Entanglement and boundary entropy in quantum spin chains with arbitrary direction of the boundary magnetic fields

J. C. Xavier¹,* and M. A. Rajabpour²

¹Universidade Federal de Uberlândia, Instituto de Física, C.P. 593, 38400-902 Uberlândia, MG, Brazil
²Instituto de Física, Universidade Federal Fluminense, Av. Gal. Milton Tavares de Souza s/n, Gragoatá, 24210-346 Niterói, RJ, Brazil

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We calculate the entanglement and the universal boundary entropy (BE) in critical quantum spin chains, such as the transverse field Ising chain and the XXZ chain, with arbitrary direction of the boundary magnetic field (ADBMF). We determine the boundary universality class that an ADBMF induces. In particular, we show that the induced boundary conformal field theory depends on the point on the Bloch sphere where the boundary magnetic field directs. We show that the classification of the directions boils down to the simple fact that the boundary field breaks the bulk symmetry or does not. We present a procedure to estimate the universal BE, based on the finite-size corrections of the entanglement entropy, which apply to ADBMF. To calculate the universal BE in the XXZ chain, we use the density matrix renormalization group. The transverse field XY chain with ADBMF after Jordan-Wigner transformation is not a quadratic free fermion Hamiltonian. We map this model to a quadratic free fermion chain by introducing two extra ancillary spins coupled to the main chain at the boundaries, which makes the problem integrable. The eigenstates of the transverse field XY chain can be obtained by proper projection in the enlarged chain. Using this mapping, we are able to calculate the entanglement entropy of the transverse field XY chain using the usual correlation matrix technique up to relatively large sizes.

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I. INTRODUCTION

Quantum entanglement in many-body systems has been studied in great detail in the last couple of decades. There are comprehensive reviews on the applications of entanglement entropy in condensed matter physics [1], quantum field theories [2], integrable models [3], and conformal field theory (CFT) [4]. There are several motivations to study quantum entanglement. For instance, entanglement is an essential ingredient in quantum computation and in many other applications [1,5]. For these reasons, the quantification of entanglement has been studied extensively. The entanglement entropy, which is one of the most used quantifiers of entanglement in pure bipartite systems, was measured recently in one-dimensional quantum systems [6,7].

The bipartite entanglement entropy is defined as \( S = -\text{tr} \rho_A \ln \rho_A \), where \( \rho_A \) is the reduced density matrix of subsystem \( A \). It is well understood for the ground state of critical and noncritical quantum chains. One of the major outcomes of all these studies was the central role of the entanglement entropy in distinguishing different phases and classifying the critical point of the continuous phase transitions into different universality classes consistent with the traditional classification based on local observables. Most of the above studies were based on the bulk properties, however, there have also been many studies regarding the entanglement entropy in systems with boundaries. In the presence of boundaries analytical and numerical calculations of the entanglement entropy are normally a bit more challenging because of the lack of translational invariance. Nevertheless, the entanglement entropy of a few quantum chains in the presence of boundaries has been studied with analytical and numerical techniques (see, for instance, Refs. [8–15] and Ref. [1] for a review).

In the presence of a boundary there is an interesting degree of freedom in which the bulk of the system can be at the critical point, but the boundary can be noncritical and flow between different fixed points under the boundary renormalization group (see Ref. [16] and references therein). In one spatial dimension this kind of flow in the language of CFT in connection with impurity problems such as the Kondo problem has already been studied [17]. The interesting observation in Ref. [17] is that for a system with its bulk at the critical point one can define a boundary entropy (BE) which decreases under the boundary renormalization group and, at the boundary fixed point, is equal to a number which is related to the universality class of the corresponding boundary condition. This BE in the context of the entanglement entropy has been studied in CFT [18–20], quantum spin chains [8–11,14,15,19,21,22], and integrable models [12]. In particular, using the density matrix renormalization-group (DMRG) technique the authors of Ref. [23] estimate the universal BE for the transverse field Ising chain with particular boundary conditions, mainly a boundary magnetic field in the \( x \) direction. In this work, we would like to generalize this idea in a few directions.

From the physics point of view, it is interesting to classify the boundary conditions in quantum spin chains when there
is a magnetic field at the boundary in an arbitrary direction. We would like to do this classification by evaluating the contribution of the BE. Precise determination of the BE, even numerically, can be challenging from the technical point of view. In this vein, we present a simple procedure to estimate the BE which is based on finite-size scaling of the entanglement entropy. In order to illustrate that the procedure works quite well, we consider the two most interesting models: the transverse field Ising chain and the XXZ chain. For the XY chain (the transverse field Ising chain is a particular case of this model) in the presence of an arbitrary direction of the boundary magnetic field (ADBMF), we were able to map the problem of the diagonalization of the model to a free fermion model which can be diagonalized in a linear time. To the best of our knowledge this problem has not been tackled before in the literature (see Ref. [24] for the solution of the XX chain with ADBMF) and it seems interesting for its own sake. After solving the XY chain with ADBMF we use a modified version of the Peschel method [25] to calculate the entanglement entropy of finite systems. In the case of the XXZ chain with ADBMF we tackle the problem with the DMRG [26,27]. Having the finite-size corrections of the entanglement entropy of those models, we show that it is possible to estimate the BE for an ADBMF and classify the corresponding boundary CFT, using relatively large system sizes.

The paper is organized as follows: In Sec. II, we first define the universal BE and introduce the relevant equations and notations. In Sec. III, we solve the Hamiltonian of the XY chain with ADBMF. Then we find the correlation functions and generalize the Peschel method to calculate the entanglement entropy. We close this section by presenting our numerical results regarding the universal BE in the transverse field Ising chain with ADBMF. In Sec. IV, we study the boundary entanglement entropy in the XXZ chain with ADBMF using the DMRG technique. Finally, in Sec. V, we summarize our findings.

II. BOUNDARY ENTROPY IN CFT

Consider a one-dimensional quantum field theory defined in a system of length $L$ with boundary conditions $a$ and $b$ at $x = 0$ and $L$, respectively. The partition function of this system at inverse temperature $\beta$ is given by the partition function of a two-dimensional system on a cylinder with particular boundary conditions. According to the Affleck-Ludwig argument [17] when we have a CFT in the limit of large $L$ and $\beta$ the free energy of the system behaves as $F = -L f + f'$, where $f'$ has, in addition to the nonuniversal contribution, also a universal BE, i.e., $f_a + f_b$, with $f_{a,b} = -\frac{1}{\beta} \ln g_{a,b}$, where $g_a = \langle B_a(0) \rangle$ and $g_b = \langle 0 | B_b \rangle$. The states $| B_{a,b} \rangle$ are the so-called conformal boundary states [28,29]. This means that the one-dimensional CFT defined on a segment has a nontrivial zero-temperature BE, or ground-state degeneracy. In other words, we have a ground-state degeneracy which should be understood as a particular behavior of the low-energy density of states in CFT. It was suggested in [17] and later proved in [30] that the quantity $g$ decreases under the boundary renormalization group for systems in which the bulk is already at the critical phase.

An equivalent description using the entanglement entropy was first suggested in [18]. The idea is as follows: Consider first the entanglement entropy of the ground state of a CFT with periodic boundary conditions (PBCs) and length $L$; then the entanglement entropy of a subsystem of length $\ell$ behaves as [18,31–33]

$$S_{\text{PBC}}(L, \ell) = \frac{c}{3} \ln \left[ \frac{L}{\pi} \sin \left( \frac{\pi \ell}{L} \right) \right] + c_{\text{PBC}} \ell^2,$$  

where $c$ is the central charge.

However, for systems with boundaries the entanglement entropy of a segment starting from one boundary and of length $\ell$ behaves as [13,14,18,23]

$$S'(L, \ell) = \frac{c}{6} \ln \left[ \frac{2L}{\pi} \sin \left( \frac{\pi \ell}{L} \right) \right] + c_{\text{PBC}} \ell^2 / 2 + \ln(g) + G_b \left( \frac{\ell}{L} \right),$$

where $s_b = \ln(g)$ is the BE and $G_b(\xi) = \lim_{n \to -1} \frac{1}{n^2} \ln F^{(n)}_\gamma$, where

$$F^{(n)}_\gamma(x) = \frac{e^{2\pi n(\pi - 1)h \gamma}}{n^{\pi n h}} \langle \prod_{k=0}^{n} \Upsilon(z_{n,k}) \Upsilon(\zeta_{n,k}) \rangle,$$  

where $z_{n,k} = e^{\xi(\pm x + 2k)}$, $k = 0, \ldots, n - 1$, and $\Upsilon$ is a chiral primary field with conformal dimension $h_\gamma$ [14].

We intend to get estimates of the BE, or equivalently the ground-state degeneracy $g$, by using the finite-size scaling of the entanglement entropies introduced above. When $G_b = 0$, this task is quite simple. First, we get the nonuniversal constant $c_{\text{PBC}}$ by using Eq. (1) and plug this result into Eq. (2) to obtain $s_b$. The authors of Ref. [23] used this procedure to extract $s_b$ of the transverse field Ising chain, with an open boundary condition (OBC) and boundary magnetic fields in the $x$ direction. However, in general, $G_b$ is nonzero, and if we do not know this function, we cannot use this procedure to determine $s_b$. Of course if we knew the nonuniversal function $G_b$, in principle, we could use the same procedure to extract $s_b$. It is important to emphasize that obtaining $G_b$, or equivalently $F^{(n)}(x)$, which depends on the model, is not a simple task. For integer values of $n$, $F^{(n)}(x)$ is known for the free boson theory as well as the transverse field Ising chain (see Refs. [34] and [14]). Note that to calculate $G_b$ it is necessary to analytically continue the function $F^{(n)}(x)$ to noninteger values of $n$, which is a nontrivial task (see, for instance, Ref. [35]).

Motivated by the above discussion, we present a procedure to obtain $s_b$ numerically, without knowing the function $G_b$, as we explain in the following. First, note that the BE is related to the entanglement entropies of systems under PBCs and with boundaries by

$$s_b = \ln(g) = S^b - \frac{S_{\text{PBC}}}{2} - \frac{c}{6} \ln(2) - G_b \left( \frac{\ell}{L} \right).$$

Due to the finite-size scaling of the entanglement entropies defined in Eqs. (1) and (2) it is convenient to define $f(x) = S^b - \frac{S_{\text{PBC}}}{2} - \frac{c}{6} \ln(2) - G_b \left( \frac{\ell}{L} \right)$. Now, inspired by the behavior of the nonuniversal function $G_b(x)$ for small values
of $x$ (see Ref. [34]), we assume that $f(x)$ behaves as

$$f(x) = \ln(g) + \frac{2\pi^2}{3} a_1 x^2 + a_2 x^4 + \frac{a_3}{x^{a_4}},$$  \hspace{1cm} (5)$$

where we have added the term $a_3/x^{a_4}$ due to the unusual corrections [36–40]. So, to get numerical estimates of the BE we fit the numerical data of the entanglement entropies to Eq. (5). We illustrate the above procedure for the transverse field Ising chain and the XXZ model with ADBMF in the next sections.

We close this section by mentioning that in order to investigate which are the conformally invariant boundary conditions, we apply boundary magnetic fields $h_b$ in the lattice models. Usually, for $0 < h_b < \infty$ the conformal invariance is lost and we can associate a crossover length $\xi \sim h_b^{-1/d}$, where $d < 1$ is the scaling dimension of the relevant boundary perturbation. The above equation is valid only for $\ell > \xi$ [41].

### A. Diagonalization of the finite chain using the ghost site technique

In this section, we show how it is possible to obtain the energies and the correlation matrices of the transverse field XY chain in the presence of an ADBMF. The route we follow is the same as the one used in Ref. [24] for the XX chain with boundary magnetic fields. For earlier use of the same technique see Refs. [42–44]. We consider the XY Hamiltonian with ADBMF,

$$H_{XY} = J \sum_{j=1}^{L-1} [(1 + \gamma) S^x_j S^x_{j+1} + (1 - \gamma) S^y_j S^y_{j+1}] - \hbar \sum_{j=1}^{L} S^z_j + \vec{b}_1 \cdot \vec{S}_1 + \vec{b}_L \cdot \vec{S}_L,$$  \hspace{1cm} (6)$$

where $S^\alpha = \frac{1}{2} \sigma^\alpha$, $\sigma^\alpha$ ($\alpha = x, y, z$) are the Pauli matrices and

$$\vec{b}_1 = b_1 (\sin \theta_1 \cos \phi_1, \sin \theta_1 \sin \phi_1, \cos \theta_1),$$  \hspace{1cm} (7)$$

$$\vec{b}_L = b_L (\sin \theta_L \cos \phi_L, \sin \theta_L \sin \phi_L, \cos \theta_L).$$  \hspace{1cm} (8)$$

The transverse field XY chain has a few interesting critical lines. On $h = \pm J$ and $\gamma \neq 0$ we have the universality of the critical Ising chain with the central charge $c = \frac{1}{2}$. On $\gamma = 0$ and $-1 < h < 1$ we have the universality class of the compactified bosons with the central charge $c = 1$. The other parts of the phase diagram are not critical, and although all the calculations of this section are valid for the full phase diagram, in later sections we concentrate mostly on the critical parts of the phase diagram.

It is convenient to rewrite the above Hamiltonian in terms of $\sigma^\pm = \frac{\sigma^x + i\sigma^y}{2}$ and $\sigma^z$ as follows:

$$H_{XY} = \frac{J}{2} \sum_{j=1}^{L-1} (\sigma_+^j \sigma_-^{j+1} + \gamma \sigma_+^j \sigma_+^{j+1} + \text{H.c.}) - \hbar \sum_{j=1}^{L} \sigma_j^z + \frac{1}{2} b_1 (\sin \theta_1 e^{-i\phi_1} \sigma_1^+ + \sin \theta_1 e^{i\phi_1} \sigma_1^- + \cos \theta_1 \sigma_1^z)$$

$$+ \frac{1}{2} b_L (\sin \theta_L e^{-i\phi_L} \sigma_L^+ + \sin \theta_L e^{i\phi_L} \sigma_L^- + \cos \theta_L \sigma_L^z).$$

Note that if we try to diagonalize the above Hamiltonian by using the Jordan-Wigner transformation we realize that the fermionic Hamiltonian is not in a bilinear form in terms of creation and annihilation operators. In order to circumvent this issue, we follow the procedure used in Ref. [24] and consider another spin Hamiltonian, $H_{\text{long}}$, which has two extra sites $(0$ and $L + 1)$, i.e., ghost sites, interacting with the spins at sites 1 and $L$, as explained in the following. We first define the following enlarged Hamiltonian:

$$H_{\text{long}} = \frac{J}{2} \sum_{j=1}^{L-1} [(\sigma_+^j \sigma_-^{j+1} + \sigma_-^j \sigma_+^{j+1}) + \gamma (\sigma_+^j \sigma_+^{j+1} + \sigma_-^j \sigma_-^{j+1})] - \hbar \sum_{j=1}^{L} \sigma_j^z$$

$$+ \frac{1}{2} b_1 (\sin \theta_1 e^{-i\phi_1} \sigma_0^+ \sigma_1^+ + \sin \theta_1 e^{i\phi_1} \sigma_0^- \sigma_1^- + \cos \theta_1 \sigma_1^z)$$

$$+ \frac{1}{2} b_L (\sin \theta_L e^{-i\phi_L} \sigma_L^+ \sigma_{L+1}^+ + \sin \theta_L e^{i\phi_L} \sigma_L^- \sigma_{L+1}^- + \cos \theta_L \sigma_{L+1}^z).$$  \hspace{1cm} (9)$$
The above Hamiltonian commutes with $\sigma_0^z$ and $\sigma_{L+1}^z$. Hence it is possible to block diagonalize $H_{\text{long}}$ in four distinct sectors, labeled by the eigenvalues of $\sigma_0^z$ and $\sigma_{L+1}^z$. We denote these sectors $(s_0, s_{L+1})$, where $s_j = \pm 1$ ($j = 0$ or $j = L + 1$) are the eigenvalues of $\sigma_j^z$, whose eigenstates are $|s_j\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |s_j\downarrow\rangle)$. Note that

$$|\Phi_{k}^{\text{long}}(+, +)\rangle = |+\rangle \otimes |\Psi_{k}^{XY}\rangle \otimes |+\rangle \quad (10)$$

are eigenstates of $H_{\text{long}}$ and $|\Psi_{k}^{XY}\rangle$ are the eigenstates of the XY chain with energy $E_{XY}$. This means that with knowledge of $|\Phi_{k}^{\text{long}}(+, +)\rangle$ it is possible to obtain $|\Psi_{k}^{XY}\rangle$ by projecting, appropriately, the state $|\Phi_{k}^{\text{long}}(+, +)\rangle$. This procedure is discussed in detail below. It is worth mentioning that the spectrum of $H_{\text{long}}$ will be at least twice degenerate due to the fact that $H_{\text{long}}$ is invariant under the transformation $\sigma_j^z \rightarrow -\sigma_j^z$ with $a = x, y$ and $\sigma_j^z \rightarrow \sigma_j^z$.

Using the Jordan-Wigner transformation

$$c_i^j = \prod_{j=0}^{l-1} \sigma_j^+ \sigma_j^-, \quad c_l = \prod_{j=0}^{l-1} \sigma_j^-, \quad (11)$$

we map the Hamiltonian $H_{\text{long}}$ to the free fermion Hamiltonian

$$H_{\text{ff}}^{\text{long}} = -\frac{J}{2} \sum_{j=1}^{L-1} (c_j^+ c_{j+1} + \gamma c_j^+ c_j c_j + c_j^+ c_j + \gamma c_j^+ c_j) - \frac{\hbar}{2} \sum_{j=1}^{L} (2c_j^+ c_j - 1)$$

$$- \frac{b_1}{2} \left[ \sin \theta_1 e^{i\phi_1} c_0^+ c_1 + \sin \theta_1 e^{-i\phi_1} c_0 c_1^+ + \sin \theta_1 e^{i\phi_1} c_0 c_1 - \cos \theta_1 (2c_1^+ c_1 - 1) \right]$$

$$- \frac{b_1}{2} \left[ \sin \theta_1 e^{i\phi_1} c_{L+1}^+ c_L + \sin \theta_1 e^{-i\phi_1} c_L c_{L+1}^+ + \sin \theta_1 e^{i\phi_1} c_L c_{L+1} - \cos \theta_1 (2c_{L+1}^+ c_L - 1) \right], \quad (12)$$

which is bilinear in terms of the creation and annihilation operators and can be diagonalized using the standard method, which is explained in the following. It is convenient to write the above Hamiltonian as

$$H_{\text{ff}}^{\text{long}} = \sum_{i,j=0}^{L+1} \left[ c_i^+ A_{ij} c_j + \frac{1}{2} c_i^+ B_{ij} c_j + \frac{1}{2} c_i^+ B_{ji} c_j \right] - \frac{1}{2} \text{Tr} A^*,$$

where the exact forms of matrices $A$ and $B$, which are crucial for later calculations and arguments, are

$$A = \begin{pmatrix}
0 & -\frac{1}{2} b_1 \sin \theta_1 e^{i\phi_1} & 0 & \ldots \\
-\frac{1}{2} b_1 \sin \theta_1 e^{-i\phi_1} & -\hbar + b_1 \cos \theta_1 & -\frac{\gamma_1}{2} & 0 & \ldots \\
0 & -\frac{\gamma_1}{2} & -\hbar & -\frac{\gamma_1}{2} & 0 & \ldots \\
. & . & . & . & . & . \\
. & . & . & . & . & . \\
. & . & . & . & . & . \\
. & . & . & . & . & . \\
0 & 0 & -\frac{\gamma_1}{2} & -\hbar & -\frac{\gamma_1}{2} & 0 & \ldots \\
. & . & . & . & . & . & . & \end{pmatrix}, \quad (13)$$

and

$$B = \begin{pmatrix}
0 & -\frac{1}{2} b_1 \sin \theta_1 e^{-i\phi_1} & 0 & \ldots \\
\frac{1}{2} b_1 \sin \theta_1 e^{-i\phi_1} & 0 & -\frac{\gamma_1}{2} & 0 & \ldots \\
0 & \frac{\gamma_1}{2} & 0 & -\frac{\gamma_1}{2} & 0 & \ldots \\
. & . & . & . & . & . & . \\
. & . & . & . & . & . & . \\
. & . & . & . & . & . & . \\
. & . & . & . & . & . & . \\
0 & 0 & -\frac{\gamma_1}{2} & 0 & -\frac{1}{2} b_1 \sin \theta_1 e^{-i\phi_1} & 0 \\
. & . & . & . & . & . & . & \end{pmatrix}. \quad (14)$$

Note that matrix $A$ is Hermitian while matrix $B$ is antisymmetric.

In order to diagonalize the above Hamiltonian, it is convenient to rewrite it in the matrix form

$$H_{\text{ff}}^{\text{long}} = \frac{1}{2} (c^+ \ M \ c) \left( c^+ \right), \quad (15)$$

where

$$M = \begin{pmatrix}
A & B \\
-B^* & -A^* \\
\end{pmatrix}. \quad (16)$$
is a \((2L + 4) \times (2L + 4)\) Hermitian matrix and we denote \((c^\dagger, c) = (c_0^\dagger, c_1^\dagger, \ldots, c_{L+1}^\dagger, c_0, c_1, \ldots, c_{L+1})\).

Due to the special form of the Hermitian matrix \(M\) one can always find a unitary matrix in the form

\[
U = \begin{pmatrix} g^* & h \\ h^* & g \end{pmatrix},
\]

which diagonalizes matrix \(M\), where \(g\) and \(h\) are \((L + 2) \times (L + 2)\) matrices. Due to this fact, one can write

\[
H_{ff}^{\text{long}} = \frac{1}{2}(c^\dagger c)U U^\dagger \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} U^\dagger \begin{pmatrix} c \\ c^\dagger \end{pmatrix} = \frac{1}{2}(\eta^\dagger \eta)A \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix},
\]

where we have introduced new fermionic operators,

\[
\begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix} = U \begin{pmatrix} c \\ c^\dagger \end{pmatrix}.
\]

Furthermore, it is easy to prove that the eigenvalues of matrix \(M\) appear in pairs, i.e., \(\pm \lambda_i\), and one can write

\[
A = \begin{pmatrix} \Lambda_1 & 0 \\ 0 & -\Lambda_1 \end{pmatrix}.
\]

Finally, one can write the diagonalized form of the Hamiltonian as

\[
H_{ff}^{\text{long}} = \sum_k \lambda_k \eta_k^\dagger \eta_k - \frac{1}{2} \text{Tr}A_1,
\]

where the modes are ordered as \(0 = \lambda_0 \leq \lambda_1 \leq \ldots \leq \lambda_{L+1}\).

It is easy to check that matrix \(M\) has \textit{at least two} eigenvectors corresponding to the zero eigenvalue, due to the form of matrices \(A\) and \(B\). They have the forms

\[
|u_0^1\rangle = \begin{pmatrix} \sqrt{ae^{i\gamma_0^1}} \\ 0 \\ \ldots \\ \sqrt{ae^{i\gamma_0^1}} \end{pmatrix}, \quad |u_0^2\rangle = \begin{pmatrix} \sqrt{\frac{1}{2} - ae^{i\gamma_0^2}} \\ 0 \\ \ldots \\ \sqrt{\frac{1}{2} - ae^{i\gamma_0^2}} \end{pmatrix},
\]

where only the elements \(1, L + 2, L + 3, \) and \(2L + 4\) are non-null, \(0 < a < \frac{1}{2}\), and

\[
a_0^1 - a_0^2 = \gamma_0^1 - \gamma_0^2.
\]

Note that these eigenstates are independent of the parameters of the XY model and we would like to choose them in such a way that Eq. (17) is preserved. For analytical calculations it should be easier to take all the angles equal to 0 and \(a = \frac{1}{4}\). For this choice, we have

\[
\eta_0 = \frac{1}{2}(c_0 + c_{L+1} + c_0^\dagger - c_{L+1}^\dagger), \quad \eta_0^\dagger = \frac{1}{2}(c_0 - c_{L+1} + c_0^\dagger + c_{L+1}^\dagger).
\]

Depending on the parameters there may be more than one zero mode. It is important that the eigenstates associated with these zero modes also preserve the form of Eq. (17). Some important examples appear later in our model.

It is worth mentioning that if we numerically diagonalize matrix \(M\) and order the eigenstates according to Eq. (20), we have no guarantee that matrix \(U\) will be in the desired form of Eq. (17). This is because each eigenstate can be defined with an arbitrary phase, \(\exp(i\theta_i)\). Thus, we would have to numerically determine the phases to get the matrix \(U\) in the desired form. A simple procedure to obtain matrix \(U\) as depicted in Eq. (17) is just to select the first \(L + 2\) eigenstates associated with the eigenvalues \(\lambda_i, i = 0, 1, \ldots, L + 1\), build the matrices \(g\) and \(h\), and then automatically we will have matrix \(U\).
We now show that for all values of \( k \), we can define the two ground states as
\[
|\tilde{G}_\pm\rangle = \frac{1}{\sqrt{2}} (|0\rangle \pm \eta_0^\dagger |\bar{0}\rangle).
\]
(27)

We now show that \( |\tilde{G}_\pm\rangle \) are eigenstates of \( \sigma_k^x \) and \( \sigma_{L+1}^x \). This fact is important, since we need the eigenstates in the \((+, +)\) sector. It is easy to show that
\[
\sigma_0^x |\tilde{G}_\pm\rangle = \pm |\tilde{G}_\pm\rangle,
\]
(28)
due to the fact that
\[
\sigma_0^x = c_0 + c_0^\dagger = \eta_0 + \eta_0^\dagger.
\]
(29)

On the other hand, to prove that \( |\tilde{G}_\pm\rangle \) is an eigenstate of \( \sigma_{L+1}^x \) is not so simple and we need some extra identities, which are presented below.

First, note that the following commutation relations hold:
\[
[\sigma_0^x, \sigma_{L+1}^x] = \left[N_k, \sigma_0^x\right] = \left[N_k, \sigma_{L+1}^x\right] = 0, \quad k \neq 0.
\]
(30)

To show the last equality we have used the fact that for \( k \neq 0 \) we have
\[
\eta_k = \sum_{j=0}^{L+1} g_{kj} c_j + h_{kj} c_j^\dagger = \sum_{j=0}^{L} (g_{kj} c_j + h_{kj} c_j^\dagger) + g_{kL+1} (c_{L+1} + c_{L+1}^\dagger),
\]
(31)
\[
\eta_k^\dagger = \sum_{j=0}^{L+1} h_{kj}^* c_j + g_{kj}^* c_j^\dagger = \sum_{j=0}^{L} (h_{kj}^* c_j + g_{kj}^* c_j^\dagger) + g_{kL+1}^* (c_{L+1} + c_{L+1}^\dagger).
\]
(32)

The last term in both of the above equations means that \( \sigma_{L+1}^{x(c)} \) does not appear in the expansion; hence we also have
\[
[\sigma_{L+1}^x, \eta_k] = [\sigma_{L+1}^{x(c)}, \eta_k] = 0, \quad k \neq 0.
\]
(33)

Using the above equation it is simple to prove the last equality in Eq. (30). There are a few other useful relations that one can prove with a little bit of calculation such as
\[
\{\sigma_0^x, \eta_k\} = \{\sigma_0^x, \eta_k^\dagger\} = 0, \quad k \neq 0.
\]
(34)

Using Eq. (30), it is now not difficult to prove that
\[
\sigma_{L+1}^x |\tilde{G}_\pm\rangle = \delta_\pm |\tilde{G}_\pm\rangle,
\]
(35)
where \( \delta_\pm = 1 \). To have a complete Hilbert space we need to have \( \delta_- = -\delta_+ \).

Now one can make the following argument: Consider \( \delta_+ = +1 \), which means that \( |\tilde{G}_\pm\rangle \) belongs to \((+, +)\); then all the states
\[
\prod_{j=1}^n \eta_{k_j}^\dagger |\tilde{G}_+\rangle, \quad n \text{ is even},
\]
(36)
also belong to \((+, +)\). Note that in the above equation \( 0 < k_j < k_{j+1} \), which means that the dimension of the space in the sector \((+, +)\) is \( 2^n \). On the other hand, when \( \delta_+ = +1 \), \( |\tilde{G}_-\rangle \) and its tower belong to the sector \((-,-)\). In other words,
\[
\prod_{j=1}^n \eta_{k_j} |\tilde{G}_-\rangle, \quad n \text{ is even},
\]
(37)
belongs to the sector \((-,-)\). The other two sectors can be built as follows:
\[
\prod_{j=1}^n \eta_{k_j}^\dagger |\tilde{G}_+\rangle, \quad n \text{ is odd}, \quad (-, +);
\]
(38)
\[
\prod_{j=1}^n \eta_{k_j}^\dagger |\tilde{G}_-\rangle, \quad n \text{ is odd}, \quad (+, -).
\]
(39)
Similarly one can show that if \( |\tilde{G}_+\rangle\) belongs to (+, –), which means that \( \delta_+ = -1 \), then one can write
\[
\prod_{j=0}^{n} \eta_{kj}^{|\tilde{G}_+\rangle}, \quad n \text{ is even, } (+, -); \tag{40}
\]
\[
\prod_{j=0}^{n} \eta_{kj}^{|\tilde{G}_-\rangle}, \quad n \text{ is even, } (-, +); \tag{41}
\]
\[
\prod_{j=1}^{n} \eta_{kj}^{|\tilde{G}_+\rangle}, \quad n \text{ is odd, } (-, -); \tag{42}
\]
\[
\prod_{j=1}^{n} \eta_{kj}^{|\tilde{G}_-\rangle}, \quad n \text{ is odd, } (+, +). \tag{43}
\]

The above argument means that to know the sector (+, +) we need to figure out the value of \( \delta_+ \). The ground state of the Hamiltonian \( H^{XY} \) will be one of the following two states of \( H^{long} \):
\[
|\tilde{G}_+\rangle, \quad \delta_+ = 1, \tag{44}
\]
\[
|\tilde{G}_-\rangle, \quad \delta_+ = -1. \tag{45}
\]

In principle, to find the right ground state we need to calculate \( \delta_+ \) as follows:
\[
\delta_+ = \langle \tilde{G}_+ | \sigma_{L+1} | \tilde{G}_+ \rangle. \tag{46}
\]

The value of \( \delta_+ \) can be found by a bit of manipulation and use of the Wick theorem. Details of the calculation are presented in Appendix A. We observed that the ground-state energies of the transverse field Ising chain \( \{ \gamma = 1 \text{ and } h = 1 \text{ in Eq. (6)} \} \) and the XX chain \( \{ \gamma = 0 \text{ and } h = 0 \text{ in Eq. (6)} \} \) correspond to the first excited-state energies of \( H^{long} \) when the boundary magnetic fields on both boundaries are the same and \( J = +1 \). In other words, the ground states of these two models are basically the state \( \eta_{kmin}^{|\tilde{G}_+\rangle} \) with \( k_{min} = 1 \) of \( H^{long} \).

**B. Correlation matrices**

In this section, we calculate the correlation functions that are necessary to calculate the entanglement entropy. In principle, we need both \( \langle \tilde{G}_+ | \sigma | \tilde{G}_+ \rangle \) and \( \langle \tilde{G}_- | \eta_{kmin} \eta_{kmin}^\dagger | \tilde{G}_- \rangle \), where \( \sigma \) is the one- and two-point functions of the fermionic operators. The rest of the correlations can be reproduced with proper use of Wick’s theorem. An easy calculation shows that
\[
\langle \tilde{G}_+ | c_j \rangle | \tilde{G}_+ \rangle = \frac{1}{2} (g_{0j} + h_{0j}), \tag{47}
\]
\[
\langle \tilde{G}_+ | c_j \rangle | \tilde{G}_+ \rangle = \frac{1}{2} (h_{0j} + g_{0j}). \tag{48}
\]

Then because of Eqs. (24) and (25) one can write
\[
\langle \tilde{G}_+ | c_j \rangle | \tilde{G}_+ \rangle = \frac{1}{2} \delta_{0j}, \tag{49}
\]
\[
\langle \tilde{G}_+ | c_j \rangle | \tilde{G}_+ \rangle = \frac{1}{2} \delta_{0j}. \tag{50}
\]

As expected, because the spin at site 0 is in the positive direction of \( \sigma^0_0 \) the above expectation values are 0 for \( j = 1, 2, \ldots, L, L + 1 \). For the expectation values of \( \langle \tilde{G}_- | \eta_{kmin} c_j (c_j)^\dagger | \eta_{kmin} \rangle | \tilde{G}_- \rangle \), the same result is correct, as expected.

To proceed and calculate the two-point correlation functions, we first define the \( \Gamma \) matrix as a block matrix which is built from the correlation functions as
\[
\Gamma_{mn} = \begin{pmatrix}
\langle a_i^\dagger a_i^\dagger \rangle - I_{x,n} & \langle a_i^\dagger a_i \rangle \\
\langle a_i^\dagger a_i \rangle & \langle a_i^\dagger a_i^\dagger \rangle - I_{x,n}
\end{pmatrix}, \tag{51}
\]
where \( a_i^\dagger = c_i^\dagger + c_i \) and \( a_i^\dagger = i(c_i - c_i^\dagger) \). One can easily find all the different elements of the \( \Gamma \) matrix. It is convenient to write the \( \Gamma \) matrix as
\[
\Gamma = \begin{pmatrix}
\Gamma_{11} & \Gamma_{12} \\
\Gamma_{21} & \Gamma_{22}
\end{pmatrix}, \tag{52}
\]
where matrices \( \Gamma_{ij} \) of dimension \( (\ell + 2) \times (\ell + 2) \), \( \ell = 0, 1, \ldots, L + 2 \), are
\[
\Gamma_{11} = F + F^\dagger + C - C^T, \tag{53}
\]
\[
\Gamma_{12} = i(-I + C + C^T - F - F^\dagger), \tag{54}
\]
\[
\Gamma_{21} = -i(-I + C + C^T + F - F^\dagger), \tag{55}
\]
\[
\Gamma_{22} = -F - F^\dagger + C - C^T, \tag{56}
\]
where \( F_{ln} = \langle c_i^\dagger c_n \rangle \) and \( C_{ln} = \langle c_i^\dagger c_n \rangle \). For states \( | \tilde{G}_\pm \rangle \) we have
\[
F_{ln}^{\pm} = \langle \tilde{G}_\pm, c_i^\dagger c_n | \tilde{G}_\pm \rangle = (h^g)_{ln} + \frac{1}{2} (g_{0l}h_{0,n}^* - h_{0,l}^*g_{0,n}), \tag{57}
\]
\[
C_{ln}^{\pm} = \langle \tilde{G}_\pm, c_i^\dagger c_n | \tilde{G}_\pm \rangle = (h^h)_{ln} + \frac{1}{2} (g_{0l}h_{0,n}^* - h_{0,l}^*g_{0,n}). \tag{58}
\]

while for states \( \eta_{kmin}^{|\tilde{G}_\pm\rangle} \) we have
\[
F_{ln}^{ex,\pm} = \langle \tilde{G}_\pm, \eta_{kmin} c_i^\dagger c_n^\dagger | \tilde{G}_\pm \rangle = (h^g)_{ln}
+ \frac{1}{2} \sum_{j=0}^{L+1} (g_{j,l}h_{j,n}^* - h_{j,l}^*g_{j,n})(j + 1), \tag{59}
\]
\[
C_{ln}^{ex,\pm} = \langle \tilde{G}_\pm, \eta_{kmin} c_i^\dagger c_n^\dagger | \tilde{G}_\pm \rangle = (h^h)_{ln}
+ \frac{1}{2} \sum_{j=0}^{L+1} (g_{j,l}h_{j,n}^* - h_{j,l}^*g_{j,n})(j + 1). \tag{60}
\]
Note that $F_{in}^{-} = F_{in}^{+}$ and $C_{in}^{-} = C_{in}^{+}$ and, also, $F_{in}^{ex} = F_{in}^{ex+}$ and $C_{in}^{ex} = C_{in}^{ex+}$. Due to these results, it is expected that both of the two degenerate sectors will give the same results for the entanglement entropy.

With a little bit of calculation one can also show that as long as $O$ does not have $c_0$ and $c_0^\dagger$, we have

$$
\langle G_+ | O | G_+ \rangle = \langle \hat{0} | O | \hat{0} \rangle,
$$
(61)
$$
\langle G_+ | c_0^\dagger c_0 O | G_+ \rangle = \langle G_+ | c_0^\dagger c_0 O | G_+ \rangle.
$$
(62)

If $O$ is derived by multiplication of an even number of creation and annihilation operators, we have

$$
\langle G_+ | c_0^\dagger c_0 O | G_+ \rangle = \frac{1}{2} \langle \hat{0} | O | \hat{0} \rangle,
$$
(63)
$$
\langle G_+ | c_0^\dagger c_0 O | G_+ \rangle = \frac{1}{2} \langle \hat{0} | O | \hat{0} \rangle,
$$
(64)
$$
\langle G_+ | c_0^\dagger c_0 O | G_+ \rangle = \frac{1}{2} \langle \hat{0} | O | \hat{0} \rangle.
$$
(65)

On the other hand, if $O$ is derived by multiplication of an odd number of creation and annihilation operators, we have

$$
\langle G_+ | c_0^\dagger c_0 O | G_+ \rangle = \langle \hat{0} | c_0 O | \hat{0} \rangle,
$$
(66)
$$
\langle G_+ | c_0^\dagger c_0 O | G_+ \rangle = \langle \hat{0} | c_0 O | \hat{0} \rangle.
$$
(67)

The right-hand-sides of the above equations can be calculated easily by using directly Wick’s theorem. Finally, it is easy to see that the elements in the first row and column of the $\Gamma$ matrix are all 0 if we include site 0.

C. Entanglement entropy

In this section, we explain how one can use the $\Gamma$ matrix to calculate the entanglement entropy of a subsystem that starts from one boundary. We emphasize that to calculate the entanglement entropy of the XY chain with ADBMF, we had to generalize the Peschel method [25,32,45,46]. We need to make a small adjustment to the Peschel method because after the projection the two ghost sites are not entangled with the rest of the system and we cannot write the projected state in an exponential form. In addition, the odd point functions of the fermionic operators with site 0 included are nonzero too.

The main idea of the Peschel method is to connect the entanglement entropy to the eigenvalues of the $\Gamma$ matrix and exploit Wick’s theorem. Here, we need to take into account the fact that the odd point functions are nonzero for site 0. Since the $\Gamma$ matrix is a skew symmetric matrix it can be block diagonalized using an orthogonal matrix, $V$, as

$$
V \Gamma V^T = \begin{pmatrix} 0 & iv \\ -iv & 0 \end{pmatrix},
$$
(68)

where $v$ is a diagonal matrix. Then we can define the fermionic operators

$$
\begin{pmatrix} d^\dagger \\ d \end{pmatrix} = \begin{pmatrix} I \\ il \end{pmatrix} V \begin{pmatrix} a^\dagger \\ a \end{pmatrix},
$$
(69)

with the correlation matrices

$$
\begin{pmatrix} \langle d^\dagger d \rangle \\ \langle d d^\dagger \rangle \end{pmatrix} = \begin{pmatrix} \frac{1+v_k}{2} & 0 \\ 0 & \frac{1-v_k}{2} \end{pmatrix}.
$$
(70)

Using Eq. (69) one can also express the one point function of fermionic operators $d_k$ and $d_k^\dagger$ in terms of the elements of matrices $g, h$, and $V$. Numerical investigation shows that

$$
\langle d_k \rangle = \frac{1}{2} T_{k,0} \delta_{k,0},
$$
(71)
$$
\langle d_k^\dagger \rangle = \frac{1}{2} T_{k,0} \delta_{k,0},
$$
(72)

where matrix $T$ is related to the unitary transformation $W$, which diagonalizes $\Gamma$, by

$$
T = 2W \begin{pmatrix} I & \nu \\ \nu & -I \end{pmatrix}.
$$
(73)

Note that we also have $\nu_0 = 0$. Having the above results in hand one can derive the following ansatz for the reduced density matrix of subsystem $A$ of size $\ell = 0, 1, 2, \ldots$:

$$
\rho_A(\ell) = \frac{T_{00} d_0 + T_{00} d_0^\dagger + I}{2} \times \prod_{k=1}^{\ell} \left( \frac{1 + v_k}{2} d_k^\dagger d_k + \frac{1 - v_k}{2} d_k d_k^\dagger \right).
$$
(74)

We note that the above ansatz also respects the generalized Wick’s theorem introduced in the previous section, which means that this reduced density matrix produces all the correlation functions correctly. Note that the reduced density matrix $\rho_A(0)$ is built with the eigenstate of $\sigma_z$, associated with the eigenvalue +1. This is evident by looking at the identity

$$
T_{00} d_0 + T_{00} d_0^\dagger = c_0 + c_0^\dagger,
$$
(75)

which we confirmed numerically for various values of the parameters.

Finally, the entanglement entropy can be written as

$$
S = -\sum_{k=1}^{\ell} \left[ \frac{1 + v_k}{2} \ln \frac{1 + v_k}{2} + \frac{1 - v_k}{2} \ln \frac{1 - v_k}{2} \right].
$$
(76)

which can also be recast as

$$
S = -\text{Tr} \left[ \frac{1 + \Gamma}{2} \ln \frac{1 + \Gamma}{2} \right] - \ln 2.
$$
(77)

In Appendix B, we present an argument showing that if the reduced density matrix is built from a pure state like $|\Psi_0^L\rangle = |+\rangle \otimes |\Psi_0^{L-1}\rangle$, we need to subtract a ln 2 term in the entanglement entropy in order to get the right result. It is convenient to mention that a similar log 2 subtraction in the entanglement entropy was also observed in the context of quantum quench of the XY chain [47]. For periodic and open systems for which one does not need to do any projection in the state, the standard method, which does not require the subtraction of ln 2, works as usual [25,32,45,46].

D. Boundary entropy: Transverse field Ising chain

In this subsection, we present our numerical estimates of the ground-state degeneracy $g \equiv g(\theta, \phi)$ of the critical transverse field Ising chain when we have arbitrary equal boundary fields on the two edges. Although the method presented in the preceding section works for arbitrary boundary conditions, in this subsection we consider the transverse field Ising chain with equal boundary conditions on the two edges.
In order to show that we are able to find quite good estimates of the ground-state degeneracy $g$ by fitting the numerical data to Eq. (5), we first consider the transverse field Ising chain with OBCs [Eq. (6)] with $\gamma = 1$, $\tilde{b}_1 = \tilde{b}_L = 0$, and $J = +1$ whose exact value of the ground-state degeneracy is $S_{\text{free}} = 1$ [23,28,29]. It is noteworthy that for $J < 0$ we have $G_b = 0$ when the edge magnetic fields are the same and are in the $x$ direction (see Ref. [14]). However, for positive values of $J$ we observed that the nonuniversal function $G_b$ is nonzero. In Fig. 1(a), we present the function $f(x)$ that we calculated numerically by using the correlation matrix method, explained in the previous section, for $L = 400$ and $L = 2000$. The anticipated scaling behaviors of the entanglement entropies in Eqs. (1) and (2) hold for $\ell \gg 1$. Moreover, Eq. (4) is valid if $x = x/L \ll 1$. For these reasons, we fit the numerical data considering $20 < \ell < 0.25L$. As shown in Fig. 1(a), we are able to fit the numerical data quite well with Eq. (5), and the obtained estimates of $g$ are very close to the expected exact one, i.e., $g = 1$.

Now we discuss the case of arbitrary direction of the boundary magnetic fields. As mentioned, we consider that the boundary magnetic fields are the same at both edges, i.e., $b_1 = b_L = b$, $\theta_1 = \theta_L = \theta$, and $\phi_1 = \phi_L = \phi$. Then the magnitude of the effective boundary magnetic fields in the directions $x$, $y$, and $z$ are $h_x^b = b \sin \theta \cos \phi$, $h_y^b = b \sin \theta \sin \phi$, and $h_z^b = b \cos \theta$, respectively, for both edges. For systems with boundaries we must be careful when we use Eq. (5) to get estimates of $g$, since Eq. (2) holds only if the crossover lengths $\xi \sim h_x^{d-1} < \ell$. The scaling dimension of the relevant boundary perturbation (in the $x$ direction) for the transverse field Ising chain is $d_x = 1/2$ [28,29]. For instance, we need to be careful when we estimate $g$ for $\theta \to 0$ and/or $\phi \to \pi/2$, since the crossover length $\xi^\phi \sim (b \sin \theta \cos \phi)^{-1/2}$, for a finite boundary magnetic field, can diverge in these regimes. Thus, we expect a huge crossover effect mainly if $\theta \to 0$ and/or $\phi \to \pi/2$ since $\xi^\phi \sim 1/\sqrt{b \sin \theta \cos \phi}$ for finite boundary magnetic field.

In Fig. 1(b), we present a representative result of the function $f(x)$ for the ADBFM case. For this particular example, where $\phi = \pi/2$ and $\theta \in (0, \pi/2)$ matrix $M$ has four 0 eigenvalues, while for $\theta = 0$ and $\phi \in [0, \pi/2]$ it has six 0 eigenvalues. In these two regimes, the correlation matrix approach (presented before) to obtain the entanglement entropy needs a bit of modification, because if one does not take into account the extra degeneracies, matrix $M$ will not necessarily be in the desired canonical form [see Eq. (17)]. We analyze these situations later. For other values of $\theta$ and $\phi$ we found that matrix $M$ has just two 0 eigenvalues, whose eigenstates are given in Eq. (22).

In Fig. 1(b), we present a representative result of the function $f(x)$ for the ADBFM case. For this particular example, where $\phi = \pi/4$, $\theta = \pi/4$, and $b = 4$, we get $g \sim 0.709$ for $L = 2000$, which is very close to the expected exact value $S_{\text{free}} = \sqrt{2}/2 = 0.7071 \ldots$ [23,28,29]. Using the explained fitting procedure, we estimated $g(\theta, \phi)$ for several other values of angles for system size $L = 2000$. The obtained values are depicted in Fig. 2. As shown in this figure, for $\phi \neq \pi/2$ and $\theta \neq 0$, we have $g \neq 0$ for $\ell < \pi/L$ as well as for $\theta \neq 0$ and $\phi \neq 0$ for $\ell < \pi/L$. The results strongly indicate that $g(\theta, \phi) \neq 0$ for very small values of $\theta$ and $\phi$, close to $\pi/2$. As already mentioned, in this region we expected a huge crossover effect for a finite-boundary magnetic field. For instance, for $\theta = 0.1\pi$ and $\phi = 0.45\pi$, and considering $b = 500$, we got $g = 0.94$ and $g = 0.83$ for $L = 400$ and $L = 2000$, respectively. We also observed that for a fixed value of $L$ the estimate of $g$ depends on the value of $b$. These finite-size effects are indicative that even for $b = 500$ and $L = 2000$ we are still not in the regime where $\xi^\phi < \ell$ for this angles.

Now we consider the case $\theta = 0$, where we have $b_i \cdot S_i = b_i \cdot c_i \cdot c_i - 1/2, i = 1$ and $L$. In this case, $b_i \cdot S_i$ is quadratic in terms of the creation and annihilation operators, so it is possible to map $H^{XY}$ to a quadratic free fermion Hamiltonian, and we can use the standard matrix correlation method to obtain the entanglement entropy. Since this perturbation is not relevant, we expect that the BE in this case will be the same as in the OBC case, i.e., $s_b = 0$ (or, equivalently, $g = 1$). Indeed, our numerical estimates of $g$, based on the fitting procedure, agree very well with the expected value. For $b = 4$
we get $g = 0.998$ and $g = 0.999$ for $L = 400$ and $L = 2000$, respectively.

Finally, we discuss the case $\phi = \pi / 2$. As mentioned, in this case we have four 0 eigenvalues. Two eigenvectors, associated with these eigenvalues, are those given in Eq. (22), and the other two are

$$
|u_0^1\rangle = \frac{1}{N_{nor}} \begin{pmatrix}
\alpha i \\
2 \\
0 \\
\vdots \\
-2 \\
-\alpha i \\
-\alpha i \\
2 \\
0 \\
\vdots \\
2
\end{pmatrix},
|u_0^2\rangle = \frac{1}{N_{nor}} \begin{pmatrix}
\alpha i \\
2 \\
0 \\
\vdots \\
2 \\
-\alpha i \\
-\alpha i \\
2 \\
0 \\
\vdots \\
2
\end{pmatrix},
$$

where $\alpha = 2b(\cot \theta - \sec \theta)$ and $N_{nor} = 2\sqrt{2}\alpha^2 + 4$. The boundary perturbation now is given by $b_i, S_i = \frac{b_i}{2}(\sin \theta \sigma_i^+ + \cos \theta \sigma_i^-)$, $i = 1$ and $L$, and is not relevant either. Thus, here too we expect that $g = 1$ along the line with $\phi = \pi / 2$. Again, our numerical data support this prediction. We found that $g \sim 1.000$ along this line.

In summary, as long as the boundary magnetic field vector is in the $yz$ plane one gets a free boundary condition. Introducing even a small boundary magnetic field in the $x$ direction, which means breaking the bulk $Z_2$ symmetry, induces a fixed boundary condition.

IV. THE XXZ CHAIN WITH ARBITRARY DIRECTION OF THE BOUNDARY MAGNETIC FIELD

In this section, we investigate the spin-1/2 XXZ chain with ADBMF given by

$$
H^{XXZ} = J \sum_{j=1}^{L-1} \left[ S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z \right] + b_1 \cdot \vec{S}_1 + b_L \cdot \vec{S}_L,
$$

where $\Delta$ is the anisotropy and we use $J = 1$ in order to fix the energy scale. The boundary magnetic fields $b_i, i = 1$ and $L$, are defined in Eqs. (7) and (8), and we consider that the magnitudes of both boundary magnetic fields are the same, i.e., $b = b_1 = b_L$. For $-1 < \Delta < 1$ the system is bulk critical with central charge $c = 1$. The OBC case corresponds to the free conformally invariant boundary condition with $g = g^{\text{free}} = \frac{1}{\pi \sqrt{\pi R}}$, where $R^2 = \frac{1}{2\kappa} \left( 1 - \frac{\Delta}{\pi^2} \right)$ [41], while the fixed conformally invariant boundary condition with $g = g^{\text{fixed}} = \frac{\pi^{1/4}\sqrt{R}}{4}$ corresponds to the case where both boundary magnetic fields are in the $x$ direction ($\phi_1 = \phi_2 = 0$ and $\theta = \frac{\pi}{2}$) with $b_1 = b_L = \infty$ [41]. Note that these predictions were obtained by the bosonization technique, and to our knowledge they were not verified by other entanglement approaches. It is important to mention that although the XXZ chain with ADBMF is exactly solvable by the thermodynamic Bethe ansatz method [48–60], it seems that in the massless regime the determination of the free boundary energy in the low-temperature regime is not simple [60]. Thus, it is highly desirable to confirm the bosonization prediction by other unbiased techniques. Furthermore, there is no prediction of the values of $g$ for other directions of the boundary magnetic fields. We intend to provide further insight into these issues in this section. It is also important to mention that, like the Ising case where the edge magnetic fields are the same and are in the $x$ direction, here too if we choose $J < 0$, the corrections in $S^\theta(L, \ell)$ are zero, i.e., $G_\theta = 0$. However, for positive values of $J$ these corrections are present.

Before presenting the results, it is convenient to mention that in the case where both boundary magnetic fields are the same, we verified, numerically, that the energies as well as the entanglement entropy of the XXZ chain do not depend on the values of the angle $\phi = \phi_1 = \phi_2$. Another important point is that in the case of the XX chain with ADBMF [$\Delta = 0$ in Eq. (79)], the Hamiltonian is the same as the one in Eq. (6) with $\gamma = 0$ and $h = 0$. Consequently, we can use the correlation matrix method developed in the previous section to obtain the entanglement entropy.

We first consider the XX chain with OBCs. In Fig. 3(a), we show the function $f(x)$ defined in Eq. (5) for the XX chain with OBCs. By fitting the numerical data to this equation we get $g = 1.0002$ and $g = 1.0001$ for $L = 600$ and $L = 2000$, respectively. Similar agreement with the bosonization prediction is found also for the XXZ under OBCs, as reported in Table I for two other values of $\Delta$. For $\Delta = 0.5$ and $\Delta = \cos (\pi / 8) = 0.9238 \ldots$, we used the DMRG to obtain the entanglement entropy. For the systems under PBCs (OBC and ADBMF) we kept up to $m = 3000$ ($m = 800$) states per block in the final sweep and did approximately six to eight sweeps.
The solid orange line corresponds to $g = 600$. (b) Estimates of $g$ for two other values of the $\Delta$ [see Fig. 3(b)] and different directions of the magnetic fields. We summarize in Fig. 3(c) all the estimates of $g$ that we obtained for the XXZ chain for different boundary conditions for system sizes $L = 600$ and $b = 1$. As shown in this figure, our results strongly support that $g = g^{\text{fixed}} = \pi^{1/4}\sqrt{R}$ for $0 < \theta < \pi/2$ and $g = g^{\text{free}} = \frac{1}{\pi^{1/4}\sqrt{2R}}$ for $\theta = 0$.

In summary, as long as the boundary magnetic field vector is in the $z$ direction, i.e., $\theta = 0$, one gets a free boundary condition. Introducing even a small boundary magnetic field in the $x$ and/or $y$ direction which breaks the bulk $U(1)$ symmetry induces a fixed boundary condition.

V. CONCLUSIONS

In this paper, we have investigated entanglement entropy in open quantum critical spin chains with arbitrary boundary magnetic fields. Evaluation of the boundary entropy in such systems, in general, is not a simple task using the thermodynamic Bethe ansatz method or the CFT approach. Here, we present a simple procedure to estimate the boundary entropy by considering the finite-size corrections of the entanglement entropies and without knowledge of the nonuniversal correction $G_h$ which is induced by the boundaries [14] [see

![Graph](image-url)
Eqs. (2)–(5)]. In particular, we calculated the boundary entropy in the critical transverse field Ising chain and the critical XXZ chain. We were able to obtain precise estimates of the universal boundary entropy of these two models that were in perfect agreement with previous analytical predictions. In particular, we provided estimates of the universal boundary entropy for directions of the boundary magnetic field that have not been investigated in the literature so far. Our results support that if the boundary magnetic field breaks the bulk symmetry, then we have a fixed boundary condition, and if it does not, we have a free boundary condition. One of our technical achievements is the exact solution of the XY chain with ADBMF, which, to the best of our knowledge, has not been tackled so far. Our exact solution gives all the spectra and the eigenstates of the Hamiltonian. Using this solution we were able to calculate the entanglement entropy using the modified version of the correlation method up to relatively large subsystem sizes, \( L = 2000 \). To do similar calculations for the XXZ chain we used the DMRG.

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APPENDIX A: CALCULATION OF \( \delta_+ \)

In this Appendix, we show how to calculate \( \delta_+ = \langle \tilde{G}_+ | \sigma_{L+1}^z | \tilde{G}_+ \rangle \). First, it is easy to see that

\[
\delta_+ = \langle \tilde{G}_+ | \sigma_{L+1}^z | \tilde{G}_+ \rangle = \langle \tilde{G}_+ | a_0^\dagger a_0 | \tilde{G}_+ \rangle \prod_{k=1}^L a_k^a a_k^a a_{L+1}^a | \tilde{G}_+ \rangle. \tag{A1}
\]

Since just \( a_0^a \) and \( a_k^a a_{L+1}^a \) depend on \( \eta_0 \) and \( \eta_0^\dagger \) one can write

\[
\delta_+ = (-i)^{L+1} \langle \tilde{G}_+ | a_0^\dagger \prod_{k=1}^L a_k^a a_k^a a_{L+1}^a | \tilde{G}_+ \rangle. \tag{A2}
\]

Because of Wick’s theorem one can write the above correlation as a Pfaffian,

\[
\delta_+ = (-i)^{L+1} \text{Pf}[\mathbf{D}], \tag{A3}
\]

where

\[
\mathbf{D} = \begin{pmatrix}
0 & \langle a_0^a a_1^a \rangle & \langle a_0^a a_2^a \rangle & \ldots & \\
\langle a_1^a a_0^a \rangle & 0 & \langle a_1^a a_2^a \rangle & \ldots & \\
\langle a_2^a a_0^a \rangle & \langle a_2^a a_1^a \rangle & 0 & \ldots & \\
\vdots & \vdots & \vdots & \ddots & \ddots \\
\langle a_{L+1}^a a_0^a \rangle & \langle a_{L+1}^a a_1^a \rangle & \langle a_{L+1}^a a_2^a \rangle & \ldots & 0
\end{pmatrix} \tag{A4}
\]

APPENDIX B: THE \( \ln 2 \) TERM IN THE ENTANGLEMENT ENTROPY

For cases where the reduced density matrix is derived using a state where one site is not entangled with the other sites, we need to be careful when we use the correlation matrix method to calculate \( S(L, \ell) \). In this Appendix, we show why we should subtract the \( \ln 2 \) in the entanglement entropy for a particular situation.

For simplicity, let us consider the following free fermion Hamiltonian:

\[
H = \sum_{i,j} \epsilon_i h_{i,j} c^\dagger_i c_j. \tag{B1}
\]

Suppose that we project the ground state of the above Hamiltonian to obtain the state \( | \Psi^{(\ell)}_0 \rangle = | \rangle | \Psi^{(0)}_0 \rangle \otimes | \Psi^{(\ell-1)}_0 \rangle \), where \( | \rangle = \frac{1}{\sqrt{2}} (|1\rangle + |0\rangle) \) and \( c_i^\dagger c_i | n \rangle = n | n \rangle, n = 0, 1 \).

Let us focus on the following density matrix:

\[
\rho = \langle | \Psi^{(\ell)}_0 | \Psi^{(0)}_0 \rangle | \Psi^{(\ell-1)}_0 | \Psi^{(0)}_0 \rangle. \tag{B2}
\]

So, the reduced density matrix is given by

\[
\rho_A = \text{tr}_B \rho = \left( \frac{1 + c_1^\dagger + c_1}{2} \right) \tilde{\rho}_A, \tag{B3}
\]

where we have defined the reduced density matrix associated with the sites \( 2, \ldots, \ell \) as

\[
\tilde{\rho}_A = \text{tr}_B | \Psi^{(\ell-1)}_0 \rangle \langle \Psi^{(\ell-1)}_0 |. \tag{B4}
\]

We assume that \( \tilde{\rho}_A \) can be written in a diagonal form in terms of a new creation/annihilation operator as

\[
\tilde{\rho}_A = \frac{e^{-\sum_{i=2}^\ell \epsilon_i d_i^\dagger d_i}}{\text{tr} \ e^{-\sum_{i=2}^\ell \epsilon_i d_i^\dagger d_i}}. \tag{B5}
\]

Hence, the eigenvalues \( \epsilon_k \) are associated with the eigenvalues \( \lambda_k \) of the correlation matrix \( C_{i,j} = \text{tr}_A (\rho_A c_i^\dagger c_j) \), with \( i, j = 2, \ldots, \ell \), by \( \lambda_k = (1 + \epsilon_i^\dagger)^{-1} \equiv \frac{1}{1 - \epsilon_k} \) [25]. And the entanglement entropy for this kind of state is given by [25]

\[
S(L, \ell) = - \sum_{k=2}^\ell \left[ \frac{1 + v_k}{2} \ln \frac{1 + v_k}{2} + \frac{1 - v_k}{2} \ln \frac{1 - v_k}{2} \right], \tag{B6}
\]

for \( \ell = 2, \ldots, L \), and for \( \ell = 1 \) we have that \( S(L, 1) = 0 \).

Now, suppose that instead of considering the correlation matrix \( C_{i,j} \), we define the correlation matrix \( \tilde{C}_{i,j} = \text{tr}_A (\rho_A c_i^\dagger c_j) \), with \( i, j = 1, 2, \ldots, \ell \). It is simple to show that \( \tilde{C}_{i,j} = 1/2 \delta_{i,j} \). Thus, the eigenvalues of matrix \( \tilde{C} \) are the same eigenvalues as for \( C \) plus the eigenvalue \( \lambda_1 = 1/2 \) (which corresponds to \( v_1 = 0 \)). So, we see that if we associate the entanglement entropy \( \tilde{S} \) with the eigenvalues of the correlation matrix \( \tilde{C} \), we realize that \( \tilde{S}(L, \ell) = \ln 2 + S(L, \ell) \).
