Entanglement of Low-Energy Excitations in Conformal Field Theory

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(Received 31 January 2011; published 17 May 2011)

In a quantum critical chain, the scaling regime of the energy and momentum of the ground state and low-lying excitations are described by conformal field theory (CFT). The same holds true for the von Neumann and Rényi entropies of the ground state, which display a universal logarithmic behavior depending on the central charge. In this Letter we generalize this result to those excited states of the chain that correspond to primary fields in CFT. It is shown that the *n*th Rényi entropy is related to a 2n-point correlator of primary fields. We verify this statement for the critical XX and XXZ chains. This result uncovers a new link between quantum information theory and CFT.

DOI: 10.1103/PhysRevLett.106.201601

PACS numbers: 11.25.Hf, 03.67.Bg, 03.67.Mn, 89.70.Cf

Entanglement is one of the central concepts in quantum physics since Schrödinger used the term in an answer to the Einstein-Podolsky-Rosen article in 1935. A particularly active line of research is concerned with the role played by entanglement in the physics of many-body systems [1]. One is typically interested in the amount of entanglement between two spatial partitions, say A and B, of a manybody system in its ground state. For a pure ground state the amount of entanglement is usually quantified with the entanglement entropy, or the von Neumann entropy of the reduced density matrix ρ_A : $S_A = -\text{tr}_A \rho_A \ln \rho_A$. Alternatively, the Rényi entropies S_n are also used: $(S_n)_A = \frac{1}{1-n} \ln r_A \rho_A^n$, the entanglement entropy being $\lim_{n\to 1} S_n$. One of the most important results in this topic is the celebrated area law [2–4], which, roughly speaking, states that ground states of gapped many-body systems with short-range interactions have an entanglement entropy proportional to the area of the hypersurface separating both partitions. The area law restricts the fraction of the Hilbert space accessible to ground states of local Hamiltonians in an essential way, allowing for their efficient numerical simulation [4].

Violations of the area law occur in gapless (critical) systems. In one dimension most of critical systems, as well as being gapless, are also conformal invariant. The attention to the entanglement properties on these systems came after the seminal result of Holzhey, Larsen and Wilczek [5], who showed that the leading behavior of the ground state entropies S_n^{gs} is proportional to the central charge of the underlying conformal field theory (CFT) governing the long-distance physics of the discrete quantum chain. If ℓ and N are the lengths of the partition A and of the total system, both measured in lattice spacing units, then the Rényi entropy of the ground state, with periodic boundary conditions, is [5–7]

$$S_n^{\rm gs}(\ell) = \frac{c(n+1)}{6n} \ln \left[\frac{N}{\pi} \sin\left(\frac{\pi\ell}{N}\right)\right] + \gamma_n, \qquad (1)$$

where *c* is the central charge of the CFT and γ_n is a nonuniversal constant.

In a critical model, the finite-size scaling of the energy of excitations is given by the scaling dimension of the corresponding conformal operators [8]. This fact suggests that also the entanglement entropy could be related to properties of these operators. Entanglement of excited states has been considered previously. In [9] it was shown that the negativity of the excited states in the *XXZ* critical model shows a universal scaling. In [10] it was shown that a violation of the area law should be expected for the low-lying excited states of critical quantum chains, and in [11], it was considered the entanglement of very large energy excitations in *XY* and *XXZ* spin chains.

In this Letter we show that the entropy S_n^{exc} of excited states associated to primary fields exhibits a universal behavior that generalizes (1). The energy of these lowlying states degenerate as 1/N in the bulk limit $N \to \infty$. We prove that the excess of entanglement, $S_n^{\text{exc}} - S_n^{\text{gs}}$, is a finite-size scaling function related to the 2n-point correlator of the primary field. These results are verified in two models: the XX and XXZ spin chains.

Entanglement of generic primary states.—Let us consider a system S of length N with periodic boundary conditions. To describe it, we introduce the complex variable $\zeta = \sigma + it$, where $0 \le \sigma \le N$ is the spatial coordinate and t is the time coordinate. S is split into two subsystems $S = A \cup B$, with $A = (\epsilon, \ell - \epsilon)$ and $B = (\ell + \epsilon, N - \epsilon)$, and where $\epsilon \ll \ell < N$ is a short-distance cutoff [5]. The world sheet of the past (t < 0), is a cylinder with two semidisks of radius ϵ cut out (denoted C and D in Fig. 1). The boundary of the world sheet of Fig. 1 is given by the union $A \cup C \cup B \cup D$. After the conformal transformations $\zeta \rightarrow w \rightarrow z$,

$$w = -\frac{\sin(\frac{\pi(\zeta-\ell)}{N})}{\sin(\frac{\pi\zeta}{N})}, \qquad z = \log w \tag{2}$$

0031-9007/11/106(20)/201601(4)

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FIG. 1 (color online). Riemann surfaces describing the past events in ζ and z. The distinguished point in z is the infinite past $\zeta_{\infty} = -i\infty$.

the ζ cylinder gets mapped into a strip of height π and width $d = 2 \log[\frac{N}{\pi\epsilon} \sin(\frac{\pi\ell}{N})]$; being *A*, *B*, *C*, *D* the boundaries of the strip in *z* space (see Fig. 1). Moreover, the point at the infinite past $\zeta_{\infty} = -i\infty$ gets mapped into $\zeta_{\infty} \rightarrow z_{\infty} = i\pi(1 - \ell/N)$. We shall consider the simplest excited states in a CFT, namely, the primary states, which are those generated acting on the vacuum $|0\rangle$ with a primary field $\Upsilon(\zeta, \overline{\zeta})$, with conformal weights (h, \overline{h}) ,

$$|\Upsilon\rangle = \lim_{\zeta,\bar{\zeta}\to -i\infty} \Upsilon(\zeta,\bar{\zeta})|0\rangle.$$
(3)

The wave function of this state $|\Upsilon\rangle$ is given by the path integral

$$\Psi_{XY}(\Upsilon) \propto \int \mathcal{D}\phi \,\Upsilon[\phi(z_{\infty})]e^{-\mathcal{A}(\phi)},\tag{4}$$

where ϕ denotes the local field whose Euclidean action is $\mathcal{A}(\phi)$. The field Y is a functional of ϕ , that is evaluated at the infinite past z_{∞} in Eq. (4) (recall Eq. (3)). X and Y denote the values of the field ϕ in the subsystems A and B respectively. Periodic boundary conditions are imposed on the C and D edges [5]. If Y were not primary, then Eq. (4) would include additional terms generated by the conformal transformations (2).

The density matrix $\rho \equiv \rho_A$ of subsystem A is obtained by tracing over the variables in B:

$$\rho_{XX'}(\mathbf{Y}) \propto \int \mathcal{D}Y \Psi_{XY}(\mathbf{Y}) \Psi^*_{YX'}(\mathbf{Y}). \tag{5}$$

Plugging (4) into (5) one finds

$$\rho_{XX'}(\mathbf{Y}) = \frac{\int \mathcal{D}\phi \,\mathbf{Y}[\phi(z_{\infty})] \mathbf{Y}^*[\phi(z'_{\infty})] e^{-\mathcal{A}(\phi)}}{Z(1) \langle \mathbf{Y}(z_{\infty}) \mathbf{Y}^{\dagger}(z'_{\infty}) \rangle}, \quad (6)$$

where $z'_{\infty} = i\pi(1 + \ell/N)$ represents the point at the infinite future. The functional integral is over a strip of height 2π and width *d*, with boundary conditions $\phi = X$ on the lower edge and $\phi = X'$ on the upper edge. The normalization factor is determined by the condition $\text{tr}\rho = 1$, which implies that Z(1) is the functional integral with no operator insertion and the top and bottom edges of the strip being identified (i.e. a torus partition function), and $\langle YY^{\dagger} \rangle$ is the two point correlator on this torus. To compute the entanglement entropy one first computes the trace of ρ_Y^n , which is given by

$$\operatorname{tr} \rho_{\Upsilon}^{n} = \frac{Z(n)}{Z(1)^{n}} \frac{\prod_{k=0}^{n-1} \langle \Upsilon(z_{\infty} + 2i\pi k) \Upsilon^{\dagger}(z_{\infty}' + 2i\pi k) \rangle_{\tau_{n}}}{\langle \Upsilon(z_{\infty}) \Upsilon^{\dagger}(z_{\infty}') \rangle_{\tau_{1}}^{n}},$$
(7)

where Z(n) denotes the partition function on a torus of lengths $2\pi n$ and d, so that the moduli parameter is given by $\tau_n = 2\pi i n/d$, and where $\langle \ldots \rangle_{\tau_n}$ denotes the expectation value in the τ_n torus. Notice that the 2*n*-point correlator of fields Y, Y[†] depends on the ratio ℓ/N and on the moduli parameter.

To further proceed one uses the expression of the partition function Z(n) of a general CFT with central charge c for chiral and antichiral sectors of the theory, $Z(n) = Z(\tau, \bar{\tau}) = \text{tr}q^{L_0 - (c/24)}\bar{q}^{\bar{L}_0 - (c/24)}$, with the nome $q = \bar{q} = \exp(2\pi i \tau)$. In the limit $d \gg 1$, it is convenient to perform the modular transformation $\tau \rightarrow -1/\tau$. The partition function is modular invariant and can be easily evaluated in terms of the nome $\tilde{q} = e^{-2\pi i/\tau} = e^{-d/n}$ [5]. In particular, for the ground state $(Y_0 = \mathbf{1})$ one gets (up to a model-dependent factor $c_n = e^{(1-n)\gamma_n}$):

tr
$$\rho_{\Upsilon_0}^n = \frac{Z(n)}{Z(1)^n} \sim e^{c/12(1/n-n)d} = \left[\frac{N}{\pi\epsilon} \sin\left(\frac{\pi\ell}{N}\right)\right]^{c/6(1/n-n)}$$
(8)

as anticipated in (1). In the general case, Eq. (7) depends on a 2*n*-point correlator of the fields Y and Y[†] on a cylinder of length $2\pi n$ along the time direction. It is now convenient to rescale this length to 2π . Afterwards, we shift the coordinates in which the fields are evaluated $z_j \rightarrow z_j - i\pi(1-x)/n$, where $x = \ell/N$. Finally, we exchange σ and t coordinates in such a way that $z_j = 2\pi j/n$ for Y and $z_j = 2\pi (j + x)/n$ for Y[†]. The ratio between the excited and the ground state traces, $F_Y^{(n)}(x) = \text{tr}\rho_Y^n/\text{tr}\rho_{Y_0}^n$, becomes, from (7)

$$F_{Y}^{(n)}(x) \equiv \frac{n^{-2n(h+\bar{h})} \langle \prod_{j=0}^{n-1} \Upsilon(\frac{2\pi j}{n}) \Upsilon^{\dagger}(\frac{2\pi (j+x)}{n}) \rangle_{\rm cy}}{\langle \Upsilon(0) \Upsilon^{\dagger}(2\pi x) \rangle_{\rm cy}^{n}}, \qquad (9)$$

where $\langle ... \rangle_{cy}$ denotes the expectation value in a cylinder of length 2π . The entanglement entropy for $|Y\rangle$ can then be computed using the replica trick: $S_1^{exc} = S_1^{gs} - \partial_n F_Y^{(n)}|_{n=1}$. The dependence of the entropies on the full operator spectrum of CFT was also observed in the ground state entropies of two disjoint segments of the quantum critical chains [12]. In the limit $x \ll 1$, the terms YY^{\dagger} appearing in (9) can be approximated by the operator product expansion (OPE) $Y \times Y^{\dagger} = \mathbf{1} + \Psi + \dots$, finding:

$$F_{\Upsilon}^{(n)}(x) \sim 1 + \frac{h + \bar{h}}{3} \left(\frac{1}{n} - n\right) (\pi x)^2 + O(x^{2\Delta_{\Psi}}),$$
 (10)

where Ψ is the operator with the smallest scaling dimension, Δ_{Ψ} . The term of order $x^{2\Delta_{\Psi}}$ depends on the OPE constants $C_{YY^{\dagger}}^{\Psi}$ and on the expectation values $\langle \Psi(0)\Psi(\frac{2\pi j}{n})\rangle_{\text{cyl}}$. If $\Delta_{\Psi} = 1$, this term is $O(x^2)$ as the first

one in Eq. (10), and eventually they may cancel one another, as we shall see in an example below. If $\Delta_{\Psi} \neq 1$ one could use (10) to infer the quantities $h + \bar{h}$, Δ_{Ψ} and $C_{YY^{\dagger}}^{\Psi}$ from the numerical computation of the entanglement.

Using $S_1^{\text{exc}} = S_1^{\text{gs}} - \partial_n F_Y^{(n)}|_{n=1}$, one finds, for the low-*x* behavior of the entanglement entropy $(\ell/N \ll 1)$:

$$S_1^{Y}(\ell) - S_1^{gs}(\ell) \sim \frac{2\pi^2}{3}(h+\bar{h})\left(\frac{\ell}{N}\right)^2 + O\left(\frac{\ell}{N}\right)^{2\Delta_{\Psi}}.$$
 (11)

Eqs. (9)–(11) are the main results of this Letter. They relate the von Neumann and *n*-Rényi entropy of the excitation represented by the primary operator Y to the 2*n*-point correlators of Y and Y[†] in the cylinder. Notice that the ratio $F_{Y}^{(n)}$ does not depend on the nonuniversal constant γ_n , which is therefore common to S_n^{gs} and S_n^{exc} .

As an example of the law (9) we shall consider a c = 1CFT given by a massless boson compactified on a circle. The primary fields are given by the vertex operators $\Upsilon_1[r, s] = e^{i(\alpha_+\phi+\alpha_-\bar{\phi})}$ (being ϕ , $\bar{\phi}$ chiral and antichiral boson fields) where $\alpha_{\pm} = r/2\sqrt{\kappa} \pm s\sqrt{\kappa}$, κ is the compactification ratio, and $r, s \in \mathbb{Z}$. The scaling dimensions of these operators are $(\alpha_+^2 + \alpha_-^2)/2 = r^2/4\kappa + s^2\kappa$. Using the chiral correlator of vertex operators on the cylinder, $\langle \prod_j e^{i\alpha_j\phi(z_j)} \rangle_{cy} = \prod_{j>k} [2\sin(z_{jk}/2)]^{-\alpha_j\alpha_k}$, it turns out that

$$F_{\Upsilon_1[r,s]}^{(n)}(x) = 1, \quad \forall \ n, r, s.$$
 (12)

Hence, all the excitations represented by vertex operators have the same entropy as the ground state. This result is not in contradiction with (10) because, in this case, $\Delta_{\Psi} = \Delta_{\partial\phi} = 1$ and both $O(x^2)$ terms in (10) cancel out due to the properties of the OPE constants. In fact, the cancellation happens to all orders in *x*.

Next, we study the operator $\Upsilon_2 = i\partial\phi$. Using its correlator on the cylinder $\langle \partial\phi(z_1)\partial\phi(z_2)\rangle_{cy} = -[2\sin(z_{12}/2)]^{-2}$ and the Wick theorem, we get, in terms of the determinant of a $2n \times 2n$ matrix:

$$F_{\Upsilon_2}^{(n)}(x) = (-1)^n \left(\frac{2}{n} \sin \pi x\right)^{2n} \det_{j \neq k} \frac{1}{e^{iz_j} - e^{iz_k}},$$
 (13)

where $z_j = \pi(2j \pm x)/n(j = 0, ..., n - 1)$. For n = 2, one finds $F_{Y_2}^{(2)}(x) = 1 - 2\mathbf{s}^2 + 3\mathbf{s}^4 - 2\mathbf{s}^6 + \mathbf{s}^8$, $\mathbf{s} \equiv \sin(\pi x/2)$. In the low- ℓ/N limit, $F_{Y_2}^{(n)}(x) \sim 1 + (\pi x)^2 \times (1/n - n)/3$, which leads to an excess of entanglement entropy given by (11) with $(h, \bar{h}) = (1, 0)$. Realizations of both types of excitations, in particular, models will be now shown, and their amount of entanglement compared with the CFT predictions (12) and (13).

Excitations in the XX and XXZ models.—The Hamiltonian of the spin-1/2 *XXZ* model is given by

$$H_{xxz} = -\frac{1}{2} \sum_{j=1}^{N} (\sigma_{j}^{x} \sigma_{j+1}^{x} + \sigma_{j}^{y} \sigma_{j+1}^{y} + \Delta \sigma_{j}^{z} \sigma_{j+1}^{z}), \quad (14)$$

where *N* is even and periodic boundary conditions are assumed (for $\Delta = 0$ we get the *XX* model). This model is integrable [13] and gapless for $-1 \leq \Delta < 1$. The corresponding CFT is given by the aforementioned bosonic CFT with $\kappa = \frac{\pi}{2} [\pi - \cos^{-1}(-\Delta)]^{-1}$. The *XX* model in the sector with magnetization $M = \frac{1}{2} \sum_{j} \sigma_{l}^{z}$ can be mapped, through a Jordan-Wigner transformation, into a system with $n_{F} = M + N/2$ free fermions in a lattice of *N* sites. We computed the entanglement and Rényi entropies of several types of excitations in these models. This task was achieved using the methods of references [7,14] in the free fermion problem and through numerical exact diagonalization in the *XXZ* case.

Let us first consider the vertex operator $Y_1[0, m]$. In the free fermion model, the result (12) is exact and can be proved analytically. Indeed, $|Y_1[0, m]\rangle$ corresponds to the umklapp excitation $\prod_{j=1}^{m} d_{k_F+(2j-1)\pi/N}^{\dagger} d_{-k_F+(2j-1)\pi/N} |0\rangle$, where $k_F = \pi n_F/N$ is the Fermi momentum, and where $|0\rangle$ is the Fermi state and d_k^{\dagger} the fermionic creation operator with momentum k. This state can be obtained from the Fermi state shifting all the momenta as $k \to k + 2m\pi/N$. Such a shift produces a global phase factor in the wave function in real space and, consequently, the entropy remains unchanged. In the XXZ model, the state $|Y_1[0, 1]\rangle$ corresponds to the ground state in the sector with n_F spins up and total momentum $P = 2\pi n_F/N$. We observe that the prediction $F_{Y_1}^{(n)}(x) = 1$ holds, up to the oscillations expected for $n \ge 2$ [15], which in this case are of the order of 10^{-3} for systems with N = 30 spins.

We will now consider the excitation $\Upsilon_1[2, 1]$. In a system of free fermions the resulting state corresponds to the addition of two fermions at the right of the Fermi point, i.e.,



FIG. 2 (color online). An illustration of the law $F_{Y_1[2,1]}^{(n)}(x) = 1$ for the XX model with N = 100, $n_F = 50$, and for the XXZ with $\Delta = -1/2$ and N = 30, $n_F = 14$ (16 for the excited state). The entropy of ground and excited states coincide and follows the law (1) (continuous lines), up to oscillations [15].



FIG. 3 (color online). The quantity $F_{Y_2}^{(2)}$ for the XX model at different filling fractions and for the XXZ ($\Delta = -1/2$, N = 30, $n_F = 14$) model, vs the CFT prediction (13). For $n_F = 250$ the oscillations around (13) are so small that both curves are indistinguishable. The inset shows S_2 for the ground and excited states (N = 500). The upper inset is a zoom of the region selected by the small rectangle over the curve in the main figure.

to the state $d_{k_F+\pi/N}^{\dagger} d_{k_F+3\pi/N}^{\dagger} |0\rangle$. Figure 2 shows that ground and excited states entropies $S_{2,3}$ coincide, up to oscillations. In the *XXZ* model, $|Y_1[2, 1]\rangle$ is the lowest eigenstate with total momentum $P = 2\pi(n_F + 2)/N$. Again in this case, oscillations of $F_{Y_1[2,1]}^{(2)}$ around one are observed (see Fig. 2).

Finally, Fig. 3 shows some numerical results for the entanglement of the excitation $Y_2 = i\partial\phi$. In the free fermion problem, $|Y_2\rangle$ corresponds to a particle-hole excitation: $d^{\dagger}_{k_F+\pi/N}d_{k_F-\pi/N}|0\rangle$, while in the *XXZ* model it corresponds to the lowest eigenstate with $P = 2\pi/N$. We observe an excellent agreement with the theoretical prediction (13) for n = 2. Similar results hold for n = 3. Moreover, we have checked, for n up to 6, that the low- ℓ/N formula (11) is very well satisfied for fermions.

In summary, we have obtained an expression for the Rényi entropies of excitations associated to any primary field. We verified the results with finite-size realizations of the XX and XXZ models up to 30 sites in the latter case, finding very good agreement with the theory.

As explained earlier, Eq. (9) can be used as a numerical method to extract information about correlators, conformal dimensions and OPE coefficients of primary fields. An interesting problem is to generalize these results to the descendent states in CFT. We expect that the Rényi entropies, at a given level of a conformal tower will depend on the particular state targeted. This can provide a method to establish the correspondence between degenerated excited states of a critical lattice model, and the descendent fields in the underlying CFT.

Equation (9) further suggests a generalization of the Rényi entropies in terms of traces of different density matrices tr[$\rho_{Y_1}\rho_{Y_2}...$]. This object would be related to the correlator: $\langle Y_1 Y_1^{\dagger} Y_2 Y_2^{\dagger} ... \rangle$ in the very same fashion as in (9). The numerical computation of the associated generalized entropies would then provide information on more general correlators in CFT, and vice-versa. Applications of the present work to other models and to nonprimary fields are in progress. This work represents a further step along the direction of deriving CFT data using quantum information methods.

We thank P. Calabrese, R. Pereira, and V. Rittenberg for discussions. This work was supported by the projects FAPESP and CNPq (Brazilian agencies), and by FIS2009-11654 and QUITEMAD (Spanish agencies).

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