Entanglement entropy in quantum spin chains with broken reflection symmetry

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We investigate the entanglement entropy of a block of L sites in quasifree translation-invariant spin chains concentrating on the effect of reflection-symmetry breaking. The Majorana two-point functions corresponding to the Jordan-Wigner transformed fermionic modes are determined in the most general case; from these, it follows that reflection symmetry in the ground state can only be broken if the model is quantum critical. The large L asymptotics of the entropy are calculated analytically for general gauge-invariant models, which have, until now, been done only for the reflection-symmetric sector. Analytical results are also derived for certain nongauge-invariant models (e.g., for the Ising model with Dzyaloshinskii-Moriya interaction). We also study numerically finite chains of length N with a nonreflection-symmetric Hamiltonian and report that the reflection symmetry of the entropy of the first L spins is violated but the reflection-symmetric Calabrese-Cardy formula is recovered asymptotically. Furthermore, for noncritical reflection-symmetry-breaking Hamiltonians, we find an anomaly in the behavior of the saturation entropy as we approach the critical line. The paper also provides a concise but extensive review of the block-entropy asymptotics in translation-invariant quasifree spin chains with an analysis of the nearest-neighbor case and the enumeration of the yet unsolved parts of the quasifree landscape.

I. INTRODUCTION

Understanding the entanglement properties of systems with many degrees of freedom, such as quantum spin chains, has been one of the main recent research topics connecting quantum information theory and condensed-matter physics [1–5]. Huge amounts of results have been accumulated about translation-invariant systems. However, the results almost exclusively correspond to reflection-symmetric systems, despite the fact that models violating reflection invariance play a prominent role in many-body theory [e.g., in describing interactions of Dzyaloshinskii-Moriya- (DM-) type or nonequilibrium steady states].

Considering a subsystem $\mathcal{S}$ of a system, which is in a pure state, the entanglement between the subsystem and its environment is characterized by the von Neumann entropy,

$$S(\rho_{\mathcal{S}}) := -\mathrm{Tr}(\rho_{\mathcal{S}} \ln \rho_{\mathcal{S}}),$$

where $\rho_{\mathcal{S}}$ denotes the density matrix of the subsystem. In the case of infinite one-dimensional critical chains, this entanglement entropy belonging to a block of L contiguous spins was shown to grow asymptotically as [1,2]

$$S_L = \frac{c}{3} \ln L + k, \qquad (1)$$

where c is the conformal charge of its universality class and k is a nonuniversal constant. For noncritical chains, the asymptotics of the entanglement entropy is bounded. This saturation value of the entropy diverges as one approaches the critical point: It increases as [2]

$$S_{\mathrm{sat}} = \frac{c}{3} \ln \xi + k', \qquad (2)$$

where ξ is the correlation length. In the case of finite chains (with open boundary conditions) consisting of N spins, the conformal field theoretic prediction for the entanglement entropy of the first L spins (at criticality) is [2,6,7]

$$S(L,N) = \frac{c}{6} \ln \left(\frac{2N}{\pi} \sin \frac{\pi L}{N} \right) + \ln g + \frac{k}{2}, \qquad (3)$$

where $\ln g$ is the boundary entropy introduced by Affleck and Ludwig [8].

In this paper, we will study the asymptotics of the entanglement entropy in chains with broken reflection symmetry. We consider quasifree models (with finite-range coupling): Their Hamiltonian can be mapped to quadratic fermionic chains by the Jordan-Wigner transformation,[1]

$$H = \sum_{i,j=1}^{N} \left(A_{i,j} b_i^{\dagger} b_j + \frac{1}{2} B_{i,j} b_i^{\dagger} b_j^{\dagger} - \frac{1}{2} B_{i,j}^{*} b_i b_j \right). \qquad (4)$$

Throughout the paper, we will assume either open boundary conditions or fermionic periodic boundary conditions ($b_i = b_{i+N}$).[2] The requirement of translation invariance implies that A and B are Toeplitz matrices ($A_{i+n,j+n} = A_{i,j}$ and $B_{i+n,j+n} = B_{i,j}$ for any $n \in \mathbb{N}$), hermiticity of H implies that A is a (possibly complex) Hermitian matrix, and B is (a possibly complex) antisymmetric matrix. Finite-ranged interaction means that there exists a positive integer n_0 such that $A_{0,l} = B_{0,l} = 0$ if $l \geqslant n_0$. Such a spin-chain Hamiltonian is not invariant with respect to the reflection transformation $R(\sigma_i^a) = \sigma_{-i}^a$ ($a = x,y,z$), iff A is not a real matrix. [One might think that the term $(b_i b_j - b_j b_i)$, with $i > j$, also breaks the translation invariance of the spin chain, but a

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[1]Throughout this paper we will use the following convention for the Jordan-Wigner transformation: $\sigma_j^x = [\prod_{l=1}^{j-1}(2b_l^{\dagger} - 1)](b_j + b_j^{\dagger})$, $\sigma_j^y = [\prod_{l=1}^{j-1}(2b_l b_l^{\dagger} - 1)]i(b_j^{\dagger} - b_j)$, $\sigma_j^z = 2b_j b_j^{\dagger} - 1$.
[2]Note that periodic boundary conditions on the fermion chain may not be mapped to a periodic boundary condition after the Jordan-Wigner transformation, as shown in Ref. [9].

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short calculation shows that its image under the Jordan-Wigner transformation is the following reflection-invariant term $\sigma_i^- \prod_{n=i+1}^{j-1} \sigma_n^z \sigma_j^- + \sigma_j^- \prod_{n=j-1}^{i+1} \sigma_n^z \sigma_i^-$]. One of the most studied quantum spin chains with broken reflection symmetry is the Ising model with transverse magnetic field and DM interaction (in the z direction) [10–13]:

$$H = \sum_{i=1}^{N} \sigma_i^x \sigma_{i+1}^x + h\sigma_i^z + D\big(\sigma_i^x \sigma_{i+1}^y - \sigma_i^y \sigma_{i+1}^x\big). \quad (5)$$

Another type of model that has been studied extensively in the literature is the model,

$$H = \sum_{i=1}^{N} \big[J\big(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y\big) + h\big(\sigma_i^z + \sigma_i^x \sigma_{i+1}^y - \sigma_i^y \sigma_{i+1}^x\big) \\ + \lambda \sigma_i^z \big(\sigma_{i-1}^y \sigma_{i+1}^x - \sigma_{i-1}^x \sigma_{i+1}^y\big)\big], \quad (6)$$

whose ground states are used to describe the energy-current-carrying eigenstates of the XX model [14–16]. Certain nonreflection-invariant quasifree states also appear as invariant states of reflection-invariant quantum cellular automata [17].

The entanglement entropy asymptotics of the models given by Eq. (4) has been studied by many authors [18–22]. The main analytic tool for tackling this problem was expressing the entropy in terms of the determinant of a Toeplitz matrix, applied first by Jin and Korepin [18]. Until now, the most general results have been achieved by Keating and Mezzadri [19], who gave a general analytic expression for the entropy asymptotics when A is real and $B \equiv 0$, and by Its *et al.* [22], who gave an analytic (although less explicit) expression even for the case of general (finite-ranged) real A and B matrices, while certain results about the d-dimensional case can be found in Ref. [23]. However, none of these studies concerned reflection-symmetry-breaking cases (i.e., when A is complex).

We will generalize the above-mentioned results by deriving an analytic expression for the general gauge-invariant case (i.e., when A is a general complex Hermitian finite-ranged Toeplitz matrix, while $B \equiv 0$). This includes, as a particular case, the model described in Eq. (6). Moreover, we will also introduce a multitude of transformations between models of Eq. (4), which allows for deriving analytic expressions for cases with nonvanishing B. A remarkable result that we obtained is that, for these quasifree models, reflection invariance can only be broken in the ground state if the model is critical. If the model is noncritical, the ground state of the model does not change if we replace $A_{i,j}$ with $\text{Re}(A_{i,j})$ in the Hamiltonian. From this, as we will show, it follows that scaling in Eq. (2) may be violated. However, we will discuss how we can reinterpret this equation to keep its validity. Furthermore, we will present numerical results in nonreflection-symmetric spin chains providing an example of broken reflection symmetry in the finite-size scaling of the entropy $S(L,N) \neq S(N-L,N)$ breaking the symmetry of Eq. (3), but we will see that this deviation goes to zero as we increase the system size.

The paper is structured as follows. In Sec. II, we calculate the Majorana two-point functions of these general (finite-ranged) quasifree models and recapitulate how one can obtain the entanglement entropy from the two-point functions. The results already known about the entanglement asymptotics of certain types of quasifree models are collected in Sec. III. We derive an analytic formula for the entanglement entropy for general gauge-invariant models in Sec. IV, whereas in Sec. V, we show how we can extend our results for certain types of nongauge-invariant models too. Section VI is an application of the foregoing to models with nearest-neighbor interactions, while in Sec. VII, we discuss how some of our analytic and numerical results conflict with formulas (2) and (3) and how we can resolve this discrepancy. Finally, Sec. VIII is devoted to the summary and the remaining open questions.

II. TWO-POINT FUNCTION OF THE MAJORANA OPERATORS AND ENTANGLEMENT ENTROPY

The entanglement entropy asymptotics of the models described by the quadratic Hamiltonians in Eq. (4) can be calculated from the ground-state expectation values $\langle m_k m_l \rangle$, where m_n's denote the so-called Majorana operators defined as

$$m_{2n} = i(b_n - b_n^\dagger), \quad m_{2n-1} = b_n + b_n^\dagger. \quad (7)$$

In this section, we will first derive these Majorana two-point functions in terms of the matrices A and B that define the Hamiltonian Eq. (4). Then, we describe how to calculate (in this quasifree setting) the entanglement entropy alone from two-point functions, and finally, we recapitulate the determinant trick of Jin and Korepin, which will allow us to obtain analytical results later.

A. The Majorana two-point functions

Let us fix our conventions used in the calculation. We will consider the fermionic periodic boundary condition: $b_i = b_{i+N}$. The Fourier and inverse transforms of the one-particle annihilation operators read

$$\tilde{b}_k = \frac{1}{\sqrt{N}} \sum_n \exp\left(-\frac{2\pi i n k}{N}\right) b_n, \quad (8)$$

$$b_n = \frac{1}{\sqrt{N}} \sum_k \exp\left(\frac{2\pi i n k}{N}\right) \tilde{b}_k. \quad (9)$$

The summation runs in the set of integers $(\frac{N-1}{2}, \frac{N-1}{2})$ $[(-\frac{N}{2}, \frac{N}{2}-1)]$ for N odd (even), and the transform of the one-particle creation operators is to be computed by means of taking the adjoint of the preceding formulas. For Toeplitz matrices, we define the Fourier transform as

$$X_k = \sum_n \exp\left(-\frac{2\pi i n k}{N}\right) X_{0,n}, \quad (10)$$

$$X_{0,n} = \frac{1}{N} \sum_k \exp\left(\frac{2\pi i n k}{N}\right) X_k. \quad (11)$$

Here, $X_{0,n}$ stands for either $A_{0,n}$ or $B_{0,n}$, and the summation again runs in the set of integers $(\frac{N-1}{2}, \frac{N-1}{2})$ $[(-\frac{N}{2}, \frac{N}{2}-1)]$ for N odd (even). Using these definitions, the Hamiltonian (4) can be written as

$$H = \sum_k \left(A_k \tilde{b}_k^\dagger \tilde{b}_k + \frac{1}{2} B_k \tilde{b}_k^\dagger \tilde{b}_{-k}^\dagger - \frac{1}{2} B_k^* \tilde{b}_k \tilde{b}_{-k} \right). \quad (12)$$

To bring this Hamiltonian into a diagonal form $H = \sum_k \Lambda_k c_k^\dagger c_k$ ($\Lambda_k \in \mathbb{R}$), one performs a Bogoliubov transformation,

$$c_k = \alpha_k \tilde{b}_k + \beta_k \tilde{b}_{-k}^\dagger, \quad \alpha_k, \beta_k \in \mathbb{C}, \tag{13}$$

where the coefficients α_k, β_k have to satisfy

$$\alpha_k \beta_{-k} + \beta_k \alpha_{-k} = 0, \tag{14}$$
$$|\alpha_k|^2 + |\beta_k|^2 = 1, \tag{15}$$

so that the canonical anticommutation relations $\{c_k, c_{k'}^\dagger\} = \delta_{kk'}$ are satisfied. The consistency conditions for the commutator $[c_k, H] = \Lambda_k c_k$ give

$$\begin{pmatrix} -A_k & B_k^* \\ B_k & A_{-k} \end{pmatrix} \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix} = \Lambda_k \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix}. \tag{16}$$

One readily extracts the one-particle spectrum,

$$\Lambda_k = \frac{A_{-k} - A_k + \sqrt{(A_k + A_{-k})^2 + 4 B_k B_k^*}}{2}, \tag{17}$$

having taken the relations $A_k^* = A_k$, $B_{-k} = -B_k$ (which are a direct consequence of $A_{j,i}^* = A_{i,j}$, $B_{j,i} = -B_{i,j}$) into account. The ground-state correlations for the two-point functions of the new Fermi operators read

$$\langle c_k^\dagger c_{k'} \rangle = \frac{1}{2}\left(-\frac{\Lambda_k}{|\Lambda_k|} + 1\right)\delta_{k,k'},$$

and all other correlations vanish. Now, using the inverse of Eq. (13) $\tilde{b}_k = \alpha_k^* c_k + \beta_{-k} c_{-k}^\dagger$, one can compute the correlations among the Fourier components $\tilde{b}_k, \tilde{b}_k^\dagger$, and substituting the solution of Eq. (16) for α_k, β_k we arrive at

$$\langle b_j b_l \rangle = \frac{1}{N}\sum_k \exp\left[\frac{2\pi i k(j-l)}{N}\right]\frac{B_k}{2\sqrt{\Delta_k}}\left(\frac{\Lambda_k}{|\Lambda_k|} + \frac{\Lambda_{-k}}{|\Lambda_{-k}|}\right),$$

$$\langle b_j^\dagger b_l \rangle = \frac{1}{N}\sum_k \exp\left[\frac{2\pi i k(j-l)}{N}\right] \tag{18}$$
$$\times \frac{2 + \left(\frac{\Lambda_k}{|\Lambda_k|} - \frac{\Lambda_{-k}}{|\Lambda_{-k}|}\right) + \frac{A_{-k}+A_k}{\sqrt{\Delta_k}}\left(\frac{\Lambda_k}{|\Lambda_k|} + \frac{\Lambda_{-k}}{|\Lambda_{-k}|}\right)}{4},$$

where $\Delta_k = (A_k + A_{-k})^2 + 4 B_k B_k^*$, and the two remaining two-point functions $\langle b_j^\dagger b_l^\dagger \rangle$ and $\langle b_j b_l^\dagger \rangle$ can be calculated directly from the previous equations. Ultimately, we would like to have a linear combination of the foregoing, the two-point functions of the self-adjoint Majorana operators defined in Eq. (7). Before writing down the final result, let us introduce some notations. We will use the combinations,

$$A_k^s = A_{-k} + A_k, \quad A_k^a = A_{-k} - A_k, \tag{19}$$
$$B_k^s = B_k + B_k^*, \quad i B_k^a = B_k - B_k^*, \tag{20}$$

and the step functions,

$$M_k = \frac{1}{2}\left(\frac{\Lambda_k}{|\Lambda_k|} - \frac{\Lambda_{-k}}{|\Lambda_{-k}|}\right), \quad P_k = \frac{1}{2}\left(\frac{\Lambda_k}{|\Lambda_k|} + \frac{\Lambda_{-k}}{|\Lambda_{-k}|}\right). \tag{21}$$

Note, that $A_k^s, A_k^a, B_k^s, B_k^a \in \mathbb{R}$ and $\Delta_k = (A_k^s)^2 + (B_k^s)^2 + (B_k^a)^2$. We now take the thermodynamic limit ($N \to \infty$) and

write the final result in a manner usually adopted in the literature,

$$\langle m_j m_l \rangle = \delta_{jl} + i C_{jl}, \tag{22}$$

where the matrix C has the following structure:

$$C = \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \\ \cdots & \Pi_0 & \Pi_{-1} & \Pi_{-2} & \Pi_{-3} & \cdots \\ \cdots & \Pi_1 & \Pi_0 & \Pi_{-1} & \Pi_{-2} & \cdots \\ \cdots & \Pi_2 & \Pi_1 & \Pi_0 & \Pi_{-1} & \cdots \\ \cdots & \Pi_3 & \Pi_2 & \Pi_1 & \Pi_0 & \cdots \\ & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{23}$$

The Π_l's are 2×2 block entries that read

$$\Pi_l = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta\, e^{-il\theta}$$
$$\times \begin{bmatrix} i M(\theta) - P(\theta)\frac{i B^s(\theta)}{\sqrt{\Delta(\theta)}} & P(\theta)\frac{A^s(\theta) - i B^a(\theta)}{\sqrt{\Delta(\theta)}} \\ P(\theta)\frac{-A^s(\theta) - i B^a(\theta)}{\sqrt{\Delta(\theta)}} & i M(\theta) + P(\theta)\frac{i B^s(\theta)}{\sqrt{\Delta(\theta)}} \end{bmatrix}, \tag{24}$$

where $\theta = 2\pi i k/N$, so all Fourier series become functions on the circle $[0, 2\pi]$ in the limit. This type of matrix C is called block Toeplitz, and the matrix argument in Eq. (24) of the integral $\varphi: S^1 \to M_2(\mathbb{C})$ is called its *symbol*.

The n-point Majorana function can be obtained from the two-point functions by the Wick rule [9]:

$$\langle m_{i_1} \cdots m_{i_{2k-1}} \rangle = 0,$$

$$\langle m_{i_1} \cdots m_{i_{2k}} \rangle = \sum_\pi \mathrm{sgn}(\pi) \prod_{l=1}^k \langle m_{\pi(2l-1)} m_{\pi(2l)} \rangle,$$

where the sum runs over all pairings of $\{1, 2, \ldots, 2k\}$ [i.e., over all permutations of the $2k$ elements, which satisfy $\pi(2l-1) < \pi(2l)$ for $l \in \{1, 2, \ldots, k\}$ and $\pi(2l-1) < \pi(2l+1)$ for $l \in \{1, 2, \ldots, k-1\}$].

Before coming to the calculation of the entropy, let us analyze the obtained result. The one-particle spectrum (17) has the form of a sum of a reflection invariant $\sqrt{\Delta(\theta)}/2$ and a noninvariant term $A^a(\theta)/2$ [note that the real-space reflection $n \to -n$ corresponds to the Fourier space one $k \to -k$ as follows from the Fourier transform (8)]. The symbol (24) characterizing the correlation matrix $\langle m_i m_j \rangle$ has a dependence on the nonreflection-invariant part of the spectrum only via $M_\theta = [\Lambda(\theta)/|\Lambda(\theta)| - \Lambda(-\theta)/|\Lambda(-\theta)|]/2$. This term, however, vanishes identically unless $\Lambda(\theta_0) = 0$ at some $\theta_0 \in [0, 2\pi]$. In other words, noncritical quasifree systems never break reflection invariance.[3] We will discuss some implications of this important fact in Secs. VI and VII.

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[3] Of course, various nonquasifree models exist with a gap that breaks reflection symmetry, see, for example, Ref. [24].

B. Calculation of the entanglement entropy from the two-point functions

Restricting the ground state to a subsystem consisting of L consecutive sites, one obtains a mixed state. Let us restrict the matrix C defined in Eq. (22) (which describes the two-point Majorana correlations) to L consecutive modes, that is, to a $2L \times 2L$ submatrix,

$$C_L = \begin{pmatrix} \Pi_0 & \Pi_{-1} & \cdots & \Pi_{-L+1} \\ \Pi_1 & \Pi_0 & \cdots & \Pi_{-L+2} \\ \vdots & \vdots & \ddots & \vdots \\ \Pi_{L-1} & \Pi_{L-2} & \cdots & \Pi_0 \end{pmatrix}, \quad (25)$$

where the Π_l's are 2×2 matrices given by Eq. (24). Let us denote, by W, the orthogonal matrix, the adjoint action of which brings the antisymmetric real matrix C_L into its canonical form, that is, for $(H_L)_{ij} = \sum_{k,l=0}^{2L-1} W_{ik}(C_L)_{kl} W_{jl}$, we have

$$H_L = \bigotimes_{k=1}^{L} \nu_k \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

where $\nu_k \in [0,1]$ $(k = 1, 2, \ldots, L)$ are the singular values of C_L. (Due to the fact that C_L is antisymmetric, the degeneracy of its singular values is always an even number, that is why we label them only from 1 to L.) The density matrix corresponding to the restricted state can be written as[4]

$$\rho_L = \prod_{j=1}^{L} \left[\frac{1+\nu_j}{2} \frac{\mathbb{1} + i\hat{m}_{2j-1}\hat{m}_{2j}}{2} + \frac{1-\nu_j}{2} \frac{\mathbb{1} - i\hat{m}_{2j-1}\hat{m}_{2j}}{2} \right],$$

where $\hat{m}_j = \sum_{k=0}^{2L-1} W_{jk} m_k$ for all $j = 0, 1, \ldots, 2L-1$. [Actually, translation invariance is not used here, the density matrix of any quasifree state (i.e., of any state for which the Wick expansion applies) can be written in this form.] The entropy can now be calculated easily. It can be written in terms of the function

$$e(x,\nu) \equiv -\frac{x+\nu}{2} \ln \frac{x+\nu}{2} - \frac{x-\nu}{2} \ln \frac{x-\nu}{2}, \quad (26)$$

as

$$S_L \equiv S(\rho_L) = \sum_{j=1}^{L} e(1, \nu_j). \quad (27)$$

The trick [18] to obtain the asymptotics of the entanglement as the size of the block grows is computing the determinant,

$$D_L(\lambda) = \det(i\lambda I + C_L) = (-1)^L \prod_{j=0}^{L-1} (\lambda^2 - \nu_i^2), \quad (28)$$

and exploiting the residue theorem by writing down the following integral:

$$\lim_{\varepsilon \to 0} \frac{1}{4\pi i} \oint_{\Gamma(\varepsilon)} e(1+\varepsilon,\lambda) \frac{d \ln[D_L(\lambda)(-1)^L]}{d\lambda}, \quad (29)$$

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[4]One can check that, for any m, $m_{i_1} m_{i_2} \cdots m_{i_k}$ $(1 \leqslant i_1, i_2, \ldots, i_k \leqslant L)$ monomial of the Majorana operators, its expectation value (given by the formulas...) is equal to $\mathrm{Tr}(\rho_L m_{i_1} m_{i_2} \cdots m_{i_k})$, hence ρ_L is indeed the density matrix of the restricted state.
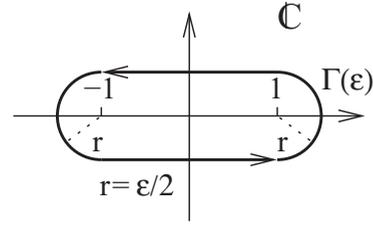

FIG. 1. The integration contour encloses a domain, where $e(1 + \varepsilon, \lambda)$ defined in Eq. (26) is analytic and contains all singular values of the matrix C_L.

where the contour $\Gamma(\varepsilon)$ is shown in Fig. 1. That contour encircles all eigenvalues of C_L, but bounds a region, in which $e(1 + \varepsilon, \lambda)$ is analytic.

Hence, the main task in all cases is to compute the determinant of the block-Toeplitz matrix

$$\widetilde{C}_L(\lambda) = i\lambda I + C_L. \quad (30)$$

Finally, we should mention that, in the gauge-invariant case (i.e., when $B = 0$), there is an easier method for the calculation of the entanglement entropy. In this case, as can be seen from Eq. (18), the nongauge-invariant two-point functions vanish ($\langle b_j b_k \rangle = \langle b_j^\dagger b_k^\dagger \rangle = 0$). If we restrict the state to L consecutive sites, and denote the corresponding restriction of the matrix $M_{ij} = \langle b_i^\dagger b_j \rangle$ by M_L and the (not necessarily real) unitary by U_L, the adjoint action of which diagonalizes M_L [$\sum_{j,k=1}^{L} U_{ij}^*(M_L)_{jk} U_{lk} = \lambda_i \delta_{il}$], then the density matrix of the restricted state reads

$$\rho_L = \prod_{i}^{L} [\lambda_i c_i^\dagger c_i + (1 - \lambda_i) c_i c_i^\dagger],$$

where $c_i = \sum_j U_{i,j} b_j$ and $\lambda_i \in [0,1]$. Hence, the entropy of the restricted state is given by

$$S_L = -\mathrm{Tr}\rho_L \ln \rho_L = -\sum_{i=1}^{L} [\lambda_i \ln \lambda_i + (1 - \lambda_i) \ln(1 - \lambda_i)]. \quad (31)$$

III. SUMMARY OF PREVIOUSLY KNOWN CASES

In this section, we shortly recapitulate what has been previously known about the entanglement entropy for quasifree models.

A. Gauge and reflection invariance

In the case of gauge- and reflection-invariant quasifree models, the matrix B is zero, while A is real, which implies $B^s(\theta) \equiv B^a(\theta) \equiv A^a(\theta) \equiv 0$, and the symbol of the Majorana two-point functions (24) reduces to

$$\varphi(\theta) = \begin{pmatrix} 0 & \frac{A^s(\theta)}{|A^s(\theta)|} \\ -\frac{A^s(\theta)}{|A^s(\theta)|} & 0 \end{pmatrix}.$$

Hence, C_L can be factorized as

$$C_L(\lambda) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \otimes G_L(\lambda), \quad (32)$$

where $G_L(\lambda)$ is the restriction of the Toeplitz matrix with scalar symbol $g(\theta) = A^s(\theta)/|A^s(\theta)|$ to an $L \times L$ block on the diagonal. From this, it follows that $\det(\widetilde{C}_L) = D_L = (-1)^L \det(\lambda I + G_L) \det(\lambda I - G_L)$. To extract the entropy asymptotics, one only needs to calculate the ($L \to \infty$ asymptotics of the) determinant of $(\lambda I \pm G_L)$ using the Fisher-Hartwig theorem, and then use the residue theorem as described in Sec. II B. This was done by Keating and Mezzadri [19,20]: They obtained the following result: Let there be number $R/2$ zeros of $A^s(\theta)$ denoted by θ_r ($r = 1, \ldots, R/2$) in the semicircle $[0,\pi]$ (implying other $R/2$ zeros in the other semicircle $[-\pi,0]$: $-\theta_r$, $r = 1, \ldots, R/2$). Then, the entanglement entropy asymptotics are given by

$$S_L(\rho_A) = \frac{R}{6} \ln L + \frac{R}{6} K - \frac{R}{2}(\ln 2)I_3, \qquad (33)$$

where

$$K = 1 + \gamma_E + \frac{1}{R} \sum_{r=1}^{R/2} \ln|1 - e^{2i\theta_r}|$$
$$- \frac{2}{R} \sum_{1 \leqslant s \leqslant r \leqslant R/2} (-1)^{r+s} \ln\left|\frac{1 - e^{i(\theta_r - \theta_s)}}{1 - e^{i(\theta_r + \theta_s)}}\right|,$$

where $\gamma_E = 0.57721\ldots$ is Euler's constant, and $I_3 = 0.0221603\ldots$, independent of $A(\theta)$ (consult Ref. [18] for its derivation).

B. Reflection invariance and real B_{ij}

The other case that has already been discussed in the literature is the case when both matrices A and B are real [i.e., when $A^a(\theta) \equiv B^s(\theta) \equiv 0$]. In this case, the symbol reads

$$\varphi(\theta) = \begin{bmatrix} 0 & \frac{A^s(\theta) - iB^a(\theta)}{|A^s(\theta) - iB^a(\theta)|} \\ -\frac{A^s(\theta) + iB^a(\theta)}{|A^s(\theta) + iB^a(\theta)|} & 0 \end{bmatrix}. \qquad (34)$$

Here, the idea, invented for the XY model in Ref. [21] and generalized for the present case in Ref. [22], is to extend the domain of $\varphi: S^1 \to M_2(\mathbb{C})$ to the complex plane and to use a theorem of Widom [25], which yields a formula of the block-Toeplitz determinant at hand, expressed in terms of Wiener-Hopf factors of the symbol: $\varphi(z) = U_+(z)U_-(z) = V_-(z)V_+(z)$, where the matrices U_+, V_+ (U_-, V_-) are analytic inside (outside) the unit circle. The factorization resides on the fact, that due to the assumption of finite-range interaction, the functions $\mathcal{A}(z) = \mathcal{A}(\exp(-i\theta)) \equiv A(\theta)$, and $\mathcal{B}(z) = \mathcal{B}(\exp(-i\theta)) \equiv B(\theta)$ are Laurent polynomials. One writes

$$\frac{\mathcal{A}^a(z) - \mathcal{B}^s(z)}{|\mathcal{A}(z) - \mathcal{B}(z)|} \equiv \frac{q(z)}{|q(z)|} = \sqrt{\frac{q(z)}{q(1/z)}} = \sqrt{\prod_{j=1}^{2n_0} \frac{z - z_j}{1 - z_j z}},$$

with z_i being the roots of the polynomial $p(z) = z^{n_0}q(z)$, where n_0 is the range of the coupling [defined after Eq. (4)]. Note that the equality in the middle is a choice of analytic continuation as $q(z)^* = q(1/z)$ holds on the unit circle [as is obvious from the general form $q(\exp -i\theta) \equiv A^s(\theta) - iB^a(\theta)$]. The nonanalytic behavior of the earlier rational function is then the only thing that has to be taken care of,

and the factorization is done with the help of theta functions living on the hyperelliptic surface of genus n_0 given by

$$w^2 = \prod_{j=1}^{2n_0} (z - z_i)(1 - zz_i). \qquad (35)$$

The XY model has $n_0 = 1$, thus, the underlying Riemann surface is a torus, while for general finite-ranged couplings, $q(z)$ can be any degree n_0 Laurent polynomial, which satisfies $q(z)^* = q(1/z)$ on the unit circle. The result (Theorem 3 of Ref. [22]) for the logarithmic derivative reads

$$\frac{d \ln D_L(\lambda)}{d\lambda} \approx -\frac{2\lambda L}{1 - \lambda^2} + \frac{1}{2\pi} \oint \text{tr}\left\{\left[\frac{dU_+(z)}{dz}U_+^{-1}(z) + V_+^{-1}(z)\frac{dV_+(z)}{dz}\right] G^{-1}(z)\right\} dz, \qquad (36)$$

and the difference between the right-hand side and the left-hand side is less than $C\rho^{-L}$ where the constant ρ satisfies $1 < \rho < \min\{|\lambda_i| : |\lambda_i| > 1\}$ [the complex numbers λ_i are the roots of $p(z)$ and their reciprocals]. The saturation entropy is given by

$$S(\rho_A) = \frac{1}{2} \int_1^\infty \ln\frac{\Theta[\beta(\lambda)\overrightarrow{e} + \frac{\tau}{2}]\Theta[\beta(\lambda)\overrightarrow{e} - \frac{\tau}{2}]}{\Theta^2(\frac{\tau}{2})} d\lambda.$$

This formula depends on the surface (35) via the theta functions (which are uniquely defined by some quasiperiodicity properties along noncontractible curves on the surface); their definition and that of their arguments will be omitted here (see Ref. [22]). We only remark that it is exactly at criticality, when the preceding surface becomes degenerate and the formula diverges.

IV. GAUGE-INVARIANT MODELS IN GENERAL

The reason why one could give an explicit formula for the entropy asymptotics in the reflection- and gauge-invariant cases [when $A^a(\theta) \equiv B^a(\theta) \equiv B^s(\theta) = 0$] and a less explicit one in the case when $A^a(\theta) \equiv B^s(\theta) \equiv 0$ was that the structure of the symbol $\varphi(\theta)$ was considerably simplified in both cases.

In the general quasifree case, it is hard to find the Wiener-Hopf factorization of the symbol, since there is no identically zero entry in the matrix function $\varphi(\theta)$. This is true even in the restricted case of gauge-invariant (but not reflection-invariant) models. However, as we will show in this section, one can circumvent this problem in this restricted case. We have seen in Sec. II B that we also can extract the entropy from the correlation matrix $C'_L \equiv \langle b_i b_j^\dagger \rangle|_{i,j=1,\ldots,L}$: It is given by $S_L = -\sum_{i=1}^{L}[\lambda_i \ln \lambda_i + (1 - \lambda_i) \ln(1 - \lambda_i)]$, where λ_i are the eigenvalues of the matrix C'_L. Now, we can use the contour integral trick again with a small alteration and write the entropy as

$$S_L = \lim_{\varepsilon \to 0} \frac{1}{2\pi i} \oint_{\Gamma(\varepsilon)} e(1 + \epsilon, \lambda)\frac{d \ln D'_L(\lambda)}{d\lambda}, \qquad (37)$$

where $D'_L(\lambda) = \det \widetilde{C}'_L(\lambda) = \det[\lambda I - (2C'_L - I)]$, the function $e(x,\lambda)$ and the contour Γ were defined in Sec. II B. Hence, the situation is analogous to Sec. III A except that $\lambda I - G_L$ is

replaced by $\lambda I - (2C'_L - I)$, which is also a Toeplitz matrix, but its symbol,

$$\lambda + 1 - 2c'(\theta) = \lambda + \frac{A(\theta)}{|A(\theta)|} \tag{38}$$

is not necessarily symmetric [$A_{i,j} \neq A_{j,i}$ implies $c'(\theta) \neq c'(-\theta)$]. Now, we can use the *Fisher-Hartwig conjecture* [26]: Suppose that the symbol $p(\theta):S^1 \to \mathbb{C}$ of a Toeplitz matrix has the following form:

$$p(\theta) = \psi(\theta) \prod_{r=1}^{R} t_{\beta_r,\theta_r}(\theta) u_{\alpha_r,\theta_r}(\theta), \tag{39}$$

with

$$t_{\beta_r,\theta_r}(\theta) = e^{-i\beta_r(\pi-\theta+\theta_r)}, \quad \theta_r < \theta < 2\pi + \theta_r,$$
$$u_{\alpha_r,\theta_r}(\theta) = [2 - 2\cos(\theta - \theta_r)]^{\alpha_r}, \quad \mathrm{Re}\,\alpha_r > -\tfrac{1}{2},$$

where the function $\psi:S^1 \to \mathbb{C}$ is smooth, nonvanishing, and has zero winding number. Then, the $L \to \infty$ asymptotic formula for the determinant reads

$$\det P_L = \left\{ \exp\left[\frac{1}{2\pi} \int_0^{2\pi} \ln \psi(\theta) d\theta \right] \right\}^L$$
$$\times \left(\prod_{i=1}^{R} L^{\alpha_i^2 - \beta_i^2} \right) \mathcal{E}[\psi, \{\alpha_i\}, \{\beta_i\}, \{\theta_i\}],$$

where

$$\mathcal{E}[\psi, \{\alpha_i\}, \{\beta_i\}, \{\theta_i\}]$$
$$= \mathcal{E}[\psi] \prod_{i=1}^{R} G_B(1 + \alpha_i + \beta_i) G_B(1 + \alpha_i - \beta_i) / G_B(1 + 2\alpha_i)$$
$$\times \prod_{i=1}^{R} [\psi_-(\exp(i\theta_i))]^{-\alpha_i - \beta_i} [\psi_+(\exp(-i\theta_i))]^{-\alpha_i + \beta_i}$$
$$\times \prod_{1 \leqslant i \neq j \leqslant R} \{1 - \exp[i(\theta_i - \theta_j)]\}^{-(\alpha_i + \beta_i)(\alpha_j - \beta_j)},$$

and the so-called Barnes function is defined by

$$G_B(1 + z) = (2\pi)^{z/2} e^{-(z+1)z/2 - \gamma_E z^2/2}$$
$$\times \prod_{n=1}^{\infty} \{(1 + z/n)^n e^{-z + z^2/(2n)}\}.$$

In our case, the symbol, defined by Eq. (38) earlier, is a step function jumping between $\lambda + 1$ and $\lambda - 1$, and the jumps occur at the zeros of $A(\theta)$. We can assume that $A(0) > 0$, as the local transformation $\hat{b}_i = b_i^\dagger$ (which keeps the entanglement entropy invariant) yields $A(0) \to -A(0)$. Using the notation for the zeros of $A(\theta)$ by θ_r, $r = 1, 2, \ldots, R$ in an increasing order in the period $(0, 2\pi]$, we can write the factors in Eq. (39) for the symbol (38),

$$u_{\alpha_r,\theta_r} = 1,$$
$$\Psi(\theta) = (\lambda + 1)\left(\frac{\lambda + 1}{\lambda - 1} \right)^{-1/2\pi \sum_j^{R/2}(\theta_{2j+1} - \theta_{2j}) - 1},$$
$$t_{\beta_r,\theta_r}(\theta) = e^{-i\beta_r(\pi - \theta + \theta_r)}, \quad \theta_r < \theta < 2\pi + \theta_r,$$

where

$$\beta_r = (-1)^r \frac{1}{2\pi i} \ln \frac{\lambda + 1}{\lambda - 1}.$$

Indeed, one can easily check that the function given by Eq. (39) with the above-defined ingredients has the value $p(0) = \lambda - 1$ and alternates between $\lambda \pm 1$ with jumps at the zeros of $A(\theta)$. Now, substituting our data in the statement of the conjecture, we get the expression for the determinant,

$$\det D'_L(\lambda)$$
$$= (\ln \Psi)^L L^{-R\beta^2} \prod_{\substack{r \neq s \\ r = s \bmod 2}} (1 - e^{i(\theta_s - \theta_r)})^{\beta^2}$$
$$\times \prod_{\substack{r \neq s \\ r \neq s \bmod 2}} (1 - e^{i(\theta_s - \theta_r)})^{-\beta^2} [G_B(1 + \beta) G_B(1 - \beta)]^R.$$

From this point, the calculation of the contour integral (37) is entirely identical to that of Refs. [18,19], and the result for entropy asymptotics reads

$$S_L = \frac{R}{6} \ln L - \frac{1}{6} \sum_{\substack{r \neq s \\ r = s \bmod 2}} \ln(1 - e^{i(\theta_s - \theta_r)})$$
$$+ \frac{1}{6} \sum_{\substack{r \neq s \\ r \neq s \bmod 2}} \ln(1 - e^{i(\theta_s - \theta_r)}) + \frac{R}{6}[(1 + \gamma_E) - 6I_3 \ln 2], \tag{40}$$

where the constants Γ_E and I_3 were given at the end of Sec. III A.

V. EXACT RESULTS FOR THE ENTROPY ASYMPTOTICS FOR CERTAIN NONGAUGE-INVARIANT MODELS

We now turn to discuss the cases of some nongauge-invariant models. In Secs. V A and V B, we will determine the entropy asymptotics for chains that are Kramers-Wannier self-dual and for those that decouple to two independent Majorana chains, by relating these cases to certain gauge-invariant models. In Secs. V C and V D, we will relate the entropy asymptotics of different nongauge-invariant models, by generalizing the XY-Ising transformation and doing local rotations.

We will make use of the fact that one can write the general (translation-invariant) quasifree Hamiltonian (4) in terms of the Majorana operators defined by Eq. (7) in the following way:

$$H = i \sum_{j,l=1}^{2N} T_{j,l} m_j m_l, \tag{41}$$

with the properties $T_{j,l} = -T_{l,j} \in \mathbb{R}$ and $T_{j+2n,l+2n} = T_{j,l}$ for all $n \in \mathbb{Z}$. The transformation between the two descriptions reads

$$T_{2j-1,2l-1} = \tfrac{1}{4} \mathrm{Im}(A_{j,l} + B_{j,l}),$$
$$T_{2j,2l} = \tfrac{1}{4} \mathrm{Im}(A_{j,l} - B_{j,l}),$$
$$T_{2j-1,2l} = \tfrac{1}{4} \mathrm{Re}(-A_{j,l} + B_{j,l}),$$
$$T_{2j,2l-1} = \tfrac{1}{4} \mathrm{Re}(A_{j,l} - B_{j,l}).$$

A. Kramers-Wannier self-dual models

The Kramers-Wannier (or disorder) spin operators on a spin chain are defined in terms of the original spin operators (Pauli matrices) as

$$\widehat{\sigma}_l^x = \prod_{i=1}^l \sigma_i^z, \quad \widehat{\sigma}_l^z = \sigma_l^x \sigma_{l+1}^x, \quad \widehat{\sigma}_l^y = -i\widehat{\sigma}_l^x\widehat{\sigma}_l^z. \quad (42)$$

These spin operators also satisfy the Pauli commutation relations $[\widehat{\sigma}_l^a, \widehat{\sigma}_k^b] = i\sum_c \delta_{kl}\epsilon_{abc}\sigma_l^c$. If the Hamiltonian is invariant with respect to the preceding transformation, then it is said to be *Kramers-Wannier self-dual*. Such self-dual Hamiltonians always describe critical models, an example is the critical point of the Ising model. A straightforward calculation shows that a quasifree Hamiltonian (41) is self-dual iff $T_{j,l} = T_{j+1,l+1}$ (recall, that translation invariance only implies $T_{j,l} = T_{j+2,l+2}$). Or, in other words, the self-dual models is the class of quasifree models, whose B matrix is real, and the equality $\text{Re}(A_{i,j} + B_{i,j}) = \text{Re}(-A_{i,j+1} + B_{i,j+1})$ is satisfied for every integer i, j. The two-point functions are then given by

$$\langle m_j m_l \rangle = \delta_{jl} + \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-i(j-l)\theta} \frac{iT(\theta)}{|T(\theta)|} d\theta, \quad (43)$$

with $T_\theta = \sum_n e^{-i\theta n} T_{0,n}$, thus, in this case, the block-Toeplitz matrix of the Majorana expectation values reduces to an ordinary Toeplitz matrix. Moreover, the previous formula is (up to a factor of 2) identical to that of $\langle b_i^\dagger b_l \rangle$ for a gauge-invariant model with the symbol given as $A(\theta) = iT(-\theta)$.

Now, let us compare the calculations of the entropy from the matrix $\langle m_i m_j \rangle$ in the general quasifree case [cf. Eq. (27)] and that from the matrix $\langle b_i^\dagger b_j \rangle$ in the gauge-invariant case Eq. (31). One can immediately conclude that the entanglement entropy of L spins in a Kramers-Wannier self-dual model defined by a matrix $T_{i,j}$ equals the entanglement entropy of $2L$ spins in a gauge-invariant quasifree model defined by $A_{i,j} = iT_{i,j}$. Thus, our result in Sec. IV applies to all Kramers-Wannier self-dual models as well. As an important example, we will apply this procedure in Sec. VI to obtain the analytic form of the entropy asymptotics for the critical Ising model with DM interaction.

B. Directly decoupled Majorana chains

Next, we turn to the case when the fermion chain decouples to two separate Majorana chains. From the form (41) of the Hamiltonian, we immediately see that, if $T_{2i,2j+1} = T_{2i+1,2j} = 0$ for all i, j, which is equivalent to having purely imaginary matrices A and B, then the fermion chain decouples to two independent Majorana chains: the one consisting of the odd modes and that of the even ones. Computing the symbol (24) corresponding to $B^a \equiv A^s \equiv 0$ gives

$$\varphi(\theta) = -i\begin{bmatrix} \frac{-A^a(\theta)-B^s(\theta)}{|-A^a(\theta)-B^s(\theta)|} & 0 \\ 0 & \frac{-A^a(\theta)+B^s(\theta)}{|-A^a(\theta)+B^s(\theta)|} \end{bmatrix}, \quad (44)$$

hence, the matrix C_L is a direct sum of two Toeplitz matrices with symbols $(-A^a \pm B^s)/|-A^a \pm B^s|$ corresponding to the two uncoupled Majorana chains. As in Sec. IV, one can again relate the Majorana expectation values to the ground-state

expectation values of the $b_i b_j^\dagger$ operators of gauge-invariant models. Namely, we have

$$\langle b_j^\dagger b_l \rangle_{-A+B} = \tfrac{1}{2} \langle m_{2j} m_{2l} \rangle, \quad (45)$$

$$\langle b_j^\dagger b_l \rangle_{-A-B} = \tfrac{1}{2} \langle m_{2j+1} m_{2l+1} \rangle, \quad (46)$$

where $\langle \cdot \rangle_{-A\pm B}$ stands for the expectation values in the gauge-invariant models with $H = \sum_{jl}(-A_{jl} \pm B_{jl})b_j^\dagger b_l$. Thus, by virtue of Eqs. (27) and (31), the entropy in the original model is given by the sum of entropies in the gauge-invariant ones before.

C. The generalized XY-Ising correspondence

There is also a less direct way certain fermion chains can be decoupled into two independent chains. Suppose that matrix T in Eq. (41) satisfies the following properties (for all i, j):

$$T_{4i,4j-1} = T_{4i,4j-2} = T_{4i-1,4j-3} = 0.$$

By defining

$$\begin{aligned} m_{2i-1}^{(1)} &= m_{4i-3}^{(1)}, \quad m_{2i}^{(1)} = m_{4i}^{(1)}, \\ m_{2i-1}^{(2)} &= m_{4i-2}^{(2)}, \quad m_{2i}^{(2)} = m_{4i-1}^{(2)}, \end{aligned} \quad (47)$$

one can see that the original quasifree Hamiltonian with $2N$ sites can be written as the sum of two other quasifree Hamiltonians with N sites:

$$\begin{aligned} H &= \sum_{i,j=1}^{4N} T_{i,j} m_i m_j \\ &= \sum_{i,j=1}^{2N} T_{i,j}^{(1)} m_i^{(1)} m_j^{(1)} + \sum_{i,j}^{2N} T_{i,j}^{(2)} m_i^{(2)} m_j^{(2)}. \end{aligned}$$

Here, the components of matrices $T^{(1)}$ and $T^{(2)}$ can be straightforwardly matched with the components of matrix T using the correspondence (47); it turns out that the decoupled subchains are also translation invariant: $T_{i,j}^{(1)/(2)} = T_{i+2,j+2}^{(1)/(2)}$. This type of decoupling is the generalization of the famous XY-Ising correspondence [27] (for another type of recent generalization of this correspondence, see Ref. [28]).

Considering the ground state in the thermodynamic limit, this type of decoupling immediately implies that the entanglement entropy of $2L$ consecutive spins in the model defined by T equals the sum of the entropies of L spins for the models defined by $T^{(1)}$ and $T^{(2)}$. This method was used for deriving the entropy asymptotics of the critical Ising model from that of the critical XY chain [29], our result generalizes this.

D. On general reflection-invariant models

As we have discussed, even for reflection-invariant chains ($A_{i,j}$ real, $B_{i,j}$ complex) there is no general formula for the entanglement entropy asymptotics. However, as we mentioned in Sec. III B, there is a formula for the saturation entropy in case the matrix B is real. In this section, we show that a subclass of models with complex B can be transformed back to the real case.

A transformation on the vector $(m_{2j-1}, m_{2j}) \equiv v^j \mapsto U v^j$ with a constant matrix $U \in U(2)$ is called canonical if the anticommutation relations $\{m_j, m_l\} = 2\delta_{jl}$ are preserved. For the two-point functions, it results in the adjoint action $\langle v^j \otimes v^j \rangle \mapsto U \langle v^j \otimes v^j \rangle U^\dagger$. Assume now that there are constants $c_x, c_y, c_z \in \mathbb{R}$ with at least one of them nonvanishing such that $c_x B^a(\theta) - c_y A^s(\theta) + c_z B^s(\theta) \equiv 0$ for all $\theta \in [0, 2\pi)$. In this case, there are rotations, which rotate the vector $c \equiv (c_x, c_y, c_z)$ into $c' \equiv (0, 0, c'_z)$ $(c'^z \neq 0)$ and consequently, $v \equiv (B^a, -A^s, B^s)$ into $v' \equiv (B'^a, -A'^s, 0)$ (as $v \perp c \Rightarrow v' \perp c'$). Furthermore, the Toeplitz symbol can be written as $\varphi = iM\mathbf{1} - iP/\sqrt{\Delta}(\sum_a \sigma^a v_a)$, $(a = x, y, z)$, so the rotation can be done by the adjoint action of SU(2) on 2×2 traceless Hermitian matrices $U_R G(v) U_R^{-1} = G(Rv)$ $[G(v) \equiv G]$. This is exactly the above-defined local transformation. Note, that the invariance of the entropy can immediately be seen from formula (36), which is invariant under the simultaneous transformation of all matrices by the adjoint action of any constant matrix (and the Wiener-Hopf factorization also remains valid). In the general case, when A^a, B^a, B^s are linearly independent Laurent polynomials of $e^{i\theta}$, this method does not work. One could, in principle, try to follow a strategy similar to that of Ref. [21] as done in Ref. [22], sketched in Sec. III B. To obtain explicit results, where physical limits can be studied, is difficult.

VI. NEAREST-NEIGHBOR COUPLING

We will now look at the general quasifree model with nearest-neighbor coupling and apply the foregoing machinery to study its entanglement entropy. Our method yields analytic expression for the Ising model with DM interaction at the critical point, while for the general noncritical case, we demonstrate that the ground state is not effected by the DM term, hence, the results [22] apply.

The Hamiltonian of the most general nearest-neighbor spin chain that can be mapped to a quasifree fermion chain is given by[5]

$$H = \sum_j \left[(1 + \gamma)\sigma_j^x \sigma_{j+1}^x + (1 - \gamma)\sigma_j^y \sigma_{j+1}^y \right.$$
$$\left. + D\left(\sigma_j^x \sigma_{j+1}^y - \sigma_j^y \sigma_{j+1}^x\right) + h\sigma_j^z \right]. \tag{48}$$

The real parameters stand for the magnetic field h, the strength D of the DM current, and the anisotropy $\gamma \in [0, 1]$. The model is mapped by the Jordan-Wigner transformation to the following fermionic one:
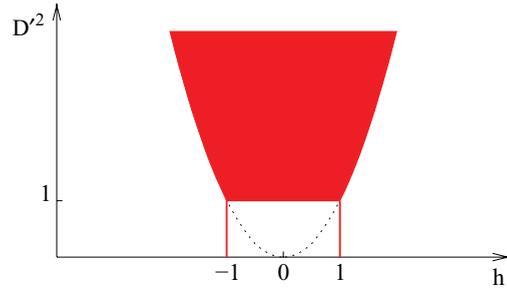
$$\frac{1}{2}H = \sum_j [b_j^\dagger b_{j+1}(1 - iD) + b_{j+1}^\dagger b_j(1 + iD)$$
$$+ \gamma(b_j^\dagger b_{j+1}^\dagger - b_j b_{j+1}) - 2hb_j^\dagger b_j]. \tag{49}$$

One can analyze whether the one-particle spectrum determined from Eq. (17):

$$\frac{\Lambda(\theta)}{2} = D\sin\theta + \sqrt{(\cos\theta - h)^2 + \gamma^2 \sin^2\theta} \tag{50}$$

---

[5]Note that the term $\sigma_j^x \sigma_{j+1}^y + \sigma_j^y \sigma_{j+1}^x$ can be eliminated by the basis change $(\sigma_j^x, \sigma_j^y) \to \left((\sigma_j^x - \sigma_j^y)/\sqrt{2}, (\sigma_j^x + \sigma_j^y)/\sqrt{2}\right)$.

vanishes or not at some θ to arrive at the following phase diagram:

The parameter D' is defined by

$$D' = \sqrt{D^2 + 1 - \gamma^2}, \tag{51}$$

and the critical regions are (i) the connected one between the $D'^2 = h^2$ parabolas and the $D'^2 = 1$ line and (ii) the $|h| = 1$ line segments. One immediately observes from the form of the two-point correlations (24) that the ground state of the noncritical regions is given by the XY model as $M(\theta) \equiv 0$ for all $\theta \in [0, 2\pi)$, and it is via $M(\theta)$ that $\langle m_j m_l \rangle$ depends on D.

Let us turn now to the special case of $\gamma = 1$, that is, the Ising model with the DM term. The phase diagram is the same as earlier with $D'^2 = D^2$. The case $h = 1$ can be solved by noticing that this case belongs to the class of models with the T matrix of the genuine Toeplitz type. We only have two nonzero elements $T_1 = 1/2$, $T_2 = -D/4$, which gives $iT(\theta) = 4\sin\theta(1 - D\cos\theta)$ for the numerator of the symbol (43). The entropy asymptotics are, thus, given by Eq. (40), with the following terms depending on the explicit form of the symbol: The number of zeros is $R = 4$, and the sum of the two sums involving their location vanishes (as a quick elementary calculation shows).

VII. SEEMING VIOLATIONS OF THE CALABRESE-CARDY FORMULAS

In this section, we will discuss two anomalies of the entropy asymptotics, which can appear at and in the vicinity of reflection-symmetry-breaking critical points and which seemingly do not fit the Calabrese-Cardy formulas. The first concerns the growth of the saturation entropy as we approach such critical points, while the second is about the breaking of reflection symmetry in the finite-size scaling of the entanglement entropy. We will discuss how we can interpret these anomalies to keep the validity of the Calabrese-Cardy formulas.

A. Anomalous behavior of the saturation entropy

As mentioned in Sec. I, the formula for the saturation value of the entanglement entropy of a block of spins near a critical point reads

$$S_{\text{sat}} = \frac{c}{3}\ln\xi + \text{const}, \tag{52}$$

where c is the central charge belonging to the critical point. We have seen in Sec. VI that considering the region $0 < D' < 1$ [see Eq. (51) for the definition of D'], the XY model with DM interaction is critical when $h = \pm 1$ and the corresponding central charge is $c_{XY-DM} = 1$, while for the model without DM interaction ($D = 0$), the central charge of the critical line (at $h = \pm 1$) is $c_{XY} = \frac{1}{2}$. However, we have also shown that when $h \neq \pm 1$, the ground state does not the depend on D in the noncritical region $0 \leqslant D' < 1$. Approaching the critical $h = \pm 1$ line in this region, the divergence of the saturation entropy (which, hence, is independent of D) is consistent with formula (52) in case the central charge is $c = \frac{1}{2}$, as can be seen from the results in Refs. [22,30]. Hence, the formula is not valid for the XY model with DM interaction, since the central charge is 1 for that model. This situation is typical for quadratic models with reflection-symmetry breaking: We have seen in Sec. II A that the ground state of the Hamiltonian Eq. (4) and the central charge do not depend on Im$A_{i,j}$ at a noncritical point, while they may depend on it at a critical one.

Hence, in order to understand the failure of formula (52), and to formulate a possible reinterpretation in the case at hand, let us first look at an other anomaly, which is, in some sense, similar. In the XX model with transverse-magnetic field,

$$H = \sum_i \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + h\sigma_i^z,$$

there is quantum phase transition at the points $h = \pm 1$. In the region $-1 < h < 1$, the ground state of the model is critical with algebraically decaying truncated correlation function $C^{xx}(n) = \langle \sigma_i^x \sigma_{i+n}^x \rangle - C_0^{xx}$ (where $C_0^{xx} = \lim_{n \to \infty} \langle \sigma_i^x \sigma_{i+n}^x \rangle$) and a diverging entropy asymptotics $S_L = \frac{1}{3} \ln L + k$, while outside this region, the ground state is either the all-spin-up or the all-spin-down state (depending on the sign of h). Hence, approaching the critical region from the noncritical one, the saturation entropy will not diverge, however, this does not contradict formula (52), since there is no diverging correlation length either. When we enter the critical region, the state will change suddenly in such a way that the correlation function $C^{xx}(n)$ that was identically zero in the noncritical region suddenly will be nonzero and even quasilong ranged (decay algebraically with n) (i.e., an infinite correlation length appears instantaneously). This is, in some sense, a degenerate situation because considering a bigger parameter space, for example, the XY model with transverse-magnetic field,

$$H = \sum_i (1+\gamma)\sigma_i^x \sigma_{i+1}^x + (1-\gamma)\sigma_i^y \sigma_{i+1}^y + h\sigma_i^z,$$

and approaching the critical line ($-1 < h < 1$, $\gamma = 0$) by fixing the value of h (between 1 and -1) and taking $\gamma \to 1$, we will observe a diverging correlation length and a diverging saturation entropy satisfying formula Eq. (52), as can be seen from the results in Refs. [22,30].

A similar situation, but in a more complicated form, occurs in the XY model with DM interactions. At the critical point, the correlation functions $C^{xx}(n)$ and $C^J(n) = \langle \sigma_i^x \sigma_{i+n}^y - \sigma_i^y \sigma_{i+n}^x \rangle$

decay algebraically. However, away from criticality, $C^J(n)$ is identically zero, while $C^{xx}(n)$ behaves "in a normal way", i.e., it decays exponentially with n and the correlation length ξ_s diverges as one approaches the critical line $h = 1$. We can think that there are two independent critical modes both with $c = \frac{1}{2}$; one is behaving normally, the other in an anomalous way, hence, in Eq. (52), we should only insert the central charge of the normally behaving mode. This picture could be made more convincing and precise, if one could show that, similar to the previously mentioned XX case, this anomalous behavior is a degenerate one by considering a bigger subspace (e.g., the XYZ chain with magnetic field and DM interaction [i.e., adding the term $\sum_i \Delta\sigma_i^z \sigma_{i+1}^z$ to Eq. (48)]). We conjecture that when approaching the mentioned critical point in such a bigger parameter space, the generic behavior induces normally diverging correlation lengths for both $C^{xx}(n)$ and $C^J(n)$, denoted by ξ_{xx} and ξ_J, respectively; and the entropy will scale according to a generalized Calabrese-Cardy formula of the form of

$$S_L = \tfrac{1}{2} \ln \xi_{xx} + \tfrac{1}{2} \ln \xi_J + \text{const.} \qquad (53)$$

We have started to study this conjecture numerically, and the results will be the subject of a forthcoming publication.

B. Breaking of reflection invariance in the finite-size scaling of the entanglement entropy

The other feature we will investigate is whether (and to which extent) the breaking of reflection invariance can be observed as a finite-size effect in the scaling of the entropy. More precisely, consider a finite-spin chain with a quadratic Hamiltonian of length N, and compute the entropy $S(L,N)$ of the restriction of the ground state to the first L sites. The Calabrese-Cardy formula (3), which has been confirmed (up to subleading corrections) analytically and numerically for many reflection-symmetric models [6,7,31], suggests a reflection-invariant form $S(L,N) = S(N-L,N)$. The questions we ask are whether this symmetry of the ground state can be broken for a quadratic Hamiltonian, which is not invariant, and whether the symmetry breaking survives the limit $N \to \infty$ (with L/N fixed)?

First, we should notice that the reflection invariance of the entropy function $S(L,N)$ can only be broken if neither the matrix A nor B is real for the following reasons. We saw that the Hamilton operator (49) is invariant (and so is the unique ground state) unless Im$A \neq 0$. For the case Im$B = 0$, one should consider the transformations $b_i \to b_{N-i}$ and $b_i \to b_i^\dagger$ and determine the transformed density matrices restricted to the first L sites of the chain. For the case Im$B = 0$, they are identical (both transformations lead to changes $A \to A^\dagger$, $B \to -B$ in the Hamiltonian). The first one corresponds to the reflection we are interested in, whereas the second is a local transformation of the chain and ,thus, preserves the entanglement entropy.

As noted in Sec. VI, the nearest-neighbor quasifree Hamiltonians can always be transformed by local transformations such that B is real. Hence, to have a symmetry-breaking entropy function, we have to consider next-to-nearest-neighbor
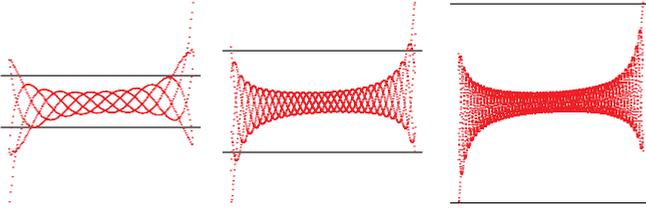
FIG. 2. (Color online) The figures show $\Delta S \equiv S(L,N) - S(N-L,N)$, the difference between the entropies of the ground state restricted to the left- and rightmost L modes of the chain with $N = 1024, 2048, 4096$. The black lines indicate $\Delta S = \pm 10^{-3}$. The plots show, in all three cases, the range $x \equiv L/N \in [0.04, 0.96]$. Besides the feature that the function $N \mapsto \Delta S(N)$ decreases for any fixed L, it also has an additional oscillating structure. One finds that the analytic function $p[N/L + N/(N-L)] \cos 2\pi L(\lambda/N - 1/5)$ fits this structure rather well with a suitable constant p for the amplitude and the N-independent wavelength λ. The explanation of this behavior is under investigation.

Hamiltonians. The particular Hamiltonian we investigated was

$$
\begin{aligned}
H = \sum_{i=1}^{N} (& t_1 b_i^\dagger b_{i+1} + t_1^* b_{i+1}^\dagger b_i + t_2 b_i^\dagger b_{i+2} + t_2^* b_{i+2}^\dagger b_i^\dagger \\
& + p_1 b_i b_{i+1} - p_1^* b_i^\dagger b_{i+1}^\dagger + p_2 b_i b_{i+2} - p_2^* b_i^\dagger b_{i+1}^\dagger + h b_i^\dagger b_i),
\end{aligned}
$$

with the following parameters: $t_1 = 7 + 28i$, $t_2 = 4 + 5i$, $p_1 = 11 + 10i$, $p_2 = 3 + 4i$, and $h = 12$.

The numerical results depicted in Fig. 2 demonstrate that the reflection symmetry of the entropy function $S(L,N)$ is indeed broken. However, it is also visible that the deviation $S(L,N) - S(N-L,N)$ goes to zero in the limit $N \to \infty$ for any fixed L. Moreover, we can see in Fig. 3 that, in this limit, the curves nicely converge to the Calabrese-Cardy formula.
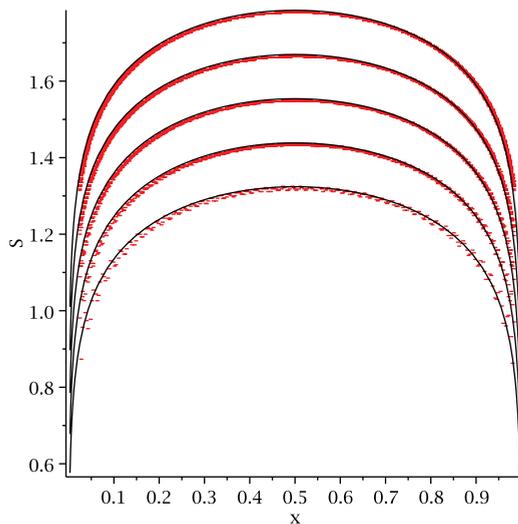

FIG. 3. (Color online) Here, we can see the entropies $S(L,N)$ for $N = 256, 512, 1024, 2048, 4096$ and the corresponding Calabrese-Cardy curves. The central charge is a fit parameter, and it converges to the physical value $c = 1$ fast (the deviation decreases roughly linearly with N from 0.038 at $N = 256$ to 0.003 at $N = 4096$).

Hence, we conclude that, according to our numerical results, the reflection symmetry of the entropy function can be broken, but its scaling limit shows no such breaking, and the Calabrese-Cardy formula is valid.

VIII. SUMMARY AND OVERVIEW

In this paper, we studied the entanglement entropy asymptotics of spin chains that can be mapped to quasifree fermionic models given by the sum of a gauge-invariant term (parametrized by a self-adjoint matrix A) and a nongauge-invariant one (parametrized by an antisymmetric matrix B). Many models of physical importance belong to the class of complex A (and B), implying the breaking of reflection symmetry). The entanglement properties of these systems have hardly been addressed in the literature before, hence, we concentrated on these cases.

We have determined the two-point functions of the Majorana operators in complete generality. An interesting result following from this investigation is that the ground state can only be reflection-symmetry breaking if it is critical.

We have been able to write down the analytic expression of the entropy asymptotics for the most general gauge-invariant models, and also extended these results for certain nongauge-invariant models. A detailed investigation of the nearest-neighbor case was carried out. We have derived the explicit form of the entanglement entropy asymptotics for the Ising model with DM interaction at the critical point, which was unknown until now. In the noncritical regime, we demonstrated that the ground state is independent of the DM coupling, thus, the entropy asymptotics given in Ref. [22] without the DM term is also valid here. This indicated violations of the formula for the saturation entropy $\sim c \ln \xi$ near the critical point $|h| = 1$. We have given a possible physical explanation for this.

Concerning the general landscape of the block-entropy asymptotics of quasifree models, we extended the general knowledge to a large extent, nevertheless, the general case remains to be a difficult unsolved mathematical problem.[6] Even when specifying the discussion to the nearest-neighbor case, there remains a surprisingly large region of the critical regime, for which the scaling of the block entropy still remains an open problem.

Finally, we carried out numerical checks for the investigation of finite-size effects. We used a model Hamiltonian with next-to-nearest-neighbor interaction, which exhibited reflection-symmetry breaking in the finite-size scaling of the entanglement entropy. The deviation was demonstrated to converge to zero quickly by increasing the size of the chain, while the block entropy converged to the asymptotic Calabrese-Cardy formula.

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[6]Assuming that three of the four polynomials $A^s(z), A^a(z)$, $B^s(z), B^a(z)$ are linearly independent, the entropy is unknown.

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