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Geometric entanglement and Affleck-Ludwig boundary entropies in critical *XXZ* and Ising chains

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We study the geometrical entanglement of the *XXZ* chain in its critical regime. Recent numerical simulations [Q.-Q. Shi, R. Orús, J. O. Fjærestad, and H.-Q. Zhou, New J. Phys. **12**, 025008 (2010)] indicate that it scales linearly with system size, and that the first subleading correction is constant, which was argued to be possibly universal. In this work, we confirm the universality of this number, by relating it to the Affleck-Ludwig boundary entropy corresponding to a Neumann boundary condition for a free compactified field. We find that the subleading constant is a simple function of the compactification radius, in agreement with the numerics. As a further check, we compute it exactly on the lattice at the *XX* point. We also discuss the case of the Ising chain in transverse field and show that the geometrical entanglement is related to the Affleck-Ludwig boundary entropy associated to a ferromagnetic boundary condition.

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I. INTRODUCTION

The geometrical entanglement (GE) is a measure of the multipartite entanglement in a wave function, and quantifies the distance to the closest *unentangled* (separable) state.[1,2] Starting from a wave function $|\Psi\rangle$ for a quantum lattice model with N sites, one defines a maximal overlap $\Lambda_{\max}$ to be

$$\Lambda_{\max} = \lim_{|\Phi\rangle} |\langle \Phi | \Psi \rangle|, \tag{1}$$

where the maximization is carried on states $|\Phi\rangle$, which are tensor products of single-site states

$$|\Phi\rangle = \bigotimes_{j=1}^{N} |\Phi_j\rangle.$$

The larger $\Lambda_{\max}$, the closer it is to a product state, and the less entangled $|\Psi\rangle$ is. The GE is then defined in logarithmic form as[3]

$$E(|\Psi\rangle) = -\log_2 \Lambda_{\max}^2.$$

This quantity allows to quantify the global multipartite entanglement of the wave function $|\Psi\rangle$, and is useful in the context of quantum computation[4–6] or state discrimination with local measurements.[7]

The GE has also recently gained interest in many-body and condensed-matter physics.[8–11] Since it generally scales linearly with the volume (N) of the system one also defines the GE per site

$$\mathcal{E}_N(|\Psi\rangle) = N^{-1} E(|\Psi\rangle).$$

As an example of interesting application, it has been shown that derivatives of $\mathcal{E}_N$ on large systems can be used to detect quantum phase transitions.[9–11]

In this Rapid Communication we focus on the case of the ground state $|\Psi\rangle = |G\rangle$ of the Hamiltonian of a periodic spin-1/2 *XXZ* chain

$$\mathcal{H} = -\sum_{j=1}^{L} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z), \tag{2}$$

where $L=N$ is the number of sites. We consider the anisotropy parameter in the range $|\Delta|<1$ so that the system is gapless (critical). In Ref. 12 it was shown numerically that the GE per spin admits the following asymptotic expansion:

$$\mathcal{E}_L(\Delta) = \mathcal{E}_\infty(\Delta) + b(\Delta)/L + O(1/L^2). \tag{3}$$

The purpose of this Rapid Communication is to show that the term $b(\Delta)$ appearing in this expansion can be computed analytically in a simple way. Using results of boundary conformal field theory (CFT),[13] we relate it to an Affleck-Ludwig (AL) boundary entropy.[14]

II. RELATION TO THE AL BOUNDARY ENTROPY

The product state $|\Phi\rangle_{\max}$ that maximizes the overlap in Eq. (1) with the ground state of Eq. (2) is known to be a spin configuration where all spins are parallel[15] and lie in the *XY* plane

$$|\Phi\rangle_{\max} = |\rightarrow \rightarrow \ldots \rightarrow\rangle = 2^{-L/2} \sum_{\{\sigma_j^z = \pm 1\}} |\sigma_1^z \sigma_2^z, \ldots, \sigma_L^z\rangle = |\text{free}\rangle_z.$$

Computing $b(\Delta)$ amounts to calculating a subleading contribution to the scalar product ${}_z\langle \text{free}|G\rangle$. To do this, we adopt a transfer-matrix point of view where $|G\rangle$ is interpreted as the dominant eigenstate of the transfer matrix M of some two-dimensional classical system (six-vertexlike in our case). The classical model is defined on a cylinder of circumference L and height $L_y \gg L$ with free boundary conditions for the spins (or the six-vertex arrows) at both edges. In this geometry the free energy $F = -\ln {}_z\langle \text{free}|M^{L_y}|\text{free}\rangle_z$ can be written[14] as $F = F_{\text{bulk}} + 2F_{\text{boundary}}$ with $F_{\text{bulk}} \sim LL_y$ and $F_{\text{boundary}} = aL + s + o(1)$. a is the boundary free-energy per unit length, and s is a subleading term in the boundary free energy.

It is easy to check that $F_{\text{boundary}} = -\ln {}_z\langle \text{free}|G\rangle$ in the limit $L_y \gg L$, where only the state $|G\rangle$ contributes. So, $b(\Delta)$ is sim-

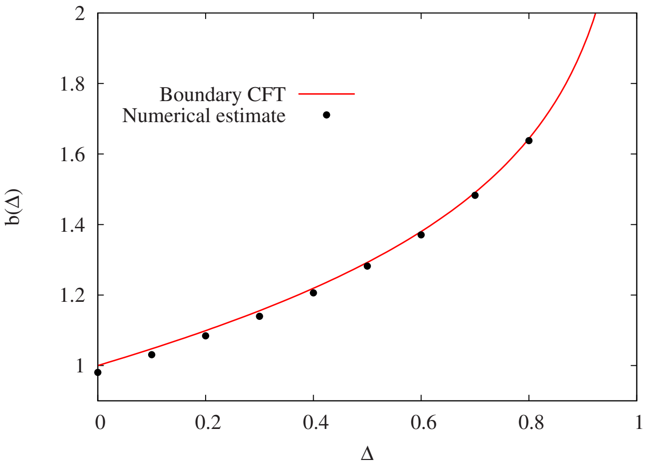

FIG. 1. (Color online) $b(\Delta)$ for the *XXZ* chain, defined in Eq. (3), as a function of the anisotropy parameter Δ. Symbols are numerical data of Ref. 12 while the solid curve is the field-theoretical calculation [Eqs. (5) and (6)]. At $\Delta=0$, an exact lattice calculation shows that $b=1$.

ply related to the constant s in the boundary free energy

$$b(\Delta) = -\frac{2}{\ln 2}s. \tag{4}$$

For critical systems s is universal and may therefore be computed in the continuum limit. In the *XXZ* chain (equivalently six-vertex case), it corresponds to a compactified free field with the following (Euclidian) Lagrangian density:

$$\mathcal{L} = \frac{1}{8\pi}(\partial_\mu \phi)^2,$$

$$\phi \equiv \phi + 2\pi R.$$

The compactification radius R is related to the decay exponents of the correlation functions and to the Luttinger parameter. In the case of Eq. (2), R is a known function of Δ (Ref. 16)

$$R(\Delta) = \sqrt{\frac{2}{\pi}\arccos(\Delta)}. \tag{5}$$

As well known in boundary CFT,[13] free boundary condition for the spins (or arrows) are encoded in the continuum limit by a Neumann boundary condition for the free field. So, the boundary entropy s is in fact the AL (Ref. 14) boundary entropy s_N associated to Neumann boundary condition. Its value is known[17] and depends solely on the compactification radius

$$s_N = \ln(g_N), \quad g_N = \sqrt{R/2},$$

where g_N is the so-called "universal noninteger ground-state degeneracy"[14] or "g factor." Combining this with Eq. (4), our prediction for $b(\Delta)$ is

$$b(\Delta) = 1 - \log_2 R(\Delta). \tag{6}$$

As can be seen in Fig. 1, this result matches very well the numerical data of Ref. 12. The slight discrepancy for small Δ is likely due to finite-size effects and/or finite-bond dimension errors in the matrix-product representation of the ground state. This can be confirmed by an exact microscopic calculation[13] of $b(\Delta)$ at the free fermion point $\Delta=0$.

The free fermion representation of the chain at $\Delta=0$ allows to obtain[18] $\mathcal{E}_L$ on the lattice, as done in Ref. 10

$$\mathcal{E}_L = 1 + \frac{2}{L \ln 2}\sum_{j=1}^{L/4} \ln \tan\left[\frac{(2j-1)\pi}{2L}\right]. \tag{7}$$

From this one gets the expansion in powers of $1/L$ using the Euler-Maclaurin formula.[19] The result is

$$\mathcal{E}_L = \mathcal{E}_\infty + \frac{b}{L} + O(1/L^2),$$

$$\mathcal{E}_\infty = 1 - \frac{2K}{\pi \ln 2} \simeq 0.158733,$$

$$b = 1,$$

where K is Catalan's constant. The result can be compared with the numerical estimations of Ref. 12: $\mathcal{E}_\infty \simeq 0.1593$ and $b \simeq 0.98$. As expected, the exact lattice calculation confirms the field theory prediction at $\Delta=0$, namely, $b(\Delta=0)=1$ [Eq. (6)].

It is also worth noticing that the calculation extends to finite magnetizations of the chain, and simply amounts to move the fermion density away from 1/2. In such a case one observes that $b(\Delta=0)=1$ is independent of the magnetization. This again matches the field theory result, since, for $\Delta=0$, the compactification radius R is indeed independent of the magnetization.

III. CRITICAL ISING CHAIN

The GE for the periodic Ising chain in transverse field at the critical point has also been considered numerically in Ref. 12. The Hamiltonian is now

$$\mathcal{H} = -\sum_{j=1}^{L} \sigma_j^x \sigma_{j+1}^x - \sum_{j=1}^{L} \sigma_j^z \tag{8}$$

and the product state which maximizes the overlap turns out to be a tilted configuration[10]

$$|\Phi\rangle_{\max} = \bigotimes_{j=1}^{N} [\cos(\xi/2)|\uparrow_j\rangle + \sin(\xi/2)|\downarrow_j\rangle],$$

$$\xi \simeq 0.897101, \tag{9}$$

where $|\uparrow_j\rangle$ and $|\downarrow_j\rangle$ are the eigenstates of σ_j^z.[20] The authors of Ref. 12 found numerically in this case $b \simeq 1.016$. We will now give an argument based on boundary CFT, similar to that presented in the case of the *XXZ* chain, which shows that $b=1$.

Again, we wish to interpret the scalar product $\Lambda_{\max}$ appearing in the GE as a boundary contribution to a classical two-dimensional free energy. When $|G\rangle$ is the ground state of

Eq. (8), the corresponding classical model is a critical two-dimensional Ising model. If we had to project $|G\rangle$ onto a state where all spins would point in the x direction (corresponding to an angle $\xi=\pm\pi$), it would correspond to a fixed ferromagnetic boundary condition for the Ising model. On the other hand, if we had to project onto a state with all the spins pointing in the z direction ($\xi=0$), it would correspond to a free boundary condition (as in the case of the *XXZ* chain). We therefore see that the tilted state of Eq. (9) somewhat corresponds to a combination of free and fixed boundary conditions for the classical model. But the important point is that $\xi\neq 0$. For this reason, $|\Phi\rangle_{\max}$ breaks the $\mathbb{Z}_2$ symmetry of the model, which exchanges the x and $-x$ directions. In such situation, where the boundary condition imposes a nonzero magnetization at the edge, the long-distance and universal properties of the boundary will be equivalent to that of a system with fixed ferromagnetic boundary condition (all spins pointing in the x direction).[14] In other words, the constant term s in the boundary free energy will be the same for the tilted boundary condition and for the ferromagnetic one. In this case, the AL entropy s_{fixed} is known to be $-\frac{1}{2}\ln 2$ (corresponding to a g factor $g_{\text{fixed}}=1/\sqrt{2}$).[14] As conjectured in Ref. 12, we therefore obtain $b=1$. This argument can also be confirmed using the exact formula of Ref. 10 for the GE, and then applying the Euler-Maclaurin formula.[21]

IV. RELATION WITH RÉNYI ENTROPIES FOR ROKHSAR-KIVELSON IN 2+1 DIMENSIONS

As we have seen in Sec. II, the GE for a critical *XXZ* chain can be expressed using a sum of scalar products with all the spin configurations $|i\rangle$ of the z basis

$$Z = 2^{L/2}\Lambda_{\max} = \sum_i \langle i|G\rangle .$$

Z can be seen as a partition function and generalized by introducing a fictitious inverse temperature $\beta>0$ (Ref. 22)

$$Z(\beta) = \sum_i (\langle i|G\rangle)^{\beta}. \tag{10}$$

It turns out that $Z(\beta)$ is related to Rényi entanglement entropies of a semi-infinite cylinder in some two-dimensional Rokhsar-Kivelson wave functions, as studied in Refs. 23 and 24 (the Rényi parameter being $n=\beta/2$). Using numerical and field-theoretical approaches, it was found that $\ln Z(\beta)$ scales as $\ln Z(\beta)=aL+\gamma$, where the constant term γ is universal and given by

$$\gamma = (1-\beta/2)\ln R + \frac{1}{2}\ln(\beta/2). \tag{11}$$

So, for the *XXZ* chain, the GE appears to be a special case $\beta=1$ of this partition function.

We finally comment on the limit $\beta\to\infty$, where only the spin configuration $|i\rangle_{\max}$ of the z basis which have the largest weight in $|G\rangle$ contributes to $Z(\beta)$. For the present *XXZ* chain, $|i\rangle_{\max}$ is the ferromagnetic state $|i\rangle_{\max}=|\uparrow\cdots\uparrow\rangle$.[23] Taking $\beta\to\infty$ in Eqs. (10) and (11) we get $\ln\langle\uparrow\cdots\uparrow|G\rangle=-\frac{1}{2}\ln R$ (omitting the extensive term). So, we see that the scalar product of $|G\rangle$ with both (i) the uniform configuration where spins point in the z direction and (ii) the configuration where spins point in the x direction, have very similar subleading terms related to the logarithm of the compactification radius. In the CFT language, the former scalar product [appearing in $Z(\beta=\infty)$] corresponds to a Dirichlet boundary condition for the free field, as opposed to Neumann for the scalar product appearing in the GE and $Z(\beta=1)$.

V. CONCLUSION

In conclusion, we have related subleading terms of the geometrical entanglement of the critical *XXZ* and Ising spin chains to their AL boundary entropies, showing that this correction is universal. Whether such universal behavior in the scaling of the geometrical entanglement (or of the scalar product of the ground state with a given separable state in general) can be found for other physical systems is an open issue that is worth pursuing.

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[15] This was demonstrated numerically in Ref. 9. Notice, however, that in this reference the antiferromagnetic chain was considered. Therefore, the result in this case is $|\Phi\rangle_{\max}=|\rightarrow\leftarrow\rightarrow\leftarrow\ldots\rightarrow\leftarrow\rangle$.

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[18] For simplicity we only consider the case $L\equiv 0 \bmod 4$. Notice that using Eq. (10), this result can also be interpreted (and recovered) as the partition function of a discretized gas of particles on an annulus interacting through a 2D Coulomb potential (discretized Dyson gas) at inverse temperature $\beta=1$. See Refs. 23 and 26 for more details.

[19] b can easily be deduced from the constant in the asymptotic expansion of $\Sigma_{j=1}^{m}\ln\tan[(j-1/2)\pi/(8m)]$. Then, a way to proceed is to cut the sum in two: $\Sigma_{j=1}^{m}=\Sigma_{j=1}^{\sqrt{m}}+\Sigma_{j=\sqrt{m}+1}^{m}$. In the first sum, the tangent can be linearized so as to apply Stirling's formula. The asymptotics of the second sum can be accessed using the Euler-Maclaurin formula. The dominant term $\mathcal{E}_\infty$ has been previously computed in Ref. 10.

[20] Introducing $f(\xi)=\sqrt{3\cos^2(\xi/2)-2}$, the optimal angle ξ is in the thermodynamic limit solution of $\cos(\xi/2)f(\xi)-\frac{2}{\pi}\text{arctanh}\left(\frac{f(\xi)}{\cos(\xi/2)}\right)=0$.

[21] For example, when L is even $\langle\Phi|G\rangle=\Pi_k[\sin^2(\xi/2)\sin(k/4)+\cos^2(\xi/2)\cot(k/2)\cos(k/4)]$, where $k=(2m+1)\pi/L$, $m\in\{0,\ldots,L/2-1\}$. The subleading constant in the asymptotic expansion of $-2\log_2\langle\Phi|G\rangle$ can be shown to be $b(\xi)=\begin{cases}0 & \xi=0 \bmod 2\pi\\ 1 & \text{otherwise.}\end{cases}$ In the boundary CFT language, $\xi=0$ corresponds to the free boundary state ($s_{\text{free}}=0$), which is unstable under the renormalization-group flow.

[22] With our (ferromagnetic) convention for the XY part of the interactions in the *XXZ* Hamiltonian, all the $\langle i|G\rangle$ are positive.

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