cos \gamma - 1)(\sigma_i^\perp \sigma_i^z + \sigma_i^z \sigma_i^\perp - 2\sin^2 \gamma [(\sigma_i^z)^2 - 2(S_i^z)^2]) \}, \quad (9)$$

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 $\sigma_i = \vec{S}_i \vec{S}_{i+1} = \sigma_i^\perp + \sigma_i^z$. The model is antiferromagnetic for $\epsilon = +1$ and ferromagnetic for $\epsilon = -1$. This is an important check for the conjecture (3) since the model has a line of critical points ($0 \leq \gamma \leq (\pi/2)$) 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 $c = 3/2$ [22] while the ferromagnetic one is ruled by a $c = 1$ CFT [23].

In Fig. 4, we show for $\epsilon = \pm 1$ the ratio $[I(\ell, L) - I(L/2, L)] / \{\ln[\sin(\pi\ell/L)/4]\}$ as a function of ℓ/L . The data are shown for the anisotropies $\gamma = \pi/3$ and $\gamma = \pi/4$ and for lattice sizes $L = 18$ and $L = 20$. We clearly see an

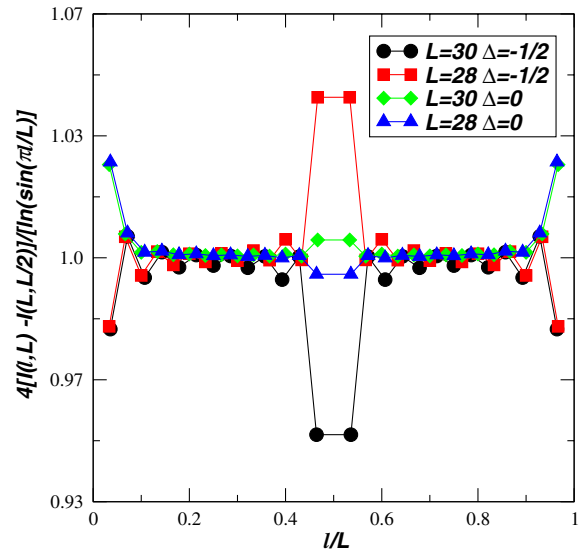


FIG. 3 (color online). Mutual information as a function of the subsystem size for the XXZ model with different values of the anisotropy Δ and lattice sizes L .

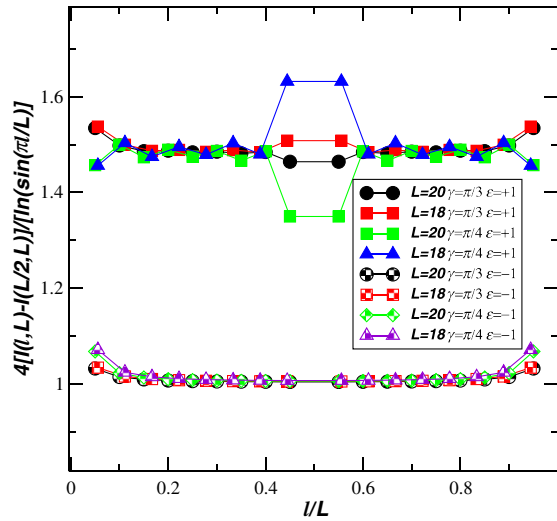


FIG. 4 (color online). Mutual information dependence with the subsystem size for the Fateev-Zamolodchikov model with different values of γ and lattice sizes.

agreement with the expected central charge of the corresponding CFT. In Table I, we give the predicted values $c(L)$, and the agreement is again quite good.

Conclusions.—All the analytical and numerical calculations presented in this Letter indicate the following properties for the Shannon mutual information of local observables for the ground state of critical quantum chains. (a) The leading dependence with the subsystem size ℓ characterizes the universality class of the critical behavior of the quantum chain. (b) The finite-size scaling function $\ln[(L/\pi)\sin(\pi\ell/L)]$ is the same as that of the entanglement entropy. (c) The finite-size scaling, similarly to the entanglement entropy, is proportional to the central charge of the underlying CFT. An overall illustration of these points is presented in Fig. 5, where we show for $2 \leq \ell < L - 1$ the finite-size behavior of the Shannon mutual information for the different models with central charge $c = 1$ presented in this Letter. This figure shows that models whose Hamiltonians act on rather distinct Hilbert spaces share the same universal behavior for the Shannon mutual information of their ground states. Our results indicate that the Shannon mutual information, similarly to the entanglement entropy, provides excellent tools for the evaluation of the central charge of conformal invariant quantum chains. Although the numerical results presented in this Letter are obtained by using the Lanczos method, we also verified that the Shannon mutual information can also be computed [24], for relatively large lattices, by using the density matrix renormalization group [25].

Finally, we mention that the conjecture (3) announced in this Letter raises several interesting questions to be answered in the future. The first one concerns its proof based on CFT calculations as done by Calabrese and Cardy [4] in the case of the entanglement entropy. In the case of

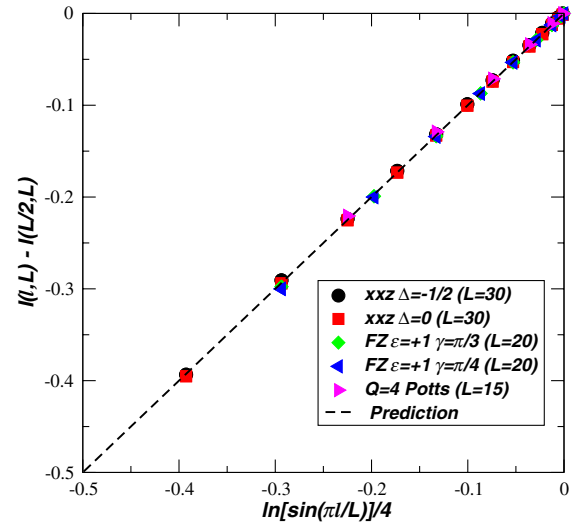


FIG. 5 (color online). Mutual information for some lattice sizes for the XXZ chain with anisotropies $\Delta = -1/2$ and $\Delta = 0$, the ferromagnetic spin-1 Fateev-Zamolodchikov model with anisotropies $\gamma = \pi/3$ and $\gamma = \pi/4$, and for the four-state Potts model. All these models are ruled by a CFT with conformal anomaly $c = 1$.

the harmonic oscillator chain, we show that in the bulk limit, the dominant part of the Shannon mutual information is the same as that of the $n = 2$ Rényi entanglement entropy. A proof of this equivalence would produce as a corollary the conjecture (3).

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