Phase transition in the Rényi-Shannon entropy of Luttinger liquids

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The Rényi-Shannon entropy allows extraction of some universal information about many-body wave functions. For a critical spin chain with central charge $c = 1$, we show that it exhibits a phase transition at some value n_c of the Rényi parameter n which depends on the Luttinger parameter R. A replica-free formulation establishes a connection to boundary entropies in conformal field theory and reveals that the transition is triggered by a vertex operator which becomes relevant at the boundary. Our numerical results (*XXZ* and J_1-J_2 spin chains) match the continuum limit prediction, confirming its universal character. The replica approach used in previous works turns out to be correct only for $n < n_c$. From the point of view of two-dimensional Rokhsar-Kivelson states, this transition reveals a singularity in the entanglement spectra.

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I. INTRODUCTION

The entanglement entropy (EE) has become an important tool for probing and characterizing many-body quantum states. In one-dimensional (1D) systems, the celebrated logarithmic divergence[1–4] of the von Neumann entropy of a long segment provides an efficient way to measure the central charge c of a critical spin chain. In higher dimensions, the EE can also be used to detect the presence of topological order,[5] which is otherwise invisible to conventional local order parameters and correlation functions. The understanding of the scaling of the EE of large subsystems has also opened a route to algorithms able to simulate efficiently these strongly interacting systems in $d > 1$.[6]

In this paper, we use a different entropy to probe the ground state of quantum spin chains, the *Rényi-Shannon entropy* (RSE) (or configuration entropy). For a normalized state $|\psi\rangle$ and a Rényi index $n > 0$ it is defined as

$$S_n = \frac{1}{1-n} \ln \left(\sum_i p_i^n \right), \quad p_i = |\langle i|\psi\rangle|^2, \tag{1}$$

where the states $|i\rangle$ form a basis of the Hilbert space. The basis states are chosen to be products of local states, and the Ising configurations ($|i\rangle = |\uparrow\uparrow\downarrow \ldots\rangle$, etc.) are the natural choice in a system with conserved particle (or S^z) number. It is also the basis in which the Rényi-Shannon entropy is identical to the (basis independent) entanglement entropy of some two-dimensional wave-function (see below).

The RSE is appealing for several reasons. Although it is basis dependent, its scaling gives some information about the universal long-distance properties.[7] It probes the system globally, without need to chose a partition and preserving all the spatial symmetries. This entropy is also the (basis-independent) EE of some particular two-dimensional (2D) states—the so-called Rokhsar-Kivelson (RK) wave functions—a fact which has allowed investigation of the EE at some 2D conformal quantum critical points.[7,8] However, here, we will mostly keep the 1D spin chain point of view.

A particularly interesting situation is that of the spin-$\frac{1}{2}$ *XXZ* chain:

$$\mathcal{H} = \sum_i \left(S_i^x \cdot S_{i+1}^x + S_i^y \cdot S_{i+1}^y \right) + \Delta \sum_i S_i^z \cdot S_{i+1}^z. \tag{2}$$

For a chain of length L, S_n has a leading term proportional to L followed by universal subleading contributions. If the chain is *periodic*, the first subleading term is $O(1)$, and was shown to be[7,9]

$$S_n^{\text{periodic}} = (\cdots)L + \ln(R) - \frac{\ln n}{2(n-1)}, \tag{3}$$

where R is the compactification radius, related to the anisotropy Δ of the *XXZ* Hamiltonian $[R(\Delta)^2 = 2 - \frac{2}{\pi}\arccos(\Delta)]$. This is a situation where the RSE gives more precise information than the single-interval EE—which gives only the central charge.[10] With *open* boundary conditions, the first subleading correction is also universal and takes the form of a logarithm of the length L of the chain:[8]

$$S_n^{\text{open}} = (\cdots)L - \tfrac{1}{4}\ln(L), \tag{4}$$

which, in the 2D RK language, confirms at $c = 1$ the arguments developed in Ref. 11 (from now on the term proportional to L will be omitted).

In this paper, however, we show that these results are correct only below a critical value n_c of the Rényi parameter. Using a replica-free formulation of the problem, we prove that the Rényi parameter n effectively modifies the compactification radius of the chain (in a sense to be defined later), and that a phase transition takes place at $n = n_c$ when a (boundary) vertex operator becomes relevant. A central result concerns the location of this transition and the behavior of the entropy above n_c:

$$n_c = d^2/R^2, \tag{5}$$

$$S_{n>n_c}^{\text{periodic}} = \frac{1}{n-1}(n \ln R - \ln d), \tag{6}$$

$$S_{n>n_c}^{\text{open}} = \ln(L)\frac{n}{n-1}\left(\frac{R^2}{4} - \frac{1}{4}\right), \tag{7}$$

where d is the degeneracy of the Ising configuration with the highest probability $p_{\max}$ in the ground state. At zero magnetization this configuration is $(d = 2)$-fold degenerate:

$$|i_{\max}\rangle = |\uparrow\downarrow\uparrow\downarrow \ldots \uparrow\downarrow\rangle \quad \text{or} \quad |i_{\max}\rangle = |\downarrow\uparrow\downarrow\uparrow \ldots \downarrow\uparrow\rangle. \tag{8}$$

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II. COMPACT FREE FIELD

To understand this transition we adopt the $(1+1)$-dimensional (Euclidean) point of view. At long distances, the model is described by a compactified "height field" $h(x,\tau)$ with Gaussian probabilities:

$$S[h] = \frac{\kappa}{4\pi}\int dx\, d\tau (\nabla h)^2, \tag{9}$$

$$\mathcal{Z} = \int \mathcal{D}[h] \exp(-S[h]), \tag{10}$$

where κ is the stiffness, r is the compactification radius ($h \equiv h + 2\pi r$), and the physical Luttinger parameter (which fixes the decay exponents of the correlations functions) is $R = \sqrt{2\kappa}r$. For periodic (open) chains, h is defined on an infinitely long cylinder (strip) of perimeter (width) L. In this language, the microscopic configurations $|i\rangle$ are replaced by configurations $\phi(x) = h(x,\tau = 0)$ of the height field at $\tau = 0$. To evaluate the probability $p[\phi]$, we decompose the field h into a harmonic function h^ϕ that satisfies the boundary condition $h^\phi_{\tau=0} = \phi$ and a "fluctuating" part δh satisfying a Dirichlet boundary condition: $h = h^\phi + \delta h$. Exploiting the Gaussian form of the action and $\Delta h_\phi = 0$, we can decouple the classical and fluctuating parts: $S[h] = S[h^\phi] + S[\delta h]$, and we get

$$p[\phi] = \exp(-S[h^\phi])\frac{\mathcal{Z}^D}{\mathcal{Z}}, \tag{11}$$

where $\mathcal{Z}^D$ is the partition function of the whole cylinder (strip) with a Dirichlet defect line at $\tau = 0$.[12] Now $p[\phi]$ is raised to the (possibly noninteger) power n,

$$p[\phi]^n = \exp(-nS[h^\phi])\left(\frac{\mathcal{Z}^D}{\mathcal{Z}}\right)^n, \tag{12}$$

and we make the observation that $\exp(-nS[h^\phi])$ is the Boltzmann weight in a system where the stiffness κ has been replaced by $\kappa' = n\kappa$. From now on we explicitly keep track of the value of the stiffness κ (as an index) and write

$$\exp(-nS_\kappa[h^\phi]) = \exp(-S_{n\kappa}[h^\phi]) = p_{n\kappa}[\phi]\frac{\mathcal{Z}_{n\kappa}}{Z^D_{n\kappa}}. \tag{13}$$

So Eq. (12) can be written as

$$(p_\kappa[\phi])^n = p_{n\kappa}[\phi]\left(\frac{\mathcal{Z}_{n\kappa}}{Z^D_{n\kappa}}\right)\left(\frac{\mathcal{Z}^D_\kappa}{\mathcal{Z}_\kappa}\right)^n. \tag{14}$$

Inserting this result in Eq. (1) and using the fact that the probabilities $p_{n\kappa}[\phi]$ are normalized, we get the main result of this section:

$$S_n = \frac{1}{1-n}\left[\ln\left(\frac{\mathcal{Z}_{n\kappa}}{Z^D_{n\kappa}}\right) - n\ln\left(\frac{\mathcal{Z}_\kappa}{Z^D_\kappa}\right)\right]. \tag{15}$$

If we assume $2n = p$ to be an integer, the partition function $Z(n) = \sum p_i^n$ has a natural interpretation in terms of p half-infinite systems glued together at their edges, forming a "book" with p sheets.[13] The derivation above, however, never assumes $2n$ to be an integer and is therefore different from the previous derivations involving a replica trick.[8,9] S_n has been reduced to ratios of standard partition functions with respectively free and Dirichlet boundary conditions at the boundary between upper ($\tau > 0$) and lower ($\tau < 0$) parts of the cylinder (or strip). The complications associated with n-sheeted surfaces[8,9] have been avoided. For a compactified free field and the cylinder geometry, the ratio $g_D^2 = \mathcal{Z}^D_\kappa/\mathcal{Z}_\kappa$ is a well-known "g factor":[14,15]

$$g_D^2 = R^{-1} = (2\kappa r^2)^{-1/2}. \tag{16}$$

Combining Eqs. (15) and (16), we find

$$S_n = \ln R - \frac{\ln n}{2(n-1)}, \tag{17}$$

in agreement with Refs. 7–9 and 16. For the strip geometry, we also recover the n-independent result of Eq. (4) by applying the Cardy-Peschel formula[17] to Eq. (15), with four angles $\gamma = \pi/2$.

III. BOUNDARY PHASE TRANSITION

Equation (15) is a combination of two g factors and therefore probes the boundary of the system (the "bookbinding" in the book picture). The action at the lattice scale is not strictly Gaussian, and other terms respecting the lattice symmetry and the periodicity $h \equiv h + 2\pi r$ are present, including vertex operators of the type $\cos(\frac{d}{r}h)$. At the boundary such an operator renormalizes to zero in the long-distance limit if $d^2 > 2\kappa r^2$.[18] Otherwise it would lock the field to a flat configuration with degeneracy d. But Eq. (15) cannot be valid anymore in this locked and massive phase since its derivation assumes Gaussian probabilities. A boundary phase transition therefore takes place when the most relevant vertex operator become marginal in the presence of a stiffness $\kappa' = n\kappa$.[19] This gives the critical value of the Rényi index:

$$n_c = \frac{d^2}{2\kappa r^2}. \tag{18}$$

In the case of the antiferromagnetic XXZ chain, the two Ising configurations $|\uparrow\downarrow\uparrow\downarrow\ldots\rangle$ and $|\downarrow\uparrow\downarrow\uparrow\ldots\rangle$ become the ground states when $\Delta \to \infty$, which shows that an operator with two minima is present at the microscopic level. Taking $2\kappa r^2 = R(\Delta)$ and $d = 2$, we find Eq. (5). We also note that the same argument applies to the J_1-J_2 (or zigzag) chain, and to any Luttinger liquid phase with umklapp terms $\sim\cos(2h/r)$.

In this locked phase, the universal contribution to S_n is given by these d configurations only, so that

$$S_{n>n_c} = \frac{1}{1-n}\ln[d(p_{\max})^n]. \tag{19}$$

In the periodic case, $p_{\max}$ simply corresponds to $g_D^2 = \mathcal{Z}^D/\mathcal{Z}$ and we recover Eq. (6).

The open chains turn out to be even more interesting. The universal contribution to $S_{n>n_c}$ is encoded in

$$p_{\max} = \lim_{\tau\to\infty}\frac{\left|\langle s|e^{-\tau H}|i_{\max}\rangle\right|^2}{\langle s|e^{-2\tau H}|s\rangle} = \frac{\mathcal{Z}(\sqcup)^2}{\mathcal{Z}(|\,|)}, \tag{20}$$

where $\mathcal{Z}(\sqcup)$ is the partition function of a semi-infinite strip with bottom boundary condition $|i_{\max}\rangle$ (see Fig. 1). The ratio in Eq. (20) is similar but not identical to the one used below the transition ($n < n_c$). As before, four corners with angle $\pi/2$ will contribute to $-\ln p_{\max}$ by a logarithm: $-\frac{1}{4}\ln L$. However, the configuration with highest probability does not exactly

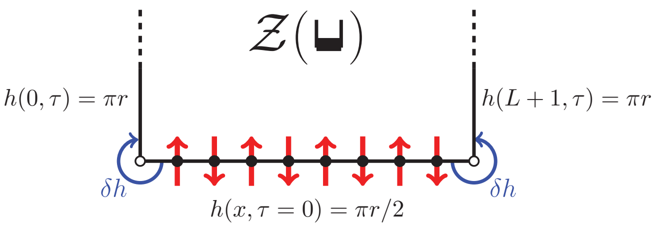

FIG. 1. (Color online) Height shift $\delta h = \pi r/2$ for the semi-infinite strip with bottom boundary condition $|i_{\max}\rangle$.

correspond to the Dirichlet condition in the continuum limit since there is a *height shift* δ between the vertical edges of the strip, and the horizontal boundary (see Fig. 1). It can be treated by subtracting a harmonic function $h_\delta(x,\tau) = (2\delta/\pi)\arg(x + i\tau)$, equal to 0 on the horizontal boundary $\tau = 0$ and δ on the vertical boundary at $x = 0$. The resulting contribution to the free energy is

$$\delta F \sim \frac{\kappa\delta^2}{2\pi^2}\ln L. \tag{21}$$

The value shift δ can be obtained by use of, for instance, a bosonization approach. The free boundary condition for the spins at the end of the open chain corresponds to the Dirichlet condition for the free field, and we have to set $h(x = 0,\tau) = h(x = L + 1,\tau) = \pi r$ to ensure vanishing spin operators at both ends.[20] Then the continuum limit of the configuration $|i_{\max}\rangle$ corresponds to locking $h(x,\tau = 0)$ to the minima of the umklapp term $\cos(2h/r)$,[21] which has two degenerate minima at $h = \pi r/2$ and $3\pi r/2$. In both cases the height difference between the $x = 0$ boundary and that at $\tau = 0$ is $\delta = \pi r/2$. Summing up the contributions coming from Eq. (21) and from the Cardy-Peschel term, we recover our main result Eq. (7). The same umklapp term – now in the *bulk* – is also responsible for the known transition to a massive Néel phase for $\Delta > 1$.[21]

IV. NUMERICS

So far, for periodic chains, only the case $n = 1$ has been investigated numerically.[7] Figure 2 shows the full n dependence of S_n (with the constant term extracted by fitting the finite-size data) for different values of Δ. Although the system sizes are very small ($L \leqslant 28$), there is a good agreement with the theoretical predictions, including the change of behavior at the predicted value of n_c (which depends on Δ). It is only close to the Heisenberg point ($\Delta = 1$) and above n_c that the finite-size results deviate from Eq. (7). We attribute these enhanced finite-size effects to the marginal operators present at the SU(2) symmetric point. To circumvent this difficulty we also studied the J_1-J_2 chain at the critical value $J_2/J_1 \simeq 0.2411$,[22] which has the same radius $R = \sqrt{2}$ but where finite-size effects are much smaller. The data again agree well with our prediction.

Open chains were investigated in Ref. 8 for various values of n and Δ, but the transition at n_c was overlooked. In Fig. 3 we see a clear tendency for the logarithmic term to approach the theoretical curves, although the finite-size data are still far from the thermodynamic limit. Interestingly, the entropy curves extracted from different system sizes cross in the immediate vicinity of the predicted value of n_c. This leads us to conjecture that the coefficient of the logarithm may take

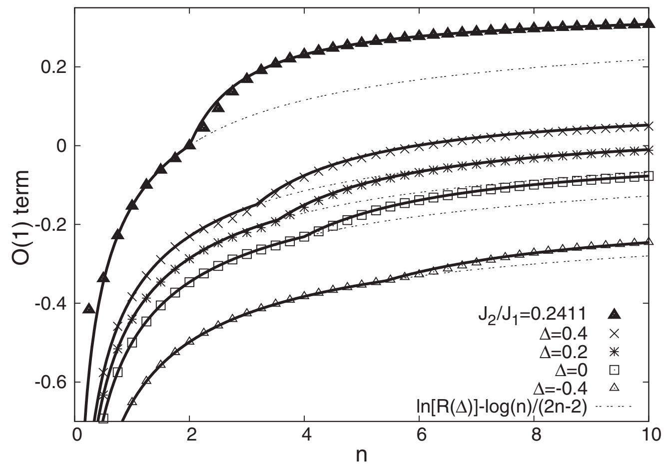

FIG. 2. Constant term in the RSE of periodic XXZ and $J_1 - J_2$ chains for different values of Δ and at the critical point $J_2/J_1 = 0.2411$. Each point comes from fitting the data for $L = 20,22,24,26$ and 28 to $aL + b + c/L + d/L^2$. Fat lines: theoretical prediction [Eq. (15)]. Eq. (3) is also plotted above n_c (dashed lines) for comparison.

a universal value at the transition point which depends only on the compactification radius R. At $\Delta = 0$ we pushed the numerics to $L = 40$ spins (see below), and the inset of Fig. 3 shows a collapse of the data for different system sizes onto a single curve in the vicinity of $n_c = 4$. This indicates a slow ($\sim L^{-1/4}$) but steady convergence toward a step function. We also get $S^{\rm open}_{n=n_c} = -(1/6)\ln L$ with a high precision at $\Delta = 0$, although we have no theoretical understanding of this value.

V. $\Delta = 0$ IN OPEN CHAINS

This corresponds to free fermions and each probability p_i is a determinant (Wick's theorem). Denoting by $\{x_k\}$

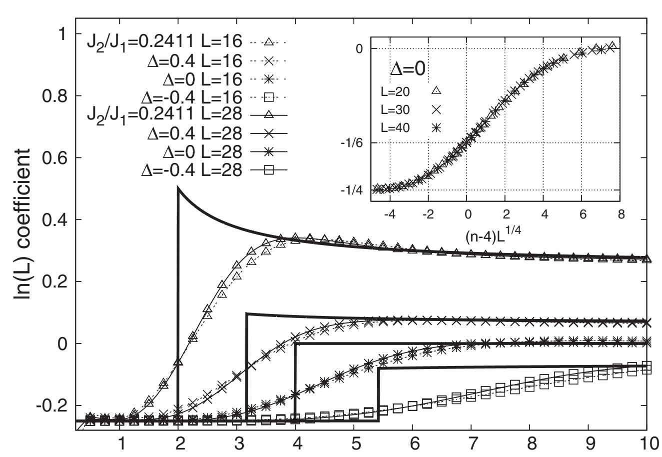

FIG. 3. Logarithmic term in the RSE of open *XXZ* and J_1-J_2 chains, extracted using $S_n \simeq aL + b\ln L + c + d/L$ with four consecutive system sizes $(L,\ldots,L-6)$ with $L = 16$ and 28. Bold lines: Eq. (15). Inset: scaling close to $n_c(\Delta = 0) = 4$.

the positions of the up spins (fermions) and setting $\theta_k = \pi x_k/(L+1)$, we have

$$p_i = p(\{\theta_k\}) = \left(\frac{2}{L+1}\right)^{L/4} \det_{1\leqslant j,k\leqslant L/2}(\sin[j\theta_k]). \qquad (22)$$

This determinant has a "simplectic Vandermonde" form[23] and can be computed exactly. As a particular case we get $p_{\max} = 2^{-L/2}$. The absence of a logarithmic term in $S_{n\to\infty} \sim -\ln p_{\max}$ is consistent with Eq. (7), because the contribution from the height shift exactly compensates for the Cardy-Peschel term at $R(\Delta = 0) = 1$. This also rigorously confirms at $\Delta = 0$ the value of δ. We also checked the validity of Eq. (7) for the square-lattice quantum dimer (2D RK) wave function, for which $d = 1$ and therefore $n_c = 1$. In this case the microscopic height representation of dimer coverings allows one to obtain δ exactly at the lattice level.

VI. CONCLUSION

We showed that the RSE problem of a compactified boson reduces to a (single-sheet) boundary entropy, but understanding the meaning of the RSE in situations where the central charge is not 1 (see Refs. 8 and 13) remains an open question. This is all the more interesting as it differs from the continuum limit of the single-interval EE, which reduces to a two-point correlation function for any c.

This study also showed that taking *powers* of the wave function gives rise to a whole line of critical points ending at a phase transition to an ordered state. In fact, going back to the 2D RK point of view, this transition reveals a rich structure in the entanglement spectrum $\{E_i\}$ of these wave functions. In some appropriate cylinder geometry,[7] the probabilities p_i are nothing else but the eigenvalues of the 2D reduced density matrix and they directly give the entanglement spectrum $E_i = -\ln p_i$. The phase transition at n_c shows that the spectrum has two distinct regions in the thermodynamic limit: at high "energy" (small inverse "temperature" $n < n_c$) the universal contributions to the probabilities are Gaussian, whereas at low energy ($n > n_c$) they are dominated by the ordered configurations. This should be compared with the fractional quantum Hall situation, where the universal part of the entanglement spectrum has only been seen at low E_i.[24] This may open new directions in the study of critical and topological wave functions—in 1D and in higher dimensions—as well as their connection to boundary critical phenomena.

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