Finite-size corrections to entanglement in quantum critical systems

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We analyze the finite-size corrections to entanglement in quantum critical systems. By using conformal symmetry and density functional theory, we discuss the structure of the finite-size contributions to a general measure of ground state entanglement, which are ruled by the central charge of the underlying conformal field theory. More generally, we show that all conformal towers formed by an infinite number of excited states (as the size of the system $L \to \infty$) exhibit a unique pattern of entanglement, which differ only at leading order $(1/L)^2$. In this case, entanglement is also shown to obey a universal structure, given by the anomalous dimensions of the primary operators of the theory. As an illustration, we discuss the behavior of pairwise entanglement for the eigenspectrum of the spin-1/2 *XXZ* chain with an arbitrary length L for both periodic and twisted boundary conditions.

I. INTRODUCTION

In recent years, the observation that entanglement may play an important role at a quantum phase transition [1–4] has motivated intensive research on the characterization of critical phenomena via quantum information concepts. In this direction, conformal invariance has brought valuable information about the behavior of block entanglement, as measured by the von Neumann entropy, in critical models. Indeed, conformal field theory (CFT) has been used as a powerful tool to determine universal properties of entanglement. Remarkably, it was shown that the entanglement entropy obeys a universal logarithmic scaling law for one-dimensional critical models both at zero and finite temperatures [5–7], which is governed by the central charge of the associated CFT. Moreover, corrections to the entanglement entropy due to finite-size effects have also been considered [6,8] for periodic and open boundary conditions. Together with approximative methods such as renormalization group (see, e.g., Refs. [9–13]) and density functional theory (DFT) [14], CFT has been settled as one of the most promising approaches for investigating the behavior of entanglement in many-body quantum critical systems.

In this work, we will exploit in a different perspective the impact of CFT methods for the evaluation of entanglement at criticality. More specifically, our approach will be based on the statement that finite size corrections to the ground state expectation values of arbitrary observables are ruled by conformal invariance. This conclusion is indeed a consequence of two results: (1) finite-size corrections to the energy spectrum of a critical theory are determined by conformal invariance [15–17]; (2) DFT techniques imply that, under certain conditions discussed below, general observables can be evaluated as a function of the first derivative of the ground state energy with respect to a Hamiltonian coupling parameter [18,19]. We then simultaneously apply these two results to obtain the finite-size corrections to ground state entanglement in critical models. As a by-product, conformal invariance determines the structure of entanglement in the presence of extra symmetries for certain higher energy states, which are the lowest energy states in each symmetrically decoupled subspace of the Hilbert space. For instance, if the Hamiltonian is translationally invariant and has a U(1) symmetry due to its commutation with the magnetization operator, we can split out the Hilbert space in sectors of fixed momentum and magnetization. More generally, we will also show that all conformal towers formed by an infinite number of excited states (as the size of the system $L \to \infty$) exhibit a unique pattern of entanglement, which differ only at leading order $(1/L)^2$. This will be based on a generalization of the Hohenberg-Kohn (HK) theorem for individual states belonging to conformal towers of critical systems. Finite-size corrections to entanglement in these excited states will obey a universal structure, given by the anomalous dimensions of the primary operators of the theory.

Since our approach is applicable for any entanglement measure, it allows in particular for the investigation of the universality properties of pairwise entanglement measures, e.g., concurrence [20] and negativity [21]. For pairwise measures, criticality was first noticed through a divergence in the derivative of entanglement, signaling a second-order phase transition [1]. For first-order phase transitions, jumps in entanglement itself indicates quantum critical points [22,23]. A general explanation for this distinct usual behavior of first-order and second-order phase transitions has been provided in Refs. [19,24] (for an explicit discussion of examples which do not obey this expected behavior, see Ref. [25]). From the point of view of CFT, we will be able to explicitly work out the finite-size corrections to pairwise entanglement measures and show how these corrections involve universal quantities, such as the central charge or the anomalous dimension of primary operators associated with the CFT. As an illustration, we will consider the spin-1/2 *XXZ* chain, where

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an analytical expression, valid up to $o(L^{-2})$, will be provided for the negativity of nearest neighboring spins as a function of the size L of the chain.

II. ENERGY SPECTRUM AND FINITE-SIZE EFFECTS IN CRITICAL QUANTUM SYSTEMS

Let us consider a critical theory in a strip of finite width L with periodic boundary conditions. The transfer matrix of the theory is written as $T=\exp(aH)$, where a denotes the lattice spacing and H is the Hamiltonian. Then, for large L, the ground state energy density $\varepsilon(L)=E_0(L)/L$ of H is provided by conformal invariance [15,16], reading

$$\varepsilon(L) = \varepsilon_\infty - \frac{\xi}{6}L^{-2} + o(L^{-2}), \qquad (1)$$

where ε_∞ is the energy density in the limit $L\rightarrow\infty$ and $o(L^{-2})$ denotes terms of any order higher than L^{-2}. In Eq. (1), c is the central charge of the Virasoro algebra (the conformal anomaly) and the parameter ξ must be fixed in such a way that the equations of motion of the theory are conformally invariant [26]. The structure of the higher energy states is determined by the primary operators of the theory [17]. For each operator O_α with anomalous dimension x_α, there corresponds a tower of states with energy densities $\varepsilon^\alpha_{j,j'}(L)$ given by

$$\varepsilon^\alpha_{j,j'}(L) = \varepsilon(L) + 2\pi\xi(x_\alpha + j + j')L^{-2} + o(L^{-2}), \qquad (2)$$

where $j,j'=0,1,\ldots$ are indices labeling the tower of states associated with the anomalous dimensions x_α. Higher-order corrections to Eqs. (1) and (2) as well as convenient generalizations for more general boundary conditions, e.g., twisted boundary conditions, may also be obtained [27,28].

III. HOHENBERG-KOHN THEOREM AND EXPECTATION VALUES OF OBSERVABLES

Let us turn now to the discussion on how DFT can be allied with conformal invariance to extract information about expectation values of observables from the energy spectrum. DFT [29,30] is originally based on the HK theorem [29] which, for a many-electron system, establishes that the dependence of the physical quantities on the external potential $v(\mathbf{r})$ can be replaced by a dependence on the particle density $n(\mathbf{r})$. The HK theorem can be extended for the context of a generic quantum Hamiltonian H on a lattice (see, e.g., Refs. [18,19]). In order to be specific, let us consider a quantum spin chain of size L governed by the Hamiltonian

$$H = H_0 + \lambda\sum_{i=1}^{L} A_i, \qquad (3)$$

where λ is a control parameter associated with the Hermitian operators A_i which act on the site i, e.g., an observable relevant to driving a quantum phase transition. Let us take, for simplicity, a translationally invariant chain (e.g., by assuming periodic boundary conditions). Then, by taking the expectation value of Eq. (3), we obtain

$$\langle H \rangle = \langle H_0 \rangle + \lambda L\langle A\rangle, \qquad (4)$$

where $\langle A\rangle \equiv \langle A_i\rangle = \langle A_j\rangle(\forall i,j)$ due to translation symmetry. Therefore

$$\varepsilon = \varepsilon_0 + \lambda\langle A\rangle, \qquad (5)$$

where $\varepsilon=\langle H\rangle/L$ and $\varepsilon_0=\langle H_0\rangle/L$ are the energy densities associated with H and H_0, respectively. For a general Hamiltonian such as given in Eq. (3), the HK theorem can be generalized to the statement that there is a duality (in the sense of a Legendre transform) between the expectation value $\langle A\rangle$ [corresponding to $n(\mathbf{r})$] and the control parameter λ [corresponding to $v(\mathbf{r})$] [18,19]. In order to specify the conditions supporting this duality let us separately consider the cases of nondegenerate and degenerate Hamiltonians.

A. Nondegenerate case

Let λ and λ' be two fixed values of the coupling parameter in Eq. (3), which correspond to nondegenerate ground states given by $|\psi\rangle$ and $|\psi'\rangle$, respectively. We assume that, for $\lambda\neq\lambda'$, we have that $|\psi\rangle\neq\alpha|\psi'\rangle$, with α a complex phase. This assumption means that different values of the coupling parameter are associated with distinct ground states. It reflects the requirement of the uniqueness of the potential (see, e.g., Ref. [31]). A general condition to ensure the uniqueness of the potential for Hamiltonian (3) will be derived below. Then, by assuming a unique potential and taking two different couplings λ and λ', the Rayleigh-Ritz variational principle allows us to write

$$\langle\psi|H|\psi\rangle < \langle\psi'|H|\psi'\rangle = \langle\psi'|H'|\psi'\rangle + (\lambda-\lambda')L\langle A\rangle', \quad (6)$$

where $\langle A\rangle'=\langle\psi'|A|\psi'\rangle$ and H and H' are the Hamiltonians associated with λ and λ', respectively. Therefore

$$\varepsilon - \varepsilon' < (\lambda-\lambda')\langle A\rangle'. \qquad (7)$$

Analogously, application of the variational principle for the ground state $|\psi'\rangle$ results into

$$\varepsilon' - \varepsilon < (\lambda'-\lambda)\langle A\rangle. \qquad (8)$$

By adding Eqs. (7) and (8) we obtain

$$\langle A\rangle' \neq \langle A\rangle. \qquad (9)$$

Equation (9) expresses the HK theorem for nondegenerate ground states, stating that distinct densities are associated with distinct potentials. In other words, we can establish the map

$$\lambda \Leftrightarrow |\psi\rangle \Leftrightarrow \langle A\rangle = \langle\psi|A|\psi\rangle. \qquad (10)$$

B. Degenerate case

In order to establish the HK theorem for degenerate ground states, let us consider two fixed values of the coupling constant, each of them associated with arbitrarily degenerate ground states:

$$\lambda \leftrightarrow q\text{-degenerate ground states:}\{|\psi_1\rangle, \ldots, |\psi_q\rangle\},$$

$\lambda' \leftrightarrow q'$-degenerate ground states: $\{|\psi'_1\rangle, \ldots, |\psi'_{q'}\rangle\}$.

Considering that any of the ground states are equally likely, we can describe them by the uniformly distributed density matrices

$$\rho = \frac{1}{q}\sum_{i=1}^{q}|\psi_i\rangle\langle\psi_i|, \quad \rho' = \frac{1}{q}\sum_{i=1}^{q'}|\psi'_i\rangle\langle\psi'_i|. \quad (11)$$

The requirement of uniqueness of the potential yields in the degenerate case the condition that ρ and ρ' are distinct. Applying the variational principle, we obtain

$$\text{Tr}(\rho H) < \text{Tr}(\rho' H) = \text{Tr}(\rho' H') + (\lambda - \lambda')L\langle A\rangle', \quad (12)$$

where, here, $\langle A\rangle' = \text{Tr}(\rho' A)$. Equation (12) implies that $\varepsilon - \varepsilon' < (\lambda - \lambda')\langle A\rangle'$. Therefore, as before, we use the complementary equation $\varepsilon' - \varepsilon < (\lambda' - \lambda)\langle A\rangle$ and obtain $\langle A\rangle' \neq \langle A\rangle$. The HK map in this case can be written as

$$\lambda \Leftrightarrow \rho \Leftrightarrow \langle A\rangle = \text{Tr}(\rho A). \quad (13)$$

C. Uniqueness of the potential

As discussed above, the condition for the uniqueness of the potential, which is fundamental for the derivation of the HK theorem, is defined by the requirement that different values of the coupling parameter λ are associated with distinct ground states of the Hamiltonian H. Here we will show that *a necessary and sufficient condition for which different values of λ are associated with distinct eigenstates of H is that the operators H_0 and $\Sigma_i A_i$, as given in Eq. (3), do not have common eigenstates.*

Sufficiency. Suppose that two distinct couplings λ and λ' yield the same eigenstate of H,

$$\left(H_0 + \lambda\sum_i A_i\right)|\psi\rangle = E(\lambda)|\psi\rangle, \quad (14)$$

$$\left(H_0 + \lambda'\sum_i A_i\right)|\psi\rangle = E(\lambda')|\psi\rangle. \quad (15)$$

Then, from Eqs. (14) and (15), we obtain

$$\sum_i A_i|\psi\rangle = \frac{E(\lambda) - E(\lambda')}{\lambda - \lambda'}|\psi\rangle. \quad (16)$$

Therefore, in this case, $|\psi\rangle$ is also an eigenstate of $\Sigma_i A_i$ (as well as an eigenstate of H_0). Hence, the condition that H_0 and $\Sigma_i A_i$ do not have common eigenstates is sufficient for ensuring the uniqueness of the potential.

Necessity. Let us suppose that H_0 and $\Sigma_i A_i$ have a common eigenstate

$$H_0|\psi\rangle = E_0|\psi\rangle, \quad (17)$$

$$\sum_i A_i|\psi\rangle = a|\psi\rangle. \quad (18)$$

Then we obtain that $(H_0 + \lambda\Sigma_i A_i)|\psi\rangle = (E_0 + \lambda a)|\psi\rangle$. Hence, by varying λ, we only change the eigenvalue (keeping the

same eigenstate), which means that distinct couplings will lead to the same eigenstate of H. Therefore, the condition that H_0 and $\Sigma_i A_i$ do not exhibit a common eigenstate is also necessary for the uniqueness of the potential. In conclusion, the sufficient and necessary condition for the uniqueness of the potential can be translated by the noncommutation relation

$$\left[H_0, \sum_i A_i\right] \neq 0. \quad (19)$$

Naturally, we disregard in Eq. (19) the rather unusual situation where H_0 and $\Sigma_i A_i$ are noncommuting observables, but $[H_0, \Sigma_i A_i]|\psi\rangle$ results in a vanishing quantum state.

D. HK theorem for conformal towers in quantum critical models

Since the HK theorem is based on a variational principle, we cannot guarantee that the expectation values of the observables in individual excited states are in general a function of the derivative of the energy of the excited state. Naturally, as previously mentioned in Sec. I, the HK theorem can be applicable in the presence of symmetries to excited states that are the minimum energy states in a given symmetric subspace of Hilbert space. In this work, we show that, under certain conditions, the HK theorem can also be extended for all the individual states of conformal towers in quantum critical models. We begin by supposing a periodic chain governed by a Hamiltonian given by Eq. (3) which is conformally invariant in a critical interval $\lambda_{c_1} \leq \lambda \leq \lambda_{c_2}$. Moreover we will assume the condition (19) for the uniqueness of the potential. Let us denote by $\{|\psi^\alpha_{j,j';d}(\lambda)\rangle\}$ the set of eigenstates associated with the energy $\varepsilon^\alpha_{j,j'}(\lambda)$, with $d = 1, \ldots, D$ labeling the D-fold degeneracy [see Eq. (2)]. We take the system in a uniformly distributed density matrix

$$\rho^\alpha_{j,j'}(\lambda) = \frac{1}{D}\sum_{d=1}^{D}|\psi^\alpha_{j,j';d}(\lambda)\rangle\langle\psi^\alpha_{j,j';d}(\lambda)|. \quad (20)$$

Our aim is to show that the potential λ uniquely specifies the density

$$\langle A\rangle^\alpha_{j,j'} = \text{Tr}[\rho^\alpha_{j,j'}(\lambda)A] = \frac{\partial\varepsilon^\alpha_{j,j'}}{\partial\lambda}. \quad (21)$$

Therefore, the derivative $\partial\varepsilon^\alpha_{j,j'}/\partial\lambda$ must be a monotonic function of λ. In order for this to occur, it is sufficient that (i) $\partial\varepsilon^\alpha_{j,j'}/\partial\lambda$ is continuous in the interval $\lambda_{c_1} \leq \lambda \leq \lambda_{c_2}$ and (ii) $\partial^2\varepsilon^\alpha_{j,j'}/\partial\lambda^2 \neq 0$. Condition (i) is usually achieved for a smooth (well-behaved) energy. Concerning condition (ii), let us take the derivative of Eq. (2), which yields

$$\frac{\partial^2\varepsilon^\alpha_{j,j'}}{\partial\lambda^2} = \frac{\partial^2\varepsilon}{\partial\lambda^2} + \frac{2\pi}{L^2}\frac{\partial^2}{\partial\lambda^2}[\xi(x_\alpha + j + j')] + o(L^{-2}). \quad (22)$$

The first term in the right-hand side of Eq. (22) concerns the second derivative of the ground state energy with respect to λ. We can show that this term is strictly negative. Indeed, from Eqs. (7) and (8), which hold for both degenerate and nondegenerate ground states, we obtain

$$\frac{\partial}{\partial\lambda}\langle A\rangle = \frac{\partial^2\varepsilon}{\partial\lambda^2} < 0, \qquad (23)$$

where $\langle A\rangle$ denotes the expectation value of A taken in the ground state. Concerning the second term in the right-hand side of Eq. (22), it is negligible for large L. Consequently, we can write

$$\frac{\partial^2\varepsilon_{j,j'}^{\alpha}}{\partial\lambda^2} \approx \frac{\partial^2\varepsilon}{\partial\lambda^2} < 0 \quad \text{(large } L\text{)}. \qquad (24)$$

Hence, $\partial^2\varepsilon_{j,j'}^{\alpha}/\partial\lambda^2$ is nonvanishing and then the derivative $\partial\varepsilon_{j,j'}^{\alpha}/\partial\lambda$ is monotonically related to λ. Therefore, a D-fold degenerate (up to order L^{-2}) eigenlevel given by α, j, and j' defines a density matrix $\rho_{j,j'}^{\alpha}$ that can be taken either as a function of λ or $\langle A\rangle_{j,j'}^{\alpha}$. This provides an extension of the HK theorem for arbitrary individual eigenstates belonging to conformal towers in quantum critical models.

IV. FINITE-SIZE CORRECTIONS TO ENTANGLEMENT IN CONFORMAL INVARIANT MODELS

The HK theorem implies a duality between the potential λ and the density $\langle A\rangle$. This behavior was revealed specially useful for the investigation of entanglement in the ground state of quantum systems undergoing quantum phase transitions [19]. In particular, the dependence of an arbitrary entanglement measure M on the parameter λ can be replaced by the dependence on the ground state expectation value $\langle A\rangle$ [19], which means that

$$M = M(\lambda) = M(\langle A\rangle) = M\left(\frac{\partial\varepsilon}{\partial\lambda}\right), \qquad (25)$$

where the Hellmann-Feynman theorem [32,33] has been used in the last equality above. As discussed in the last section, in the case of critical models, the HK theorem can also be applied to any state of conformal towers, which allows us to write the entanglement of such states as

$$M_{j,j'}^{\alpha} = M_{j,j'}^{\alpha}(\lambda) = M_{j,j'}^{\alpha}(\langle A\rangle_{j,j'}^{\alpha}). \qquad (26)$$

Equation (26) can be rewritten by observing that

$$\langle A\rangle_{j,j'}^{\alpha} = \frac{\partial\varepsilon_{j,j'}^{\alpha}}{\partial\lambda} = \langle A\rangle + \frac{2\pi}{L^2}\frac{\partial}{\partial\lambda}[\xi(x_\alpha + j + j')] + o(L^{-2}) \qquad (27)$$

By inserting Eq. (27) into Eq. (26) and performing a series expansion, we obtain

$$M_{j,j'}^{\alpha} = M(\langle A\rangle) + \frac{2\pi}{L^2}\frac{\partial}{\partial\lambda}[\xi(x_\alpha + j + j')]\left[\frac{\partial M_{j,j'}^{\alpha}}{\partial\lambda}\right]_{\lambda=\langle A\rangle} + o(L^{-2}). \qquad (28)$$

This means that the entanglement corresponding to all the eigenstates in the conformal towers are nearly the same as that of the ground state, with corrections of order L^{-2}. Moreover, it follows that finite-size effects for an arbitrary mea-

sure of entanglement are ruled by conformal invariance.

In order to evaluate entanglement at a point $\lambda = \lambda_c$, we should be able to perform a derivative of the energy with respect to λ taken at λ_c. Therefore, note that we will have that Eqs. (1) and (2) are the starting point to determine finite-size corrections to entanglement if and only if the theory is critical in an interval around λ_c. For the case of a single critical point (e.g., Ising spin-1/2 chain in a transverse field) instead of a critical region (e.g., XXZ spin-1/2 chain in the anisotropy interval $-1 < \Delta < 1$), more general expressions for the energy should be used, which take into account a mass spectrum (see, e.g., Ref. [34]).

V. ENTANGLEMENT IN THE FINITE-SIZE SPIN-1/2 XXZ CHAIN

As an illustration of the previous results, let us consider the spin-1/2 XXZ chain, whose Hamiltonian is given by

$$H_{XXZ} = -\frac{J}{2}\sum_{i=1}^{L}(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \Delta\sigma_i^z\sigma_{i+1}^z), \qquad (29)$$

where periodic boundary conditions (PBC) are assumed. We will set the energy scale such that $J = 1$. Entanglement for spin pairs can be quantified by the negativity [21], which is defined by

$$\mathcal{N}(\rho^{ij}) = 2\max(0, -\min_\alpha(\mu_\alpha^{ij})), \qquad (30)$$

where μ_α^{ij} are the eigenvalues of the partial transpose ρ^{ij,T_A} of the density operator ρ^{ij}, defined as $\langle\alpha\beta|\rho^{T_A}|\gamma\delta\rangle = \langle\gamma\beta|\rho|\alpha\delta\rangle$. For the XXZ model, $U(1)$ invariance ($[H, \Sigma_i\sigma_z^i] = 0$) and translation invariance ensure that the reduced density matrix for spins i and j reads

$$\rho^{ij} = \begin{pmatrix} a^{ij} & 0 & 0 & 0 \\ 0 & b^{ij} & z^{ij} & 0 \\ 0 & z^{ij*} & b^{ij} & 0 \\ 0 & 0 & 0 & d^{ij} \end{pmatrix}, \qquad (31)$$

where

$$a^{ij} = \frac{1}{4}(1 + 2G_z + G_{zz}^{ij}),$$

$$b^{ij} = \frac{1}{4}(1 - G_{zz}^{ij}),$$

$$d^{ij} = \frac{1}{4}(1 - 2G_z + G_{zz}^{ij}),$$

$$z^{ij} = \frac{1}{4}[(G_{xx}^{ij} + G_{yy}^{ij}) + i(G_{xy}^{ij} - G_{yx}^{ij})], \qquad (32)$$

where $G_z = \langle\sigma_z^i\rangle$ is the magnetization density (computed for any site i) and $G_{\alpha\beta}^{ij} = \langle\sigma_\alpha^i\sigma_\beta^j\rangle$ ($\alpha, \beta = x, y, z$), with the expectation value taken over an arbitrary quantum state of the system. Moreover, invariance of H_{XXZ} under the discrete trans-

formations $\sigma_x \rightarrow -\sigma_x$, $\sigma_y \rightarrow \sigma_y$, and $\sigma_z \rightarrow -\sigma_z$ implies that $G_{xy}^{ij} = 0$ and $G_{yx}^{ij} = 0$. Therefore, the element z^{ij} in Eq. (32) is real, namely, $z^{ij} = z^{ij*} = 1/4(G_{xx}^{ij} + G_{yy}^{ij})$. Then, evaluation of the negativity for spins i and j from Eq. (31) yields

$$\mathcal{N}(L) = \frac{1}{2} \max(0, \sqrt{4G_z^2 + |G_{xx}^{ij} + G_{yy}^{ij}|^2} - G_{zz}^{ij} - 1). \quad (33)$$

From now on, we will be interested in computing the negativity for nearest-neighbor spins. The generalized HK theorem discussed in Sec. III implies that we can consider Δ as the external potential and $\langle \sigma_i^z \sigma_{i+1}^z \rangle$ (for any site i) as the relevant density. Thus, $\mathcal{N}(L)$ can be written as a function of $\partial \varepsilon / \partial \Delta$ for the ground state as well as for any minimum energy state in a sector of magnetization m ($m = 0, \pm 2, \ldots, \pm L$) and momentum $P = (2\pi/L)p$ ($p = 0, 1, \ldots, L-1$). In this direction, it is convenient to write the correlation functions $G_{\alpha\beta}^{i,i+1}$ in terms of $\partial \varepsilon / \partial \Delta$, which results into

$$G_{zz}^{i,i+1} = -2 \frac{\partial \varepsilon}{\partial \Delta},$$

$$G_{xx}^{i,,i+1} + G_{yy}^{i,i+1} = -2 \left(\varepsilon - \Delta \frac{\partial \varepsilon}{\partial \Delta} \right). \quad (34)$$

A. Ground state entanglement

For the ground state, we have that $G_z = 0$. Then, by using Eq. (34) and Eq. (33), negativity reads

$$\mathcal{N}(L) = -\varepsilon(L) + (\Delta + 1) \frac{\partial \varepsilon(L)}{\partial \Delta} - \frac{1}{2}, \quad (35)$$

where we have used that $|G_{zz}^{i,i+1}| \leq 1$ and $G_{xx}^{i,i+1} + G_{yy}^{i,i+1} \geq 0$ (Marshall-Peierls rule). Note that, in Eq. (35), the energy density $\varepsilon(L)$ can be seen as a function of $\partial \varepsilon / \partial \Delta$ by the HK theorem, which is explicitly shown in Fig. 1. Indeed, this implies that the negativity can be taken as a function of $\partial \varepsilon / \partial \Delta$, which illustrates the duality between potential and density established in Eq. (25) for entanglement measures. The XXZ model is critical in the interval $-1 \leq \Delta < 1$, with central charge $c = 1$. Then, from Eq. (35), we can determine an approximate analytical expression for the negativity in terms of energy as given by Eq. (1). The parameter ξ appearing in Eq. (1) can be obtained analytically [35] for the XXZ chain, reading

$$\xi = \pi \frac{\sin \gamma}{\gamma}, \quad (36)$$

where γ is defined by

$$\Delta = -\cos \gamma, \quad \gamma \in [0, \pi]. \quad (37)$$
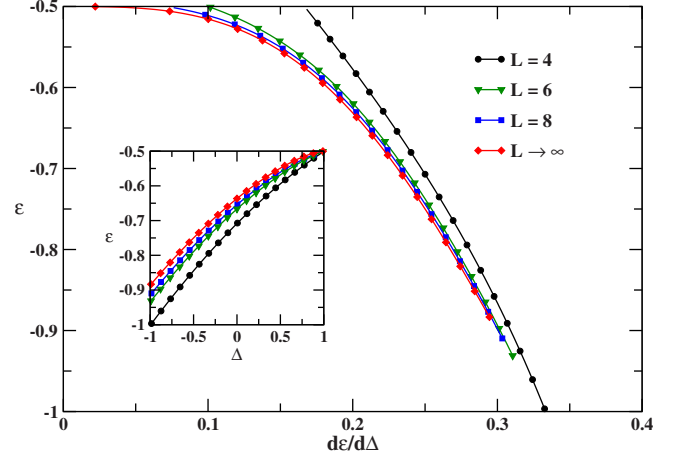
Then, substitution of Eq. (1) into Eq. (35) yields

FIG. 1. (Color online) Density energy ε as a function of $\partial \varepsilon / \partial \Delta$ as given by the solution of the Bethe equations for finite-size chains as well as in the thermodynamic limit (values plotted in the range $-1 < \Delta < 1$). For finite chains with lattice sizes $L > 8$, the curves become nearly superposed with the curve for the infinite chain. Inset: Density energy ε versus anisotropy parameter Δ. Note that ε can be taken either as a function of Δ (the potential) or $\partial \varepsilon / \partial \Delta$ (the density). Units are chosen such that $J = 1$.

$$\mathcal{N}_{CFT}(L) = \mathcal{N}_\infty + \frac{\pi^2 c}{6\gamma L^2} \left(\sin \gamma + \frac{1 + \Delta}{\gamma} + \frac{\Delta \sqrt{1 + \Delta}}{\sqrt{1 - \Delta}} \right) + o(L^{-2}), \quad (38)$$

where $\mathcal{N}_\infty$ can be computed from Eq. (35), with ε_∞ and $\partial \varepsilon_\infty / \partial \Delta$ directly given by the solution of the model at the thermodynamic limit [36]. An exact value for the negativity $\mathcal{N}(L)$ can be obtained from Eq. (35) by computing $\varepsilon(L)$ and $\partial \varepsilon(L) / \partial \Delta$ via Bethe ansatz equations for each length L. Naturally, this amounts to a much harder computational effort for a general Δ, while Eq. (38) directly provides the negativity for a finite chain up to order L^{-2} with no need of solving the Bethe ansatz equations for each length L. A comparison between $\mathcal{N}(L)$ and $\mathcal{N}_{CFT}(L)$ for $\gamma = \pi/2$ and $\gamma = \pi/3$ is exhibited in Tables I and II.

TABLE I. Comparison between $\mathcal{N}(L)$ and $\mathcal{N}_{CFT}(L)$ for $\gamma = \pi/2$ (the XX model). For an infinite chain, we have that negativity is given by $\mathcal{N}(\infty) = 0.339\,262\,139\,652$.

L	$\mathcal{N}(L)$	$\mathcal{N}_{CFT}(L)$
4	0.457106781187	0.446378653269
8	0.366669830087	0.366041268056
16	0.345995599194	0.345956921753
32	0.340938243195	0.340935835178
64	0.339680713890	0.339680563534
128	0.339366755018	0.339366745623
256	0.339288291732	0.339288291145
512	0.339268677562	0.339268677525
1024	0.339263774123	0.339263774121

TABLE II. Comparison between $\mathcal{N}(L)$ and $\mathcal{N}_{CFT}(L)$ for $\gamma = \pi/3$. For an infinite chain, we have that negativity is given by $\mathcal{N}(\infty) = 3/8 = 0.375$.

L	$\mathcal{N}(L)$	$\mathcal{N}_{CFT}(L)$
4	0.489830037812	0.478556230132
8	0.401639244141	0.400889057533
16	0.381525197365	0.381472264383
32	0.376621871264	0.376618066096
64	0.375404791436	0.375404516524
128	0.375101148980	0.375101129131
256	0.375025283711	0.375025282283
512	0.375006320673	0.375006320571
1024	0.375001580150	0.375001580143

B. Twisted boundary conditions

We can also use the results obtained for PBC to investigate the finite-size corrections to the negativity with more general boundary conditions. We will consider here the so-called twisted boundary conditions (TBC), which can be achieved as the effect of a magnetic flux through a spin ring [37]. Remarkably, it has recently been shown that TBC may improve multiparty quantum communication via spin chains [38]. In order to consider TBC, it is convenient to rewrite the Hamiltonian in Eq. (29) (with $J=1$) in the following form:

$$H_{XXZ} = -\frac{1}{2}\sum_{i=1}^{L}[2(\sigma_i^+\sigma_{i+1}^- + \sigma_i^-\sigma_{i+1}^+) + \Delta\sigma_i^z\sigma_{i+1}^z], \quad (39)$$

where $\sigma_j^\pm = (\sigma_j^x \pm i\sigma_j^y)/2$ and $\sigma_{L+1}^\pm = e^{\pm i\Phi}\sigma_1^\pm$ $(0 \leq \Phi < 2\pi)$, with Φ denoting a phase. The quantum chain given by Eq. (39) is solvable by the Bethe ansatz [28]. In presence of TBC, Eq. (1) still holds, but with an effective central $\hat{c}(\Phi)$ [28], which is given by

$$\hat{c}(\Phi) = 1 - \frac{3\Phi^2}{2\pi(\pi-\gamma)}, \quad (40)$$

with γ defined as in Eq. (37). Let us take the following canonical transformations [39]:

$$\tilde{\sigma}_j^\pm = e^{\mp i\Phi j/L}\sigma_j^\pm, \quad \tilde{\sigma}_j^z = \sigma_j^z \ (j=1,\ldots,L). \quad (41)$$

In terms of this new set of operators, the original chain with TBC is now given by the periodic chain

$$H_{XXZ} = -\frac{1}{2}\sum_{j=1}^{L}[e^{-i\Phi/L}\tilde{\sigma}_j^+\tilde{\sigma}_{j+1}^- + e^{i\Phi/L}\tilde{\sigma}_j^-\tilde{\sigma}_{j+1}^+ + \Delta\tilde{\sigma}_j^z\tilde{\sigma}_{j+1}^z],$$
$$(42)$$

where $\tilde{\sigma}_{L+1}^\pm = \tilde{\sigma}_1^\pm$. Defining the operators $\tilde{\sigma}_j^x$ and $\tilde{\sigma}_j^y$ through $\tilde{\sigma}_j^\pm = (\tilde{\sigma}_j^x \pm i\tilde{\sigma}_j^y)/2$, the Hamiltonian can be put in the form

$$H_{XXZ} = -\frac{1}{2}\sum_{j=1}^{L}\left[\cos\left(\frac{\Phi}{L}\right)\frac{(\tilde{\sigma}_j^x\tilde{\sigma}_{j+1}^x + \tilde{\sigma}_j^y\tilde{\sigma}_{j+1}^y)}{2}\right.$$
$$\left. -\sin\left(\frac{\Phi}{L}\right)\frac{(\tilde{\sigma}_j^x\tilde{\sigma}_{j+1}^y - \tilde{\sigma}_j^y\tilde{\sigma}_{j+1}^x)}{2} + \Delta\tilde{\sigma}_j^z\tilde{\sigma}_{j+1}^z\right]. \quad (43)$$

Note that the Hamiltonian in Eq. (43) is both U(1) invariant ($[H,\Sigma_j\tilde{\sigma}_j^z]=0$) and translationally invariant (H_{XXZ} exhibits PBC in terms of the set $\{\tilde{\sigma}_j^\pm, \tilde{\sigma}_j^z\}$). Therefore, the two-spin reduced density matrix keeps the form given in Eq. (31), with the correlation functions $G_{\alpha\beta}^{ij}$ replaced by $\tilde{G}_{\alpha\beta}^{ij} = \langle\tilde{\sigma}_\alpha^i\tilde{\sigma}_\beta^j\rangle$. Then, the negativity for nearest-neighbor spins governed by Hamiltonian (43) can be computed similarly as before. By using that $G_z = 0$ (ground state) and $|G_{zz}^{i,i+1}| \leq 1$ we obtain

$$\mathcal{N} = 2\max(0,|z|-a), \quad (44)$$

where $a = (1+\tilde{G}_{zz})/4$ and $z = (\tilde{G}_\| + i\tilde{G}_\perp)/4$, with $\tilde{G}_{zz} = \tilde{G}_{zz}^{i,i+1}$, $\tilde{G}_\| = \tilde{G}_{xx}^{i,i+1} + \tilde{G}_{yy}^{i,i+1}$, and $\tilde{G}_\perp = \tilde{G}_{xy}^{i,i+1} - \tilde{G}_{yx}^{i,i+1}$ ($\forall i$). In order to write entanglement in terms of the derivatives of the energy density, it is convenient to define $\bar{H}_{XXZ} = H_{XXZ}/\cos(\Phi/L)$. Then

$$\bar{\varepsilon} = -\frac{1}{2}(\tilde{G}_\| - \eta\tilde{G}_\perp + \bar{\Delta}\tilde{G}_{zz}), \quad (45)$$

where $\bar{\varepsilon} = \langle\bar{H}_{XXZ}\rangle/L$, $\eta = \tan(\Phi/L)$, and $\bar{\Delta} = \Delta/\cos(\Phi/L)$. From Eq. (45) we obtain

$$\tilde{G}_{zz} = -2\frac{\partial\bar{\varepsilon}}{\partial\bar{\Delta}},$$

$$\tilde{G}_\perp = 2\frac{\partial\bar{\varepsilon}}{\partial\eta},$$

$$\tilde{G}_\| = 2\left(-\bar{\varepsilon} + \eta\frac{\partial\bar{\varepsilon}}{\partial\eta} + \bar{\Delta}\frac{\partial\bar{\varepsilon}}{\partial\bar{\Delta}}\right). \quad (46)$$

Therefore, the contribution $(|z|-a)$ for expression for the negativity in Eq. (44) reads

$$|z|-a = \frac{1}{2}\left[\sqrt{\left(-\bar{\varepsilon}+\eta\frac{\partial\bar{\varepsilon}}{\partial\eta}+\bar{\Delta}\frac{\partial\bar{\varepsilon}}{\partial\bar{\Delta}}\right)^2 + \left(\frac{\partial\bar{\varepsilon}}{\partial\eta}\right)^2} + \frac{\partial\bar{\varepsilon}}{\partial\bar{\Delta}} - \frac{1}{2}\right].$$
$$(47)$$

In order to obtain the results in terms of Φ and Δ, we make use of the expressions

$$\frac{\partial\bar{\varepsilon}}{\partial\eta} = \cos\left(\frac{\Phi}{L}\right)\left[L\frac{\partial\varepsilon}{\partial\Phi} + \tan\left(\frac{\Phi}{L}\right)\varepsilon\right], \quad (48)$$

$$\frac{\partial\bar{\varepsilon}}{\partial\bar{\Delta}} = \frac{\partial\varepsilon}{\partial\Delta}. \quad (49)$$

Hence, finite-size corrections to entanglement can be found now by using Eq. (1) [replacing the central charge c by the effective central charge $\hat{c}(\Phi)$ as in Eq. (40)] into Eq. (47).

TABLE III. Comparison between the exact evaluation of $\mathcal{N}(L)$ and the approximate expression $\mathcal{N}_{CFT}(L)$ (up to order L^{-2}) for $\gamma = \pi/2$ and $\Phi = \pi/2$.

L	$\mathcal{N}(L)$	$\mathcal{N}_{CFT}(L)$
4	0.406774810601	0.446378653269
8	0.354315234931	0.366041268056
16	0.342922395530	0.345956921753
32	0.340170924101	0.340935835178
64	0.339488945731	0.339680563534
128	0.339318816833	0.339366745623
256	0.339276307427	0.339288291145
512	0.339265681501	0.339268677525
1024	0.339263025109	0.339263774121

Examples comparing the negativity $\mathcal{N}_{CFT}(L)$ for nearest neighbors up to $o(L^{-2})$ and the exact value of the negativity $\mathcal{N}(L)$ (obtained through the numerical solution of the Bethe ansatz equations derived in Ref. [28]) are exhibited in Tables III and IV below.

Note from Tables I and III that, for $\gamma = \pi/2$, $\mathcal{N}_{CFT}(L)$ gives the same result either for $\Phi = 0$ (PBC) or $\Phi = \pi/2$, which is an indication that TBC should not affect the negativity [up to $o(L^{-2})$] in the case of the XX model. Indeed, this can be analytically proved. In this case, the anisotropy is $\Delta = 0$, which implies that $\gamma = \pi/2$ and $\xi = 2$. Then, from Eqs. (1) and (40), we have

$$\varepsilon(L) = \varepsilon_\infty - \frac{\pi \hat{c}(\Phi)}{3} L^{-2} + o(L^{-2}),$$

$$\frac{\partial \varepsilon}{\partial \Phi} = \frac{2}{\pi} \frac{\Phi}{L^2} + o(L^{-2}),$$

$$\frac{\partial \varepsilon}{\partial \Delta} = \left. \frac{\partial \varepsilon_\infty}{\partial \Delta} \right|_{\Delta=0} + \frac{2}{3L^2} + o(L^{-2}). \quad (50)$$

By inserting the above equations into Eqs. (48) and (49), it can be shown that the negativity as given by Eq. (44) becomes

TABLE IV. Comparison between the exact evaluation of $\mathcal{N}(L)$ and the approximate expression $\mathcal{N}_{CFT}(L)$ (up to order L^{-2}) for for $\gamma = \pi/3$ and $\Phi = 2\pi/3$.

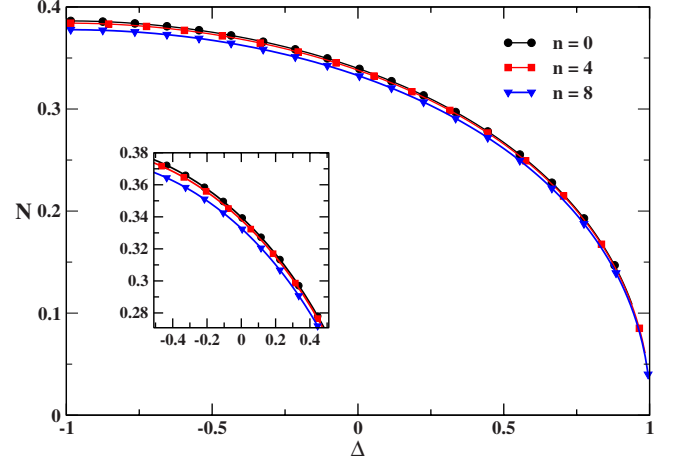| L	$\mathcal{N}(L)$	$\mathcal{N}_{CFT}(L)$
4	0.400000000000	0.452230707893
8	0.381121448251	0.394307676973
16	0.376577662094	0.379826919243
32	0.375405200439	0.376206729811
64	0.375102994373	0.375301682453
128	0.375025983614	0.375075420613
256	0.375006526789	0.375018855153
512	0.375001635654	0.375004713788
1024	0.375000409414	0.375001178447

FIG. 2. (Color online) Negativity for minimum energy states as a function of the anisotropy Δ for $L=256$ sites. Note that the curves are nearly the same, indicating a unique entanglement pattern in the critical region. Inset: Negativity as a function of Δ in a larger zoom scale. Units are chosen such that $J=1$.

$$\mathcal{N}_{CFT} = |\varepsilon_{(\Phi=0)}| + \left. \frac{\partial \varepsilon_\infty}{\partial \Delta} \right|_{\Delta=0} + \frac{2}{3L^2} - \frac{1}{2} + o(L^{-2}), \quad (51)$$

where $|\varepsilon_{(\Phi=0)}| = \sqrt{\varepsilon_\infty^2 - 2\varepsilon_\infty \pi \xi/(6L^2)}$. Hence, Eq. (51) implies that the negativity for the XX model with TBC is not affected by the phase Φ up to order $1/L^2$.

C. Excited states

Let us consider now the structure of the negativity for the excited states in the XXZ model with PBC. The $U(1)$ and translation symmetries allow us the decomposition of the associated eigenspace of H_{XXZ} into disjoint sectors (fixed magnetization and momentum) labeled by the quantum numbers $r = 0, 1, 2, \ldots, L$ and $p = 1, 2, \ldots, L-1$, which give the number of spins up in the σ_z basis and the eigenvalue of the momentum $P = (2\pi/L)p$, respectively. An exact evaluation of the negativity for nearest-neighbor spins can be performed from Eq. (33) by taking a nonvanishing magnetization density G_z and by using Eq. (34), where the energy of the excited state is obtained through the solution of the Bethe ansatz equations. This is illustrated in Fig. 2, where we plot the negativity between nearest neighbors in a chain of length $L = 256$ sites for minimum energy states with zero momentum in several magnetization sectors. These states have anomalous dimensions x_n given by [28]

$$x_n = n^2 \frac{(\pi - \gamma)}{2\pi}, \quad (52)$$

where $n = L/2 - r$ and $j + j' = p = 0$ in Eq. (2). Remarkably, note that the negativities for the minimum energy states plotted are nearly the same, indicating a unique entanglement pattern in the critical region. Indeed, this is a more general result, which holds also for other excited states. For instance, let us take the so-called marginal state [28], which is a state that will be taken in the sector $n=0$ with anomalous dimension $x=2$ (independently of γ) and $j, j' = 0$. Exact computa-

TABLE V. Comparison between $\mathcal{N}(\Delta)$ for the marginal state and $\mathcal{N}(\Delta)$ for the ground state in a chain with $L=256$ sites.

Δ	Marginal state	Ground state
0.505023772863	0.265447369819	0.266151418398
0.205023772863	0.315358910123	0.316005319520
0.005023772863	0.338660739066	0.339288291732
−0.204976227137	0.357090720201	0.357706303640
−0.504976227137	0.374867541783	0.375473489099

tion in Table V shows that its negativity is also close to the values found in Fig. 2. Indeed, we can show that entanglement in the critical region of the *XXZ* chain will exhibit a unique pattern for all states accessible via the CFT associated with the model. As discussed in Sec. II, each primary operator of the theory corresponds to a tower of states with energies given by Eq. (2). All these states in the towers will have energies which differ at order L^{-2} [see Eqs. (1) and (2)]. According to Eq. (33), such a difference is also reflected in the negativity of nearest-neighbor spins, which explains the behavior displayed in both Fig. 2 and Table V. This can explicitly be shown by inserting Eq. (2) into Eq. (33). As an illustration, we take the minimum energy states with zero momentum in a given magnetization sector labeled by n. For this case, the negativity can be evaluated as

$$\mathcal{N}_n(L) = \mathcal{N}_n^\infty + \frac{|G_\infty|^{-1}}{6\gamma L^2}\left[3\gamma n^2 + \pi \sin \gamma G_\infty z_n + \pi(\Delta G_\infty + |G_\infty|)\right.$$

$$\left. \times \left(\frac{w_n}{\gamma} - z_n \cot \gamma \right) \right] + o(L^{-2}),$$

where

$$w_n = \pi(c - 6n^2), \quad \mathcal{N}_n^\infty = |G_\infty| + \partial \varepsilon_n^\infty / \partial \Delta - 1/2,$$

$$z_n = [\pi c - 6n^2(\pi - \gamma)], \quad G_\infty = -\varepsilon_n^\infty + \Delta \partial \varepsilon_n^\infty / \partial \Delta,$$

with ε_n^∞ denoting the energy density of the excited state as $L \to \infty$. Note that this unique pattern of entanglement, which has been explicitly derived here, is in agreement with the general discussion of Sec. IV. This is indeed exhibited in Eq. (28). Naturally, similar expressions can be obtained for excited states higher than the minimum energy states.

VI. CONCLUSION

In conclusion, we have investigated the computation of finite-size corrections to entanglement in quantum critical systems. These corrections were shown to depend on the central charge of the model as well as the anomalous dimensions of the primary operators of the theory. Our approach has naturally arisen as a general consequence of the application of CFT and DFT methods in critical theories. This framework has been illustrated in the *XXZ* model, where we have shown that (i) entanglement in spin chains with arbitrary finite sizes can be analytically computed up to order $o(L^{-2})$ with no need of solving the Bethe ansatz equations for each length L; (ii) conformal towers of excited states displays a unique pattern of entanglement in the critical region. Indeed, we have been able to provide a general argument according to which this unique pattern of entanglement should appear in all conformally invariant models. Further examples in higher dimensional lattices and higher spin systems are left for future investigation.

ACKNOWLEDGMENTS

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