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 is calculated analytically for general gauge-invariant models, which has, until now, been done only for the reflection symmetric sector. Analytical results are also derived for certain non-gauge-invariant models, e.g., for the Ising model with Dzyaloshinskii-Moriya interaction. We also study numerically finite chains of length $N$ with a non-reflection-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 non-critical 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 amount of results have been accumulated about translation-invariant systems. However, the results almost exclusively correspond to reflection symmetric systems, despite the fact that 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 type or non-equilibrium steady states.

Considering a subsystem $S$ of a system, which is in a pure state, the entanglement between the subsystem and its environment is characterised by the von Neumann entropy

$$S(\rho_S) := -\text{Tr}(\rho_S \ln \rho_S) ,$$

where $\rho_S$ 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]

$$S_L = \frac{c}{3} \ln L + k ,$$

where $c$ is the conformal charge of its universality class and $k$ is a non-universal constant. For non-critical 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]

$$S_{\text{sat}} = \frac{c}{3} \ln \xi + k' ,$$

where $\xi$ 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]

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

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 [32]

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

Throughout the paper we will assume either open boundary conditions or "fermionic" periodic boundary conditions ($b_i = b_{i+N}$) [33]. 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) anti-symmetric matrix. Finite-ranged interaction means that there exists a positive integer $n_0$ such that $A_{0,l} = B_{0,l} = 0$ if $l \geq n_0$. Such a spin-chain Hamiltonian

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is not invariant with respect to the reflection transformation $R(\sigma_{ij}^a) = \sigma_{ji}^a$ ($a = x,y,z$), if $A$ is not a real matrix. (One might think that the term $(b_ib_j - b_jb_i)$, with $i > j$ also breaks the translation invariance of the spin chain, but a short calculation shows that its image under the Jordan-Wigner transformation is the following reflection-invariant term $\sigma_i^z \Pi_{n=i+1}^{i-1} \sigma_n^a \sigma_j^+ + \sigma_j^- \Pi_{n=j-1}^{i+1} \sigma_n^a \sigma_i^-$). One of the most studied quantum spin chain with broken reflection symmetry is the Ising model with transverse magnetic field and Dzyaloshinskii-Moriya (DM) interaction (in the $z$-direction) [10–13]:

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

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

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

whose ground states are used to describe the energy current carrying eigenstates of the $XX$ model [14–16]. Certain non-reflection 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, Mo, and Mezzadri [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 [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 non-vanishing $B$. 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 non-critical 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 non-reflection-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 that this deviation goes to zero as we increase the system size.

The paper is structured as follows. In Section 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 Section III. We derive an analytic formula for the entanglement entropy for general gauge-invariant models in Section IV, whereas in Section V we show how we can extend our results for certain types of non-gauge-invariant models too. Section VI is an application of the above to models with nearest neighbor interactions, while in Section VII we discuss how some of our analytic and numerical results conflict with the formulas (2) and (3) and how we can “resolve” this discrepancy. Finally, Section 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 later to obtain analytical results.

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

$$b_k = \frac{1}{\sqrt{N}} \sum_n \exp \left(-\frac{2\pi i nk}{N}\right) b_n, \quad (8)$$

$$b_n = \frac{1}{\sqrt{N}} \sum_k \exp \left(\frac{2\pi i nk}{N}\right) \tilde{b}_k, \quad (9)$$
the summation runs in the set of integers $[\frac{N-1}{2}, \frac{N+1}{2}]$ for $N$ odd (even) and the transform of the one-particle creation operators are to be computed by means of taking the adjoint of the above formulae.

For Toeplitz matrices we define the Fourier transform as

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

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

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

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

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

$$c_k = \alpha_k \hat{b}_k + \beta_k \hat{b}_k^\dagger \ , \ \alpha_k, \beta_k \in \mathbb{C} \ , \tag{13}$$

where the coefficients $\alpha_k, \beta_k$ 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

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

having taken the relations $A_k^* = A_k$, $B_{-k} = -B_k$ (which are 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

$$\langle c_k^\dagger c_{k'} \rangle = \frac{1}{2} \left( -\frac{\Lambda_k}{|\Lambda_k|} + 1 \right) \delta_{kk'} \tag{18}$$

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

$$\langle b_j b_i \rangle = \frac{1}{N} \sum_k \frac{2\pi i k (j-l)}{N} B_k \left( \frac{A_k}{|\Lambda_k|} + \frac{A_{-k}}{|\Lambda_k|} \right) \times$$

$$\langle b_j^\dagger b_i \rangle = \frac{1}{N} \sum_k \frac{2\pi i k (j-l)}{N} \times$$

$$2 + \frac{\left( A_k \Lambda_k - A_{-k} \Lambda_{-k} \right)}{4 \sqrt{\Delta_k \Delta_{-k}}} \left( \frac{\Lambda_k}{|\Lambda_k|} + \frac{\Lambda_{-k}}{|\Lambda_{-k}|} \right) \ , \tag{19}$$

where $\Delta_k = (A_k + A_{-k})^2 + 4B_k B_k^*$, and the two remaining two-point functions $\langle b_j^\dagger b_i \rangle$ and $\langle b_j b_i \rangle$ can be calculated directly from the above equations. Ultimately, we would like to have a linear combination of the above, 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

$$A_k^e = A_{-k} + A_k , \ A_k^o = A_{-k} - A_k \ , \tag{20}$$

and the step functions

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

Note, that $A_k^e, A_k^o, B_k^e, B_k^o \in \mathbb{R}$ and $\Delta_k = (A_k^e)^2 + (B_k^e)^2 + (B_k^o)^2$. We now take the thermodynamic limit $(N \to \infty)$ and write the final result in a manner usually adopted in the literature

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

where the matrix $C$ has the following structure

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

The $\Pi_l$'s are $2 \times 2$ block entries that read

$$\Pi_l = \frac{i}{2} \int_{-\pi}^{\pi} d\theta e^{-il\theta} \times$$

$$\begin{pmatrix} iM(\theta) - P(\theta) & iB^*(\theta) & \frac{iB^*(\theta)}{\sqrt{\Delta(\theta)}} & \frac{iA^*(\theta) - iB^*(\theta)}{\sqrt{\Delta(\theta)}} \\ P(\theta) - A^*(\theta) - iB^*(\theta) & iM(\theta) + P(\theta) \end{pmatrix} \tag{24}$$

where $\theta = 2\pi ik/N$, 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 (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]:

$$\langle m_{i_1} \ldots m_{i_{2k-1}} \rangle = 0 \ , \tag{25}$$

$$\langle m_{i_1} \ldots m_{i_{2k}} \rangle = \sum_{\pi} \text{sgn}(\pi) \prod_{l=1}^{k} \langle m_{\pi(2l-1)} m_{\pi(2l)} \rangle \ , \tag{26}$$

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 analyse the obtained result. The one particle spectrum (17) has the form of a sum of a reflection invariant \( \sqrt{\Delta(\theta)/2} \) and a non-invariant 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 \((m_i m_j)\) has a dependence on the non-reflection 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, non-critical quasifree systems never break reflection invariance [34]. We will discuss some implications of this important fact in Sections VI and VII.

### 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

\[
C_L = \begin{pmatrix}
\Pi_0 & \Pi_{-1} & \cdots & \Pi_{-L+1} \\
\Pi_1 & \Pi_0 & \cdots & \Pi_{-L+2} \\
\vdots & \vdots & \ddots & \vdots \\
\Pi_{L-1} & \Pi_{L-2} & \cdots & \Pi_0 \\
\end{pmatrix},
\]

(25)

where the \( \Pi_i \)'s are \( 2 \times 2 \) matrices given by Eq. (24). Let us denote by \( W \) the orthogonal matrix, the adjoint action of which diagonalizes the antisymmetric real matrix \( C_L \) into its canonical form, i.e., 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 [35]

\[
\rho_L = \prod_{j=1}^{L} \left[ \frac{1 + \nu_j}{2}, \frac{1 + \nu_j}{2} \right] = \prod_{j=1}^{L} \frac{1 + \nu_j}{2}, \frac{1 - \nu_j}{2} \cdot \frac{1 - \nu_j}{2}. \]

where \( \nu_j = \sum_{k=0}^{2L-1} W_{jk} m_k \) 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 easily calculated. It can be written in terms of the function

\[
e(x, \nu) = -\frac{x + \nu}{2} \ln \frac{x + \nu}{2} - \frac{x - \nu}{2} \ln \frac{x - \nu}{2},
\]

(26)

as

\[
S_L \equiv S(\rho_L) = \sum_{j=1}^{L} e(1,\nu_j).
\]

(27)

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

\[
D_L(\lambda) = \det (i\lambda I + C_L) = (-1)^L \prod_{j=0}^{L-1} (\lambda^2 - \nu_j^2),
\]

(28)

and exploiting the residue theorem by writing down the following integral

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

(29)

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

\[
\tilde{C}_L(\lambda) = i\lambda I + C_L
\]

(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 non-gauge-invariant two-point functions vanish \( \langle b_j b_k \rangle = \langle \bar{b}_j^\dagger \bar{b}_k^\dagger \rangle = 0 \). If we restrict the state to \( L \) consecutive sites, and denote by \( M_L \) the corresponding restriction of the matrix \( M_{ij} = \langle \bar{b}_i^\dagger b_j \rangle \) and by \( U_L \) the (not necessarily real) unitary, the adjoint action of which diagonalizes \( M_L \) \( (\sum_{k=0}^{2L} U_{i}^\dagger (M_L)_{jk} U_{ik} = \lambda_i \delta_{ik}) \), then the density matrix of the restricted state reads

\[
\rho_L = \prod_i \left( \lambda_i c_i^\dagger c_i + (1 - \lambda_i) e_i^\dagger e_i \right),
\]
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

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

(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 \( B^2(\theta) \equiv B^2(\theta) \equiv A^2(\theta) \equiv 0 \) and the symbol of the majorana two-point functions (24) reduces to

\[
\varphi(\theta) = \begin{pmatrix}
0 & A^2(\theta) \\
-A^2(\theta) & 0
\end{pmatrix} .
\]

Hence, \( C_L \) can be factorized as

\[
C_L(\lambda) = \begin{pmatrix}
0 & 1 \\
-1 & 0
\end{pmatrix} \otimes G_L(\lambda) ,
\]

(32)

where \( G_L(\lambda) \) is the restriction of the Toeplitz matrix with scalar symbol \( g(\theta) = A^2(\theta)/|A^2(\theta)| \) to an \( L \times L \) block on the diagonal. From this it follows that \( \det(C_L) = D_L = (-1)^L \det(\lambda I + G_L) \det(\lambda I - G_L) \). 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 Section II B. This was done by Keating and Mezzadri [19, 20]: they obtained the following result: Let there be number \( R/2 \) zeros of \( A^2(\theta) \) denoted by \( \theta_r \) \( (r = 1, \ldots, R/2) \) in the semi-circle \( [0, \pi] \) (implying another \( R/2 \) zeros in the other semi-circle \( [-\pi, 0] \): \( -\theta_r, r = 1, \ldots, R/2 \). Then the entanglement entropy asymptotics is given by

\[
S_L(\rho_A) = \frac{R}{6} \ln L + \frac{R}{6} K - \frac{R}{2} (\ln 2) I_3 ,
\]

(33)

where

\[
K = 1 + \gamma_E + \frac{1}{R} \sum_{r=1}^{R/2} \ln |1 - e^{i2\theta_r}| -
\]

\[
\frac{2}{R} \sum_{1 \leq s \leq r \leq R/2} (-1)^{r+s} \ln \left| \frac{1 - e^{i(\theta_r - \theta_s)}}{1 - e^{i(\theta_s + \theta_r)}} \right| ,
\]

where \( \gamma_E = ... \) is Euler’s constant, and \( I_3 = 0.0221603... \), independent of \( A(\theta) \) (consult [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 matrix \( A \) and \( B \) are real, i.e., when \( A^2(\theta) \equiv B^2(\theta) \equiv 0 \). In this case, the symbol reads

\[
\varphi(\theta) = \begin{pmatrix}
0 & A^2(\theta) + B^2(\theta) \\
A^2(\theta) - B^2(\theta) & 0
\end{pmatrix} .
\]

(34)

Here the idea, invented for the XY model in [21] and generalized for the present case in [22], is to extend the domain of \( \varphi : S^1 \to M_2(\mathbb{C}) \) to the complex plane and use a theorem of Widom [26], 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 \( A(z) = A(\exp(-i\theta)) \equiv A(\theta), \text{and} B(z) = B(\exp(-i\theta)) \equiv B(\theta) \) are Laurent polynomials. One writes

\[
\frac{A^2(z) - B^2(z)}{|A(z) - B(z)|} = \frac{q(z)}{|q(z)|} = \sqrt{\frac{q(z)}{q(1/z)}} = \prod_{j=1}^{2n_0} \frac{z - z_j}{1 - z_j z}
\]

with \( z_j \) being the roots of the polynomial \( p(z) = z^{n_0}q(z) \), where \( n_0 \) is the range of the coupling (defined after (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 \( q(\exp(-i\theta)) \equiv A^2(\theta) - iB^2(\theta) \). The non-analytic behaviour of the above 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

\[
w^2 = \prod_{j=1}^{2n_0} (z - z_j)(1 - z z_j) .
\]

(35)

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

\[
\frac{d \ln D_L(\lambda)}{d \lambda} \approx - \frac{2M}{1 - \lambda^2} +
\]

\[
\frac{1}{2 \pi} \text{tr} \left[ \left( \frac{dU^{-1}_{\pm}(z)}{dz} U_{\pm}^{-1}(z) + V_{\pm}^{-1}(z) \frac{dV_{\pm}(z)}{dz} \right) G^{-1}(z) \right] dz
\]

(36)

and the difference \( (\text{rhs.} - \text{lhs.}) < C \rho^{-L} \) where the constant \( \rho \) satisfies \( 1 < \rho < \min\{|\lambda_i| : |\lambda_i| > 1\} \) (the complex numbers \( \lambda_i \) are the roots of \( p(z) \) and their reciprocals). The saturation entropy is given by

\[
S(\rho_A) = \frac{1}{2} \int_1^\infty \Theta(\beta(\lambda) \frac{\theta}{\beta} + \frac{\beta}{\theta}(\lambda) \frac{\theta^2}{2} - \frac{\beta}{\theta}(\frac{\theta}{2})) \theta^2 d\lambda .
\]
This formula depends on the surface (35) via the theta functions (which are uniquely defined by some quasi-periodicity properties along non-contractible curves on the surface); their definition and that of their arguments will be omitted here (see [22]). We only remark that it is exactly at criticality, when the above 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 case (when $A^a(\theta) \equiv B^a(\theta) \equiv B^*(\theta) = 0$) and a less explicit one in the case when $A^a(\theta) \equiv B^*(\theta) \equiv 0$ 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 of 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 section II B that we can extract the entropy also from the problem in this restricted case. We have seen in section II B that we can extract the entropy also from the correlation matrix $C_L = \langle b_i^\dagger b_j \rangle_{i,j=1,L}$: it is given by

$$S_L = \lim_{\epsilon \to 0} \frac{1}{2\pi i} \int_{\Gamma(\epsilon)} \epsilon(1, \epsilon, \lambda) \frac{d\ln D'_L(\lambda)}{d\lambda},$$

where $D'_L(\lambda) = \det C'_L(\lambda) = \det(\lambda I - (2C'_L - I))$, the function $\epsilon(x, \lambda)$ and the contour $\Gamma$ were defined in Section II B. Hence the situation is analogous to section III A except that $M - G_L$ is replaced by $M - (2C'_L - I)$, which is also a Toeplitz matrix, but its symbol

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

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 [25]: Suppose that the symbol $p(\theta) : S^1 \to \mathbb{C}$ of a Toeplitz matrix has the following form

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

with

$$t_{\beta_r, \theta_r}(\theta) = e^{-i\beta_r(\pi - \theta + \theta_r)}, \quad \theta_r < \theta < 2\pi + \theta_r,$$

$$u_{\alpha_r, \theta_r}(\theta) = \left(2 - 2\cos(\theta - \theta_r)\right)^{\alpha_r}, \quad \Re \alpha_r > \frac{1}{2},$$

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

$$\det P_L = \left(\exp \left(\frac{1}{2\pi} \int_0^{2\pi} \ln \psi(\theta)d\theta\right)\right)^L \times \prod_{i=1}^R \left(1 + \frac{1}{2\pi} \int_0^{2\pi} \ln \left(1 - e^{-\theta}b_i^\dagger b_i\right) d\theta\right)^{\beta_i} \times \prod_{i=1}^R \left(1 - e^{i\theta_i - \theta_j}\right)^{-(\alpha_i + \beta_i)(\alpha_j - \beta_j)},$$

and the so-called Barnes function is defined by

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

In our case the symbol, defined by Eq. (38) above, 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 $b_i = b_i^\dagger$ (which keeps the entanglement entropy invariant) yields $A(0) \to -A(0)$. Using the notation for the zeros of $A(\theta)$ by $\theta_r$, $r = 1, 2, \ldots, R$ in an increasing order in the period $(0, 2\pi]$ we can write the factors in (39) for the symbol (38)

$$u_{\alpha_r, \theta_r} = 1,$$

$$\Psi(\theta) = (\lambda + 1 + \frac{1}{\lambda - 1}) \left(1 - \left(\frac{\lambda + 1}{\lambda - 1}\right)^{\beta_r}\right) - \frac{1}{2\pi} \int_0^{2\pi} \ln \frac{\lambda + 1}{\lambda - 1} d\theta,$$

$$t_{\beta_r, \theta_r}(\theta) = e^{-i\beta_r(\pi - \theta + \theta_r)}, \quad \theta_r < \theta < 2\pi + \theta_r,$$

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 (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

$$\det D'_L(\lambda) = (\ln \Psi)^L L^{-R\beta^2} \prod_{r \neq s \mod 2} \left(1 - e^{i(\theta_r - \theta_s)}\right)^{\beta^2} \times \prod_{r \neq s \mod 2} \left(1 - e^{i(\theta_r - \theta_s)}\right)^{\beta^2} (G_B(1 + \beta)G_B(1 - \beta))^R.$$
From this point, the calculation of the contour integral (37) is entirely identical to that of [18, 19], and the result for entropy asymptotics reads

\[ S_L = \frac{R}{6} \ln L - \frac{1}{6} \sum_{r<x \mod 2} \ln(1 - e^{i(\theta_r - \theta_r)}) + \]
\[ \frac{1}{6} \sum_{r \neq x \mod 2} \ln(1 - e^{i(\theta_r - \theta_r)}) + \frac{R}{6} \left( 1 + \gamma_E \right) - 6I_3 \ln 2 \]

where the constants \( \Gamma_E \) and \( I_3 \) were given at the end of section III A.

V. EXACT RESULTS FOR THE ENTROPY ASYMPOTICS FOR CERTAIN NON-GAUGE-INVARINAT MODELS

We now turn to discuss the cases of some non-gauge-invariant models. In the first two subsections we will determine the entropy asymptotics for chains that are Kramers-Wannier selfdual and for those that decouple to two independent majorana chains, by relating these cases to certain gauge-invariant models. In the last two subsections we will relate the entropy asymptotics of different non-gauge-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 (7) in the following way:

\[ H = i \sum_{j=1}^{2N} T_{j,i} m_j m_l \] (41)

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

\[ T_{2j-1,2l-1} = \frac{1}{4} \text{Im}(A_{j,i} + B_{j,i}) \]
\[ T_{2j,2l} = \frac{1}{4} \text{Im}(A_{j,i} - B_{j,i}) \]
\[ T_{2j-1,2l} = \frac{1}{4} \text{Re}(-A_{j,i} + B_{j,i}) \]
\[ T_{2j,2l-1} = \frac{1}{4} \text{Re}(A_{j,i} - B_{j,i}) \].

A. Kramers-Wannier selfdual models

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

\[ \tilde{\sigma}_i^r = \prod_{i=1}^{l} \sigma_i^r, \quad \tilde{\sigma}_i^q = \sigma_i^r \sigma_{i+1}^r, \quad \tilde{\sigma}_i^q = -i \tilde{\sigma}_i^r \tilde{\sigma}_i^r. \] (42)

These spin operators also satisfy the Pauli commutation relations \( [\tilde{\sigma}_i^r, \tilde{\sigma}_j^q] = i \sum \delta_{ij} \epsilon_{abc} \sigma_j^a \). If the Hamiltonian is invariant with respect to the above transformation then it is said to be Kramers-Wannier selfdual. Such selfdual 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 selfdual iff \( T_{j+l} = T_{j+1,j+l+1} \) (recall, that translation invariance only implies \( T_{j,l} = T_{j+2,l+2} \)). Or in other words, the selfdual models is the class of quasifree models, whose \( \tilde{B} \) 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 integers \( i,j \). The two-point functions are then given by:

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

with \( T_{\theta} = \sum_n e^{-in\theta} T_{0,n} \), thus in this case the block-Toeplitz matrix of the majorana expectation values reduces to an ordinary Toeplitz matrix. Moreover, the above formula is (up to a factor of 2) identical to that of \( \langle b_{i,j}^* b_j \rangle \) 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 \( \langle b_{i,j}^* b_j \rangle \) in the gauge-invariant case Eq. (31). One can immediately conclude that the entanglement entropy of \( L \) spins in a Kramers-Wannier selfdual model defined by a matrix \( T_{i,j} \) equals half the entanglement entropy of \( 2L \) spins in a gauge-invariant quasifree model defined by \( A_{i,j} = iT_{i,j} \). Thus our result in Section IV applies to all Kramers-Wannier selfdual models as well. As an important example, we will apply this procedure in Section 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 \( T_{2n+2,2n+2} + T_{2n+1,2n+1} = 0 \) 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 \( B' \equiv A^* \equiv 0 \) gives

\[ \varphi(\theta) = -i \left( \begin{array}{cc} -A^*(\theta) & -B^*(\theta) \\ A^*(\theta) & B^*(\theta) \end{array} \right) \]

hence the matrix \( C_L \) is a direct sum of two Toeplitz matrices with symbols \(-A^* \pm B^*\) corresponding to the two uncoupled majorana chains. As in the
previous section, one can again relate the majorana expectation values to the ground state expectation values of the \(b_i b_j\) operators of gauge-invariant models. Namely, we have
\[
\langle b_j^i b_i^\dagger \rangle_{-A+B} = \frac{1}{2} \langle m_{2j} m_{2i} \rangle \tag{45}
\]
\[
\langle b_j^i b_i^\dagger \rangle_{-A-B} = \frac{1}{2} \langle m_{2j+1} m_{2i+1} \rangle \tag{46}
\]
where \(\langle \cdot \rangle_{-A\pm B}\) stand for the expectation values in the gauge invariant models with \(H = \sum_j ( -A_j \pm B_j ) b_i^j b_i^\dagger \). Thus, by virtue of Equations (27) and (31) the entropy in the original model is given by the sum of entropies in the gauge invariant ones above.

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
\[
m_{2i-1}^{(1)} = m_{4i-3}^{(1)} , \quad m_{2i}^{(1)} = m_{4i}^{(1)} ,
\]
\[
m_{2i-1}^{(2)} = m_{4i-2}^{(2)} , \quad m_{2i}^{(2)} = m_{4i-1}^{(2)} ,
\]
(47)
one can see that the original quasifree Hamiltonian with 2\(N\) sites can be written as the sum of two other quasifree Hamiltonians with \(N\) sites:
\[
H = \sum_{i,j=1}^{4N} T_{i,j} m_i m_j =
\]
\[
= \sum_{i,j=1}^{2N} T_{i,j}^{(1)} m_i^{(1)} m_j^{(1)} + \sum_{i,j=1}^{2N} T_{i,j}^{(2)} m_i^{(2)} m_j^{(2)} .
\]
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: \(T^{(1)/(2)}_{i,j} = T_{i+2,j+2}\). This type of decoupling is the generalization of the famous XY-Ising correspondence [27] (for an other type of recent generalization of this correspondence, see [28]).

Considering the ground state in the thermodynamic limit, this type of decoupling immediately implies that the entanglement entropy of 2\(L\) 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 Section III B, there is a formula for the saturation entropy in case the matrix \(B\) is real. In this subsection 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 anti-commutation relations \(\{ m_i, m_j \} = 2 \delta_{ij}\) are preserved. For the two point functions it results in the adjoint action \((v_j \otimes v_j^\dagger) \mapsto U (v_j \otimes v_j^\dagger) U^\dagger\). Assume now that there are constants \(c_x, c_y, c_z \in \mathbb{R}\) with at least one of them non-vanishing, such that \(c_x B^a(\theta) - c_y A^a(\theta) + c_z B^a(\theta) \equiv 0\) for all \(\theta \in [0, 2\pi)\). In this case there are rotations, which rotate the vector \(v \equiv (c_x, c_y, c_z)\) into \(v' \equiv (0, 0, c_z)\) \((c_z^2 \neq 0\) and consequently \(v' \equiv (B^a, -A^a, B^a)\) into \(v' \equiv (B^a, -A^a, 0)\) \((v' \mapsto v' \mapsto c'\)). Further, the Toeplitz symbol can be written as \(\varphi = iM 1 - iP/\sqrt{\Lambda} (\sum_a \sigma^a v_a)\), \((a = x, y, z)\), so the rotation can be done by the adjoint action of \(SU(2)\) on 2 \times 2 traceless Hermitian matrices \(U_R G(v) V_{R}^{-1} = G(Rv) (G(v) \equiv G)\). This is exactly the above defined local transformation. Note, that the invariance of the entropy can be immediately seen from the 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 remains also valid). The general case, when \(A^a, B^a, C^a\) 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 [21] as was done in [22] sketched in section 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 neighbour coupling and apply the above 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 non-critical 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 neighbour spin chain that can be mapped to a quasi-free fermion chain is given by [36]
\[
H = \sum_j \left( (1 + \gamma) \sigma_j^x \sigma_{j+1}^x + (1 - \gamma) \sigma_j^y \sigma_{j+1}^y + D (\sigma_j^x \sigma_{j+1}^y - \sigma_j^y \sigma_{j+1}^x) + h \sigma_j^z \right) . \tag{48}
\]
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:

\[
\frac{1}{2} H = \sum_j (b_j^\dagger b_{j+1} (1 - iD) + b_j^\dagger b_j (1 + iD) +
\gamma (b_j^\dagger b_{j+1} - b_j b_{j+1}) - 2h b_j^\dagger b_j).
\]

(49)

One can analyse whether the one-particle spectrum determined from (17):

\[
\Lambda(\theta) = D \sin \theta + \sqrt{(\cos \theta - h)^2 + \gamma^2 \sin^2 \theta}
\]

vanishes or not at some \( \theta \) to arrive at the following phase diagram:

\[
D^2
\]

\[
\begin{array}{c}
1 \\
0 \\
-1
\end{array}
\]

\[
\begin{array}{c}
D \quad h
\end{array}
\]

The parameter \( D' \) is defined by

\[
D' = \sqrt{D^2 + 1 - \gamma^2},
\]

(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 non-critical regions are 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 DM term. The phase diagram is the same as above with \( D'^2 = D^2 \). The case \( h = 1 \) can be solved by noticing that this case belongs to the class of models with \( T \) matrix of the genuine Toeplitz type. We have only two non-zero elements \( T_1 = 1/2, T_2 = -D/4 \), which gives \( i T(\theta) = 4 \sin \theta (1 - D \cos \theta) \) for the numerator of the symbol (43). The entropy asymptotics for this class is given via \( S_L = S_{2L}^{A=2T}/2 \), as explained after Eq. (43), the superscript refers to the gauge-invariant model, whose Toeplitz symbol is \( A \). Its entropy is given by given by Eq. (40). The final result reads

\[
S_L = \begin{cases}
\frac{1}{3} \ln L + \frac{1}{12} \ln (1 + \frac{1}{12}) + C_{IsDM} |D| > 1 \\
\frac{1}{6} \ln L + C_{Is} |D| \leq 1
\end{cases}
\]

(52)

with

\[
C_{IsDM} = \frac{1}{3} (1 + \gamma_E + (1 - 6I_3) \ln 2) \approx 0.726067
\]

\[
C_{Is} = \frac{1}{6} (1 + \gamma_E + (2 - 6I_3) \ln 2) \approx 0.478558
\]

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 the Introduction, the formula for the saturation value of the entanglement entropy of a block of spins near a critical point reads

\[
S_{sat} = \frac{c}{3} \ln \xi + \text{const},
\]

(53)

where \( c \) is the central charge belonging to the critical point. We have seen in the previous section 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 \( c_{XY} = 1/2 \). However, we have also shown that when \( h \neq \pm 1 \) the ground state does not depend on \( D \) in the non-critical region \( 0 \leq D' < 1 \). Approaching the critical \( h = \pm 1 \) line in this region, the divergence of the saturation entropy (which is hence independent of \( D \)) is consistent with formula (53) in case the central charge is \( c = 1/2 \), as can be seen from the results in [22, 30]. Hence the formula is not valid for the XY model with DM interaction, since for that model the central charge is 1. This situation is typical for quadratic models with reflection symmetry breaking: We have seen in Section II.A that the ground state of the Hamiltonian Eq. (4) and the central charge do not depend on \( \text{Im}A_{i,j} \) at a non-critical point, while they may depend on it at a critical one.

Hence, in order to understand the failure of formula (53), 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 \( C_{XX}(n) = \langle \sigma_i^x \sigma_{i+n}^x \rangle \) 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 all-spin-down state (depending on the sign of \( h \)). Hence approaching the critical region from the non-critical one, the saturation entropy will not diverge, however, this does not contradict formula (53), 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 quasi-long-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, e.g., 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 \( \gamma \rightarrow 1 \), we will observe a diverging correlation length and a diverging saturation entropy satisfying formula Eq. (53), as can be seen from the results in [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 \( C^J(n) = (\sigma_i^x \sigma_{i+n}^x - \sigma_i^y \sigma_{i+n}^y) \) 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 \( \xi_1 \), characterizing the exponential decay, 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. (53) 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, similarly to the previously mentioned XX case, this anomalous behaviour 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 \( \sum_i \Delta \sigma_i^x \sigma_{i+1}^x \) to the Eq. (48). We conjecture that 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 \( \xi_{xx} \) and \( \xi_J \), respectively; and the entropy will scale according to a "generalized" Calabrese-Cardy formula of the form of

\[
S_L = \frac{1}{2} \ln \xi_{xx} + \frac{1}{2} \ln \xi_J + \text{const}.
\]

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 question we ask is 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 \( N \rightarrow \infty \) (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 \( \text{Im} A \neq 0 \). For the case \( \text{Im} B = 0 \), one should consider the transformations \( b_i \rightarrow b_{N-i} \) and \( b_i \rightarrow b_i^\dagger \) and determine the transformed density matrices restricted to the first \( L \) sites of the chain. For the case \( \text{Im} B = 0 \) they are identical (both transformations lead to changes \( A \rightarrow A^\dagger \), \( B \rightarrow -B \) 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 those preserve 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 neighbour Hamiltonians. The particular Hamiltonian we investigated was

\[
H = \sum_{i=1}^N \left( t_1 b_i^\dagger b_{i+1} + t_2 b_{i+1}^\dagger b_i + t_2 b_i^\dagger b_{i+2} + t_3 b_{i+2}^\dagger b_i + p_1 b_i^\dagger b_{i+1} - p_1 b_{i+1}^\dagger b_i + p_2 b_i b_{i+2} - p_2 b_{i+2} b_i + h b_i^\dagger b_i \right),
\]

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 \( N \rightarrow \infty \) for any fixed \( L \). Moreover, we can see in Fig. 3 that in this limit the curves nicely converge to the Calabrese-Cardy formula. 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
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. A novelty 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 non-gauge-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 Dzyaloshinskii-Moriya 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 [22] without the DM term is valid also here. This indicated violations of the formula for the saturation entropy \( \sim c \log \xi \) 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 [37]. 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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\[ \Delta S \equiv S(L, N) - S(N - L, N) \]

Many models of physical importance belong to the class of complex \( A \) (and \( B \)), implying

FIG. 2: 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 \( x \equiv L/N \in [0.04, 0.96] \). Beside 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 \( \lambda \). The explanation of this behaviour is under investigation.

FIG. 3: 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 \( N = 4096 \)).

quasifree fermionic models given by the sum of a gauge-invariant term (parametrized by a selfadjoint matrix \( A \)) and a non-gauge-invariant one (parametrized by an anti-symmetric matrix \( B \)). Many models of physical importance belong to the class of complex \( A \) (and \( B \)), implying

\[ \Delta S \equiv S(L, N) - S(N - L, N) \]

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 \( N = 4096 \)).
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[32] Throughout this paper we will use the following convention for the Jordan-Wigner transformation:
\[ \sigma_j^x = \left( \prod_{i=1}^{j-1} (2b_i b_i^\dagger - 1) \right) (b_j + b_j^\dagger), \]
\[ \sigma_j^y = \left( \prod_{i=1}^{j-1} (2b_i b_i^\dagger - 1) \right) i (b_j^\dagger - b_j), \]
\[ \sigma_j^z = 2 b_j b_j^\dagger - 1. \]
[33] Note that periodic boundary conditions on the fermion chain may not be mapped to periodic boundary condition after the Jordan-Wigner transformation, as was shown in [9].
[34] Of course, various non-quasifree models exist with a gap that break reflection symmetry, see e.g., [24].
[35] One can check that for any \( m_{i_1} m_{i_2} \cdots m_{i_k} (1 \leq i_1, i_2, \ldots, i_k \leq L) \) monomial of the majorana operators its expectation value (given by the formulas ...) is equal to \( \text{Tr} (\rho L m_{i_1} m_{i_2} \cdots m_{i_k}) \), hence \( \rho L \) is indeed the density matrix of the restricted state.
[36] Note, that the term \( \sigma_j^x \sigma_j^z + \sigma_j^z \sigma_{j+1}^z \) can be eliminated by the basis change \( (\sigma_j^x, \sigma_j^y) \rightarrow (\sigma_j^x - \sigma_j^y)/\sqrt{2}, (\sigma_j^x + \sigma_j^y)/\sqrt{2} \).
[37] Assuming that three of the four polynomials \( A^z(z), A^x(z), B^z(z), B^x(z) \) are linearly independent, the entropy is unknown.