Entanglement in fermionic chains with finite-range coupling and broken symmetries

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We obtain a formula for the determinant of a block Toeplitz matrix associated with a quadratic fermionic chain with complex coupling. Such couplings break reflection symmetry and/or charge conjugation symmetry. We then apply this formula to compute the Rényi entropy of a partial observation to a subsystem consisting of contiguous sites in the limit of large size. The present work generalizes similar results due to Its, Jin, and Korepin [Fields Institute Communications, Universality and Renormalization, Vol. 50, p. 151, 2007] and Its, Mezzadri, and Mo [Commun. Math. Phys. **284**, 117 (2008)]. A striking feature of our formula for the entanglement entropy is the appearance of a term scaling with the logarithm of the size. This logarithmic behavior originates from certain discontinuities in the symbol of the block Toeplitz matrix. Equipped with this formula we analyze the entanglement entropy of a Dzyaloshinski-Moriya spin chain and a Kitaev fermionic chain with long-range pairing.

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I. INTRODUCTION

The ability of controlling parts or subsystems of a quantum system is the main resource of a future quantum computer with processing superiority over today's computers. Such ability presupposes the control of local operations on parts of the system and its effects due to quantum correlations on other parts of the system. Such quantum correlations among distinct parts of the system are encoded by the keyword entanglement—the characteristic trait of quantum mechanics, in the words of Schrödinger. It is therefore of great interest to be able to quantify or measure how entangled the parts of the system are. This is the reason for the great effort being carried out to elucidate the notion of quantum entanglement.

Entanglement has been studied in diverse systems, the simplest and most studied being those associated with quadratic spinless fermionic chains. These are related via a (nonlocal) Jordan-Wigner transformation to simple spin systems such as Ising, XX, and XY with an external magnetic coupling. It is fair to say that nowadays we have a good control of almost all aspects of quantum correlations in such systems. Such achievements were possible due to the sophisticated resolution of diverse mathematical problems, most of them associated with the computation of the determinant of correlation matrices–usually of the block Toeplitz type due to translational symmetry. The sophistication may be appreciated by noting that such computations are instances of the Riemann-Hilbert problem (RHP). This fact brings in a geometrical flavor to the study of entanglement entropy for such systems. It is a question of the analysis of the topology of a certain Riemann surface associated to the system.

In the framework of this successful ideology, we can find two classes of block Toeplitz matrices [1]. On one hand, those that can be reduced to a pure Toeplitz one, with scalar symbol, where the Fisher-Hartwig theorem [2] is the key to obtain an asymptotic expansion of our determinant. That is the case of spinless fermionic chains described by a Hamiltonian which preserves the fermionic number. In this way, Jin and Korepin [3] obtained a formula for the von Neumann entropy associated to a set of contiguous sites in the XX spin chain. Using the same philosophy, the Rényi entropy of an interval for every stationary state of a general quadratic spinless fermionic Hamiltonian which preserves the fermionic number of excitations is obtained in Ref. [4]. On the other hand, we have those block Toeplitz matrices that cannot be reduced to a scalar one; as usually happens when the above number symmetry is broken. In general, we cannot bypass the RHP. Confronting it, Its, Jin, and Korepin [5] obtained a formula for the von Neumann entanglement entropy associated to a set of contiguous sites in the XY spin chain. An expression for the Rényi entropy was then written down by Franchini, Its, and Korepin [6]. Later the von Neumann entropy for the case of quadratic spinless fermionic chains with finite-range coupling was provided by Its, Mezzadri, and Mo [7]. In a different spirit, using a duality transformation, Peschel [8] obtained the same kind of formula for the XY spin chain.

Later on, Kádar and Zimborás [9] started a systematic analysis of the entanglement entropy for self-dual models with broken reflection symmetry. It is interesting to note that in this self-dual case the block Toeplitz matrix analysis reduces to that of a scalar Toeplitz matrix.

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In this work, we extend further the above sequence of complexities by considering the Rényi entanglement entropy for quadratic spinless fermionic chains with complex finite-range couplings. Due to the complex nature of the couplings, some alternate possibilities appear. We have to deal with some interesting challenges associated with some discontinuities in the symbol of a block Toeplitz matrix. As a resolution of these challenges we here propose a formula for the determinant of such Toeplitz matrix with 2×2 symbol (23):

$$\ln D_X(\lambda) = \frac{|X|}{2\pi} \int_{-\pi}^{\pi} \ln \det[\lambda I - \mathcal{G}(\theta)] d\theta + \ln |X| \sum_{j=1}^{J} b_j + \cdots ,$$

where b_j encapsulates the information due to the discontinuities of the symbol. The important fact of this formula is its logarithmic scaling with the size of the subsystem $|X|$. As an application of this formula, we proceed to an exhaustive analysis of the entropy computation of a spin chain with Dzyaloshinski-Moriya (DM) coupling and a Kitaev fermionic chain with long-range pairing.

As stated by Its, Mezzadri, and Mo in Ref. [7], the core of our derivation of the entropy of entanglement is the computation of determinants of Toeplitz matrices for a wide class of 2×2 matrix symbols. The 2×2 matrix character of these symbols stems from the noninvariance of the fermionic number. This is a distinctive feature of the XY model. We also consider finite-range couplings: the Kitaev chain with long-range pairing being an example. Our work deals with the complex nature of the couplings. This feature allows one to consider systems with broken reflection and/or charge conjugation. An example of a system with broken reflection symmetry is the DM spin chain.

When considering such systems with broken reflection and/or charge conjugation, we obtain a wider moduli of system, among those one may encounter systems with critical behavior. Such systems are expected to display an entropy that scales logarithmically with the size of the system. This is indeed what we obtain when we use our proposed formula for the determinant of the block Toeplitz matrix in the Rényi entropy formula.

We organize this paper as follows. In Sec. II, we present the general Hamiltonian for a spinless fermionic chain with finite-range coupling and define the Fock space of states; in Sec. III, we review the well-known relation between the entropy and the correlation matrix and in (12) we derive the latter for a general stationary state. In Sec. IV, we compute the determinant of the block Toeplitz matrix, first in the smooth case where the Its, Mezzadri, and Mo's formula (19) applies, and then by extending it in (23) to the case where discontinuities are present; later we use this result to obtain our general expression (26) for the asymptotic behavior of the entanglement entropy in a critical theory with long-range couplings and the above broken symmetries. In Secs. V and VI, we apply the formulas of previous section for an analysis of the entropy in the DM spin chain model and in a Kitaev chain with long range pairing respectively. Finally, Sec. VII contains our conclusions.

II. FINITE-RANGE HAMILTONIAN

Let us consider an N-site chain of size ℓ with N spinless fermions described by a quadratic, translational invariant Hamiltonian with finite-range couplings ($L < N/2$)

$$H = \frac{1}{2} \sum_{n=1}^{N} \sum_{l=-L}^{L} (2A_l a_n^\dagger a_{n+l} + B_l a_n^\dagger a_{n+l}^\dagger - \overline{B}_l a_n a_{n+l}). \quad (1)$$

Here a_n and $a_n^\dagger$ represent the annihilation and creation operators at the site n. The only nonvanishing anticommutation relations are

$$\{a_n^\dagger, a_m\} = \delta_{nm},$$

and in (1) we assume $a_{n+N} = a_n$.

In order that H is Hermitian, the hopping couplings must satisfy $A_{-l} = \overline{A}_l$. In addition, without loss of generality, we may take $B_l = -B_{-l}$. When $B_l = 0$, $\forall l$, our Hamiltonian preserves the fermionic number. The reflection symmetry ($P : a_n \mapsto i\, a_{N-n}$) is broken when A_l is not real; the imaginary part of B_l breaks reflection-charge conjugation ($PC : a_n \mapsto i\, a_{N-n}^\dagger$), where we define charge conjugation by ($C : a_n \mapsto a_n^\dagger$).

We can express H in terms of uncoupled fermion modes. First, given the translational invariance of the Hamiltonian, we introduce the Fourier modes

$$b_k = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{-i\theta_k n} a_n; \qquad \theta_k = \frac{2\pi k}{N}, \quad k \in \mathbb{Z}.$$

Notice that by construction $b_k = b_{k+N}$. The Hamiltonian in (1) can now be written as

$$H = \mathcal{E} + \frac{1}{2} \sum_{k=0}^{N-1} (b_k^\dagger, b_{-k}) \begin{pmatrix} F_k & G_k \\ \overline{G}_k & -F_{-k} \end{pmatrix} \begin{pmatrix} b_k \\ b_{-k}^\dagger \end{pmatrix},$$

with

$$F_k = \sum_{l=-L}^{L} A_l e^{i\theta_k l}, \quad (2)$$

which is real,

$$G_k = \sum_{l=-L}^{L} B_l e^{i\theta_k l}, \quad (3)$$

which is an odd function of k, i.e., $G_{-k} = -G_k$, and

$$\mathcal{E} = \frac{1}{2} \sum_{k=0}^{N-1} F_k. \quad (4)$$

The matrix

$$R_k = \begin{pmatrix} F_k & G_k \\ \overline{G}_k & -F_{-k} \end{pmatrix}$$

is Hermitian and satisfies

$$R_{-k} = -\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \overline{R}_k \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Therefore we can introduce the dispersion relation Λ_k, with $\Lambda_{k+N} = \Lambda_k$, such that the diagonalization of R_k is given by

$$U_k R_k U_k^\dagger = \begin{pmatrix} \Lambda_k & 0 \\ 0 & -\Lambda_{-k} \end{pmatrix},$$

with U_k a unitary matrix. The order ambiguity in the eigenvalues is fixed if we demand that $\Lambda_k^S \equiv (\Lambda_k + \Lambda_{-k})/2 \geqslant 0$. Thus the dispersion relation is univocally determined.

We can now write the Hamiltonian in diagonal form by performing a Bogoliubov transformation to the new modes

$$\begin{pmatrix} d_k \\ d_{-k}^\dagger \end{pmatrix} = U_k \begin{pmatrix} b_k \\ b_{-k}^\dagger \end{pmatrix},$$

in terms of which H reads

$$H = \mathcal{E} + \sum_{k=0}^{N-1} \Lambda_k \left(d_k^\dagger d_k - \frac{1}{2} \right).$$

Λ_k can be derived from the relations

$$\Lambda_k^A \equiv \frac{\Lambda_k - \Lambda_{-k}}{2} = \frac{F_k - F_{-k}}{2} \equiv F_k^A,$$

and

$$\Lambda_k^S = \sqrt{\left(F_k^S\right)^2 + |G_k|^2} \geqslant 0,$$

with

$$F_k^S \equiv \frac{F_k + F_{-k}}{2}.$$

Finally we get

$$\Lambda_k = \sqrt{\left(F_k^S\right)^2 + |G_k|^2} + F_k^A. \tag{5}$$

An eigenstate of H is determined by a subset of occupied modes $\mathbf{K} \subset \{0, \ldots, N-1\}$. If we denote by $|0\rangle$ the vacuum of the Fock space for the new modes, i.e., $d_k |0\rangle = 0$, the stationary state

$$|\mathbf{K}\rangle = \prod_{k \in \mathbf{K}} d_k^\dagger |0\rangle \tag{6}$$

has energy

$$E_{\mathbf{K}} = \mathcal{E} + \frac{1}{2} \sum_{k \in \mathbf{K}} \Lambda_k - \frac{1}{2} \sum_{k \notin \mathbf{K}} \Lambda_k.$$

In particular, the ground state will be obtained by filling the modes with negative energy (Dirac sea)

$$|\hat{\mathbf{K}}\rangle = \prod_{\Lambda_k < 0} d_k^\dagger |0\rangle,$$

with energy

$$E_{\hat{\mathbf{K}}} = \mathcal{E} - \frac{1}{2} \sum_{k=0}^{N-1} |\Lambda_k|.$$

Note that if $|F_k^A| < \sqrt{(F_k^S)^2 + |G_k|^2}$ the dispersion relation is positive and the ground state of H is $|0\rangle$. On the contrary, if there are some momenta with $|F_k^A| > \sqrt{(F_k^S)^2 + |G_k|^2}$ a Dirac sea develops, hence the ground state has occupied modes and differs from the Fock space vacuum. In this case, the ground state is not invariant under reflection in momentum space $k \leftrightarrow N - k$. As we shall see in the next section, this fact has important consequences for the evaluation of the entanglement entropy and its behavior near the boundaries of the critical region.

III. ENTANGLEMENT ENTROPY AND CORRELATION MATRIX

The main goal of this paper is to study the Rényi entanglement entropy for the ground state of a Hamiltonian of the kind analysed in the previous section. For the moment, however, we keep the general discussion by considering a general stationary state $|\mathbf{K}\rangle$ as defined in (6).

Given a subsystem X of contiguous sites of the fermionic chain, with complementary set Y we have the corresponding factorization of the Hilbert space $\mathcal{H} = \mathcal{H}_X \otimes \mathcal{H}_Y$. If the system is in the pure state $|\mathbf{K}\rangle$, the reduced density matrix for X is obtained by taking the partial trace with respect to $\mathcal{H}_Y$, $\rho_X = \mathrm{Tr}_Y |\mathbf{K}\rangle \langle \mathbf{K}|$. The Rényi entanglement entropy of X is defined by

$$S_\alpha(X) = \frac{1}{1-\alpha} \ln \mathrm{Tr} \left(\rho_X^\alpha\right). \tag{7}$$

In order to compute $S_\alpha(X)$ we take advantage of the fact that the state $|\mathbf{K}\rangle$ satisfies the Wick decomposition property and, as it is well known [10,11], the reduced density matrix can be obtained from the two-point correlation function.[1]

For any pair of sites $n,m \in X$, we introduce the following correlation matrix,

$$\begin{aligned} (V_X)_{nm} &= 2\left\langle \begin{pmatrix} a_n \\ a_n^\dagger \end{pmatrix} (a_m^\dagger, a_m) \right\rangle - \delta_{nm}\, I \\ &= \begin{pmatrix} \delta_{nm} - 2\langle a_m^\dagger a_n \rangle & 2\langle a_n a_m \rangle \\ 2\langle a_n^\dagger a_m^\dagger \rangle & 2\langle a_n^\dagger a_m \rangle - \delta_{nm} \end{pmatrix}. \end{aligned}$$

Notice that V_X is a $2|X| \times 2|X|$ matrix.

Following Refs. [10,11] one can show that the Rényi entanglement entropy reads

$$S_\alpha(X) = \frac{1}{2(1-\alpha)} \mathrm{Tr} \ln \left[\left(\frac{\mathbb{I} + V_X}{2} \right)^\alpha + \left(\frac{\mathbb{I} - V_X}{2} \right)^\alpha \right], \tag{8}$$

where $\mathbb{I}$ is the $2|X| \times 2|X|$ identity matrix.

From the numerical side, this formula supposes a drastic improvement of computational capabilities. In fact, the dimension of ρ_X is $2^{|X|}$, so the cost of calculating $S_\alpha(X)$ grows, in principle, exponentially with the length of the interval.

[1]This construction of a density matrix out of correlation functions represents an instance of a general procedure known as Gelfand-Naimark-Segal (GNS) construction: one is given an algebra of observables and a positive linear functional acting on this algebra, and the outcome is the construction of a Hilbert space, where the algebra is represented, and a density matrix representing the positive linear functional. In Refs. [22,23] it is discussed a unified approach to compute the entropy due to a partial observation, which is associated with a restriction to a subalgebra of observables. In particular, this framework allows the study of entropy respecting the statistics of particles.

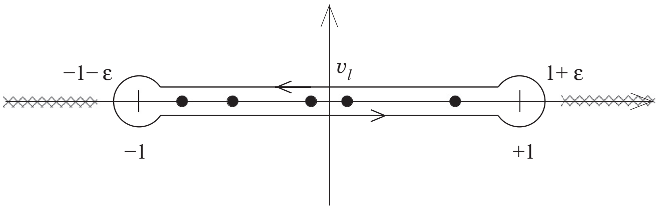

FIG. 1. Contour of integration, cuts and poles for the computation of $S_\alpha(X)$. The cuts for the function f_α extend to $\pm\infty$.

However, V_X has only dimension $2|X|$, allowing one to reach larger sizes of X.

We can derive a useful way of implementing (8) by applying Cauchy's residue theorem, so that

$$S_\alpha(X) = \lim_{\varepsilon\to 0^+} \frac{1}{4\pi i}\oint_{\mathcal{C}} f_\alpha(1+\varepsilon,\lambda)\frac{d\ln D_X(\lambda)}{d\lambda}d\lambda, \quad (9)$$

where $D_X(\lambda) = \det(\lambda\mathbb{I} - V_X)$,

$$f_\alpha(x,y) = \frac{1}{1-\alpha}\ln\left[\left(\frac{x+y}{2}\right)^\alpha + \left(\frac{x-y}{2}\right)^\alpha\right], \quad (10)$$

and $\mathcal{C}$ is the contour depicted in Fig. 1 which surrounds the eigenvalues v_l of V_X, all of them lying in the real interval $[-1,1]$.

In order to compute V_X we first rewrite it in the Fourier basis,

$$(V_X)_{nm} = \frac{1}{N}\sum_{k=0}^{N-1}\mathcal{G}_k e^{i\theta_k(n-m)},$$

with

$$\mathcal{G}_k = 2\left\langle\begin{pmatrix} b_k \\ b_{-k}^\dagger\end{pmatrix}(b_k^\dagger, b_{-k})\right\rangle - I.$$

Or in terms of the Bogoliubov modes

$$\mathcal{G}_k = 2U_k^\dagger\left\langle\begin{pmatrix} d_k \\ d_{-k}^\dagger\end{pmatrix}(d_k^\dagger, d_{-k})\right\rangle U_k - I.$$

We now compute the expectation value in the stationary state $|\mathbf{K}\rangle$ associated to the occupation $\mathbf{K}\subset\{0,1,\ldots,N-1\}$, so that

$$\left\langle\begin{pmatrix} d_k \\ d_{-k}^\dagger\end{pmatrix}(d_k^\dagger, d_{-k})\right\rangle = \begin{pmatrix} 1-\chi_{\mathbf{K}}(k) & 0 \\ 0 & \chi_{\mathbf{K}}(N-k)\end{pmatrix}, \quad (11)$$

where $\chi_{\mathbf{K}}(k)$ is the characteristic function of $\mathbf{K}$, i.e., it is 1 or 0 according to whether k belongs to $\mathbf{K}$ or not. Now, introducing

$$M_k \equiv U_k^\dagger\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}U_k = \frac{1}{\sqrt{(F_k^S)^2 + |G_k|^2}}\begin{pmatrix}F_k^S & G_k \\ \overline{G}_k & -F_k^S\end{pmatrix},$$

we finally arrive at

$$\mathcal{G}_k = \begin{cases} -M_k, & \text{if } k\in\mathbf{K} \text{ and } N-k\in\mathbf{K},\\ -I, & \text{if } k\in\mathbf{K} \text{ and } N-k\notin\mathbf{K},\\ M_k, & \text{if } k\notin\mathbf{K} \text{ and } N-k\notin\mathbf{K},\\ I, & \text{if } k\notin\mathbf{K} \text{ and } N-k\in\mathbf{K}.\end{cases} \quad (12)$$

Notice that the symbol of V_X at momentum k depends not only on the occupation number at k but also at $N-k$. This is a general fact that, to our knowledge, has been overlooked in the literature. We believe that there are two reasons for that. First, if $F^A(k)=0$ and we are interested in a ground state like that in Refs. [5,7], then we have $\mathbf{K}=\emptyset$. Hence any consideration on the occupation numbers is superfluous. The symbol is M_k and that is all. The second situation corresponds to general stationary states, like in Refs. [4,12] where the whole casuistics in the computation of the symbol would play a role. However in these papers, like in Ref. [13], one has $G_k = 0$, therefore M_k is diagonal, the symbol can be considered scalar instead of a 2×2 matrix and the discussion above is not necessary.

In this paper we are interested in computing $S_\alpha(X)$ for the ground state. As it is well known, it contains information on the critical properties of the system. Following the previous discussion, it is determined by the occupation set

$$\hat{\mathbf{K}} = \{k\,|\,\Lambda_k < 0\}.$$

Since $\Lambda_k = \Lambda_k^S + F_k^A$, with $\Lambda_k^S = \Lambda_{N-k}^S \geqslant 0$ and $F_k^A = -F_{N-k}^A$, applying the general expression in (12), we obtain

$$\hat{\mathcal{G}}_k = \begin{cases} -I, & \text{if } -\Lambda_k^S > F_k^A,\\ M_k, & \text{if } -\Lambda_k^S < F_k^A < \Lambda_k^S,\\ I, & \text{if } F_k^A > \Lambda_k^S.\end{cases} \quad (13)$$

Note that for the vacuum state, and due to the fact that $\Lambda_k^S \geqslant 0$, one can not have that Λ_k and Λ_{N-k} are both negative implying that the first case in (12) never happens.

In the so-called thermodynamic limit, $N\to\infty$, $\ell\to\infty$ with N/ℓ fixed, the previous N-tuples, like Λ_k, F_k, G_k and the others, become 2π-periodic functions determined by the relation $\Lambda(\theta_k) = \Lambda_k$, $\theta_k = 2\pi k/N$ and analogously for $F(\theta), G(\theta), \ldots$.

IV. BLOCK TOEPLITZ DETERMINANT AND ENTANGLEMENT ENTROPY

In this section we compute an expression for $D_X(\lambda) \equiv \det(\lambda\mathbb{I} - V_X)$ for large $|X|$. This enters in the formula (9) so that we can obtain the asymptotic behavior of $S_\alpha(X)$ for large $|X|$.

There exists a generalization for block Toeplitz matrices of the Szegö theorem [14] that allows to compute the linear dominant term of $D_X(\lambda)$. According to it,

$$\ln D_X(\lambda) = \frac{|X|}{2\pi}\int_{-\pi}^{\pi}\ln\det[\lambda I - \hat{\mathcal{G}}(\theta)]d\theta + \cdots, \quad (14)$$

where the dots denote sublinear contributions. If we apply this general result to our case, the integrand with $\hat{\mathcal{G}}(\theta)$ read from (13) becomes the simple result:

$$\det[\lambda I - \hat{\mathcal{G}}(\theta)] = \begin{cases} (\lambda+1)^2, & \text{if } -\Lambda_k^S > F_k^A,\\ \lambda^2 - 1, & \text{if } -\Lambda_k^S < F_k^A < \Lambda_k^S,\\ (\lambda-1)^2, & \text{if } F_k^A > \Lambda_k^S.\end{cases} \quad (15)$$

After inserting this result into (14) and then (9) we immediately see that the linear, dominant contribution to the entropy vanishes. Therefore, in order to determine its asymptotic behavior one is forced to compute the subdominant terms for the determinant that are hidden in the dots of (14).

Case 1: $F^A(\theta)^2 < F^S(\theta)^2 + |G(\theta)|^2$, *for all* $\theta \in (-\pi,\pi]$. We first discuss the case in which $F^A(\theta)^2 < F^S(\theta)^2 + |G(\theta)|^2$, for all $\theta \in (-\pi,\pi]$. The symbol $\hat{\mathcal{G}}(\theta)$ is therefore continuous.

This situation has been analysed before in the notable papers [5,7] when $F(\theta) = F(-\theta)$ and $G(\theta)$ is imaginary. Their results can be straightforwardly generalized to our case provided

$$\overline{G(\theta)} = -e^{i\psi} G(\theta). \tag{16}$$

The generalization goes as follows. We first define the meromorphic complex functions

$$\Phi(z) = \sum_{l=-L}^{L} A_l z^l, \quad \Xi(z) = \sum_{l=-L}^{L} B_l z^l,$$

which are related to F and G, from (2) and (3), by $F(\theta) = \Phi(e^{i\theta})$ and $G(\theta) = \Xi(e^{i\theta})$. We also introduce the symmetric and antisymmetric part of Φ, $\Phi^S(z) = \frac{1}{2}(\Phi(z) + \Phi(z^{-1}))$, $\Phi^A(z) = \frac{1}{2}(\Phi(z) - \Phi(z^{-1}))$. Since $\overline{A_l} = A_{-l}$ and $B_{-l} = -B_l$, these functions satisfy

$$\Phi^S(z^{-1}) = \Phi^S(z), \quad \overline{\Phi^S(z)} = \Phi^S(\overline{z}), \quad \Xi(z^{-1}) = -\Xi(z),$$

and this, together with (16), implies

$$\overline{\Xi(z)} = e^{i\psi}\,\Xi(\overline{z}).$$

We now define the polynomial

$$\begin{aligned} P(z) &= z^{2L}[\Phi^S(z) + e^{i\psi/2}\Xi(z)][\Phi^S(z) - e^{i\psi/2}\Xi(z)] \\ &= K\prod_{j=1}^{4L}(z - z_j), \end{aligned} \tag{17}$$

with $K = \frac{1}{4}(A_L + \overline{A_L})^2 - |B_L|^2$. From the symmetries of Φ and Ξ one can show that $\Phi^S(z) \pm e^{i\psi/2}\Xi(z)$ have real coefficients. Moreover, the roots of $P(z)$ come in pairs z_j and z_j^{-1}.

We include the possibility of a global phase ψ for completeness, but actually it is easy to get rid of it by performing a redefinition of the creation and annihilation operators. In fact, by introducing $a_n' = e^{i\psi/4}a_n$ the new meromorphic functions are $\Phi' = \Phi$, $\Xi' = e^{i\psi/2}\Xi$, therefore

$$\overline{\Xi'(z)} = \Xi'(\overline{z}),$$

and the global phase is absent.

We assume that $P(z)$ is generic in the sense that it has $4L$ different simple roots. Then the complex curve

$$w^2 = P(z) \tag{18}$$

defines a Riemann surface of genus $g = 2L - 1$.

As it is shown in Ref. [7], in the limit of large $|X|$, $D_X(\lambda)$ can be expressed in terms of analytic invariants of the Riemann surface. Namely, we make a choice of branch cuts in the z plane that do not cross the unit circle and a basis of fundamental cycles such that every a cycle surrounds anticlockwise one of the cuts with the last L of them corresponding to the cuts outside the unit circle. Associated to this choice we have a canonically defined ϑ function, $\vartheta : \mathbb{C}^g \to \mathbb{C}$, given by

$$\vartheta(\vec{s}) \equiv \vartheta(\vec{s}|\Pi) = \sum_{\vec{n}\in\mathbb{Z}^g} e^{i\pi\vec{n}\cdot\Pi\vec{n} + 2i\pi\vec{s}\cdot\vec{n}},$$

where Π is the $g \times g$ period matrix. Now, one has the following expression for the asymptotic value of the determinant (Proposition 1 of Ref. [7]):

$$\begin{aligned} \ln D_X(\lambda) &= |X|\ln(\lambda^2 - 1) \\ &\quad + \ln\frac{\vartheta\left[\beta(\lambda)\vec{e} + \frac{\vec{\tau}}{2}\right]\vartheta\left[\beta(\lambda)\vec{e} - \frac{\vec{\tau}}{2}\right]}{\vartheta\left(\frac{\vec{\tau}}{2}\right)^2} + \cdots, \end{aligned} \tag{19}$$

where the dots represent terms that vanish in the large $|X|$ limit. The argument of the ϑ function contains

$$\beta(\lambda) = \frac{1}{2\pi i}\ln\frac{\lambda + 1}{\lambda - 1}, \tag{20}$$

$\vec{e} \in \mathbb{Z}^g$, which is a g-dimensional vector whose first $L - 1$ entries are 0 and the last L are 1 and the constant g-tuple $\vec{\tau}$ is determined once we fix which of the roots of $P(z)$ are also roots of its first factor $z^L[\Phi^S(z) + e^{i\psi/2}\Xi(z)]$ (see Ref. [7] for details).

Case 2: $F^A(\theta)^2 > F^S(\theta)^2 + |G(\theta)|^2$, *for some* $\theta \in (-\pi,\pi]$. We move on now to discuss the other case, in which $F^A(\theta)^2 > F^S(\theta)^2 + |G(\theta)|^2$, for some open intervals in $(-\pi,\pi]$. The symbol now has discontinuities at the boundaries of the interval where $F^A(\theta)^2 = F^S(\theta)^2 + |G(\theta)|^2$.

Up to now, in the presence of such discontinuities none of the known results on block Toeplitz matrices can be applied to obtain the asymptotic behavior for the determinant. We here propose a procedure that covers this gap in the literature, so that one can compute the asymptotics of the determinant in this case.

Before presenting the new procedure, let us recap some facts about Toeplitz matrices with scalar symbol with discontinuities and the corresponding Fisher-Hartwig theorem [2].

We therefore consider a genuine Toeplitz matrix, i.e., one with a scalar symbol $g(\theta)$. Furthermore, we assume $g(\theta)$ is a piecewise smooth symbol with jump discontinuities at θ_j, $j = 1,\ldots,J$ and lateral limits t_j^-, t_j^+ at the discontinuities. Then from the discontinuities we get a logarithmic contribution to $D_X(\lambda)$, whose asymptotic expansion reads

$$\begin{aligned} \ln D_X(\lambda) &= \frac{|X|}{2\pi}\int_{-\pi}^{\pi}\ln[\lambda - g(\theta)]d\theta \\ &\quad + \ln|X|\sum_{j=1}^{J}\frac{1}{4\pi^2}\left(\ln\frac{\lambda - t_j^-}{\lambda - t_j^+}\right)^2 + \cdots, \end{aligned} \tag{21}$$

where now the dots represent finite contributions in the large $|X|$ limit, that can be computed explicitly but are not going to be necessary for us. The crucial fact is that contrary to the linear term (and also the constant one) the logarithmic contribution only depends on the behavior of the symbol near its discontinuities, more concretely on its lateral limits.

The previous observation can be used to compute the logarithmic term for a block Toeplitz matrix in some particular cases. Assume that a two-dimensional symbol $\mathcal{G}(\theta)$ presents a discontinuity at say $\tilde{\theta}$. We shall assume that the lateral limits, $\mathcal{G}^- = \lim_{\theta\to\tilde{\theta}^-}\mathcal{G}(\theta)$ and $\mathcal{G}^+ = \lim_{\theta\to\tilde{\theta}^+}\mathcal{G}(\theta)$, commute. If the two matrices commute there is a basis where both are diagonal. Call $\tau_1^\pm$ and $\tau_2^\pm$ the corresponding eigenvalues at each side of the discontinuity. Inspired by the Fisher-Hartwig theorem for the scalar case, we argue that the contribution of this discontinuity to the logarithmic term of the determinant only depends on the value of $\mathcal{G}(\theta)$ at each side of the jump or more concretely on its eigenvalues. Explicitly the contribution of the discontinuity to the coefficient of the logarithmic term of $\ln D_X(\lambda)$ is

$$b = \frac{1}{4\pi^2}\left[\left(\ln\frac{\lambda-\tau_1^-}{\lambda-\tau_1^+}\right)^2 + \left(\ln\frac{\lambda-\tau_2^-}{\lambda-\tau_2^+}\right)^2\right]. \tag{22}$$

Now if we have several discontinuities with commuting lateral limits there is a logarithmic contribution b_j, like the one above, for each of them. Then, the asymptotic form of the block Toeplitz determinant up to finite contributions should be

$$\ln D_X(\lambda) = \frac{|X|}{2\pi}\int_{-\pi}^{\pi}\ln\det[\lambda I - \mathcal{G}(\theta)]d\theta + \ln|X|\sum_{j=1}^{J} b_j + \cdots. \tag{23}$$

This result is crucial for the computation of the asymptotic behavior of the entanglement entropy for the general free fermionic model with finite-range coupling. It is one of the main contributions of this work. It would be very interesting to extend this to the case when the two lateral limits do not commute. So far we have been unable to accomplish this goal. Fortunately, in order to study the fermionic chain that we consider in this paper, the stated result is enough.

After this general discussion we proceed to study the asymptotic behavior for the entanglement entropy in the ground state of the Hamiltonian (1) when the symbol in the thermodynamic limit is not continuous. The latter can be written

$$\hat{\mathcal{G}}(\theta) = \begin{cases} -I, & \text{if } -\Lambda^S(\theta) > F^A(\theta),\\ M(\theta), & \text{if } -\Lambda^S(\theta) < F^A(\theta) < \Lambda^S(\theta),\\ I, & \text{if } F^A(\theta) > \Lambda^S(\theta). \end{cases} \tag{24}$$

The first thing one should notice is that if $\mathcal{G}$ has a discontinuity at θ it has also another one at $-\theta$. Therefore, discontinuities come in pairs except those at $\theta = 0$ or π. We will now analyze the type of discontinuities and their contribution to the logarithmic term.

The first situation is when the two lateral limits are $M(\theta)$ and $\pm I$. Obviously, the two limits commute and we can therefore apply (22). The eigenvalues of $M(\theta)$ are ± 1 [indeed, $\det M(\theta) = -1$ and $\mathrm{Tr}\, M(\theta) = 0$], which implies that its contribution to the $\ln|X|$ term of (23) is

$$b_{MI} = \frac{1}{4\pi^2}\left(\ln\frac{\lambda+1}{\lambda-1}\right)^2.$$

The second type of discontinuity is when the lateral limits are $+I$ and $-I$, in this case the two eigenvalues ± 1 are different in both sides and we get a contribution

$$b_{II} = 2b_{MI}.$$

Finally, it is also possible that the matrix $M(\theta)$ itself is discontinuous. This may happen when F^S and G vanish for some values of θ and at least one of them goes linearly to zero. In this case the two lateral limits have opposite sign and the contribution to the logarithmic term is

$$b_{MM} = 2b_{MI}.$$

From the above ingredients we can compute the asymptotic behavior of the determinant for the four archetypical situations sketched in Fig. 2.

In Fig. 2(a) we represent a double change of sign for the dispersion relation for positive values of θ. We have four discontinuities of the kind MI, which one can deduce from (24). This is depicted with the lines with arrows below the plot. The contribution to the logarithmic term of $\ln D_X(\lambda)$ is $b_a = 4b_{MI}$.

In Fig. 2(b) we consider the case in which Λ changes sign at $\theta = 0$ (the case $\theta = \pi$ is analogous). We now have two discontinuities of the type MI and one II with a contribution $b_b = 2b_{MI} + b_{II} = 4b_{MI}$.

In Fig. 2(c) we represent the case in which Λ^S vanishes at two symmetric values of the angle, it produces two discontinuities of the type MM and hence a contribution $b_c = 2b_{MM} = 4b_{MI}$.

Finally, it may happen that Λ^S vanishes at $\theta = 0$ or π in which case we have only a discontinuity of the type MM and a contribution $b_d = 2b_{MI}$. Altogether we have

$$b_T = 2(2n_a + 2n_b + 2n_c + n_d)b_{MI} \equiv N_T b_{MI},$$

where n_i, $i = a,\ldots,d$, are the number of discontinuities of the corresponding type i (see Fig. 2). This leads to

$$\ln D_X(\lambda) = |X|\ln(\lambda^2-1) + \ln|X| b_T + \cdots. \tag{25}$$

Therefore, the asymptotic behavior of the Rényi entanglement entropy is

$$S_\alpha(X) = N_T\frac{\alpha+1}{24\alpha}\ln|X| + \cdots, \tag{26}$$

where we have used the identity

$$\lim_{\varepsilon\to0^+}\frac{1}{4\pi i}\oint_C f_\alpha(1+\varepsilon,\lambda)\frac{db_{MI}}{d\lambda}d\lambda = \frac{\alpha+1}{24\alpha}.$$

To close this section we would like to discuss how the existence of discrete symmetries may affect our results. First, note that the Hamiltonian is P (reflection) invariant if and only if $F^A(\theta) = 0$. Then we are in case 1 above. On the other hand, PC is a symmetry when $G(\theta)$ is purely imaginary, so that case 1 above applies. Finally, one should notice that in case 2 (which implies the absence of P symmetry) the existence or not of PC symmetry is irrelevant here.

V. EXAMPLE 1: DZYALOSHINSKI-MORIYA COUPLING

As an application of the previous results we will study the XY spin chain with transverse magnetic field and

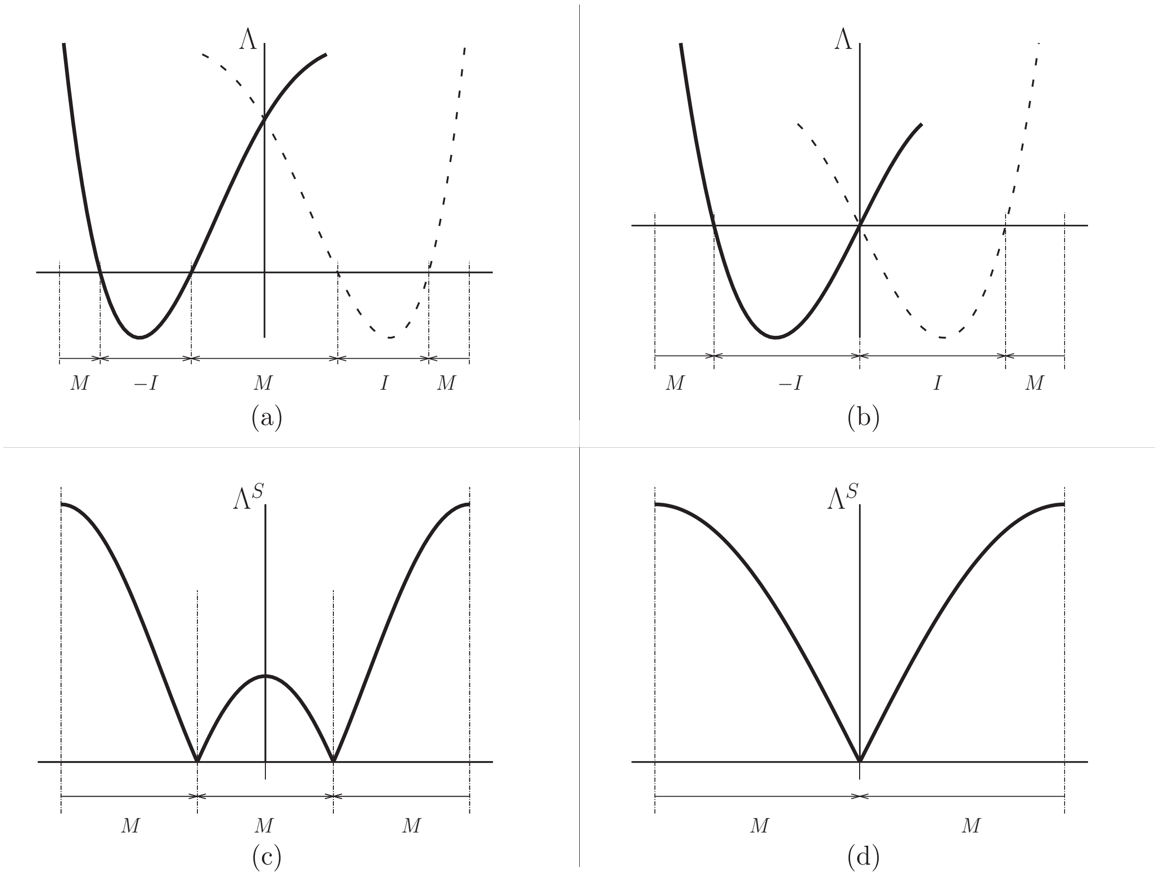

FIG. 2. Four archetypical discontinuities for the symbol $\hat{\mathcal{G}}(\theta)$ of the correlation matrix. In (a) and (b) the dispersion relation $\Lambda(\theta)$ is represented by the solid curve while the dashed curve depicts $\Lambda(-\theta)$. In (c) and (d) the solid curve stands for $\Lambda^S(\theta)$. The lines with arrows, directly below the plots, mark the angle θ where the discontinuities happen.

Dzyaloshinski-Moriya (DM) coupling [9,17]. The Hamiltonian reads

$$H_{\rm DM} = \frac{1}{2}\sum_{n=1}^{N}\big[(t+\gamma)\sigma_n^x\sigma_{n+1}^x + (t-\gamma)\sigma_n^y\sigma_{n+1}^y + s\big(\sigma_n^x\sigma_{n+1}^y - \sigma_{n+1}^x\sigma_n^y\big) + h\sigma_n^z\big].$$

The coupling constants h, t, s, and γ are assumed to be real.

As it is well know, a Jordan-Wigner transform allows to write this Hamiltonian in terms of fermionic operators. Namely

$$H_{\rm DM} = \sum_{n=1}^{N}[(t+is)a_n^\dagger a_{n+1} + (t-is)a_n^\dagger a_{n-1} + \gamma(a_n^\dagger a_{n+1}^\dagger - a_n a_{n+1}) + h a_n^\dagger a_n] - \frac{Nh}{2}, \quad (27)$$

which can be described as a Kitaev chain with complex hopping couplings that break the reflection symmetry. It is also well known that the entanglement entropy of connected spin subchains coincide with its corresponding fermionic one and, therefore, for our purposes the two models are completely equivalent.

The Hamiltonian of (27) is a particular case of (1) with $L = 1$ and then we can apply the preceding section's results. The meromorphic functions are in this case

$$\Phi^S(z) = tz + h + tz^{-1}, \quad \Phi^A(z) = -is(z - z^{-1}),$$
$$\Xi(z) = \gamma(z - z^{-1}).$$

Therefore, the dispersion relation is

$$\Lambda(\theta) = \Lambda^S(\theta) + 2s\sin\theta, \quad \text{with}$$
$$\Lambda^S(\theta) = \sqrt{(h + 2t\cos\theta)^2 + 4\gamma^2\sin^2\theta}. \quad (28)$$

In the following we will fix the invariance under rescaling of the coupling constants by taking $t = 1$.

With a simple inspection of (28) we deduce that the system has no mass gap when

$$\Delta = s^2 - \gamma^2 > 0, \quad \text{and} \quad (h/2)^2 - \Delta < 1; \quad \text{(region A)},$$

or when

$$\Delta < 0, \quad \text{and} \quad h = 2; \quad \text{(region B)}.$$

In Fig. 3 we depict regions A and B (actually a line) in the (γ,h) plane for a fixed s.

In region A the dispersion relation becomes negative in some interval (Dirac sea) and therefore the energy is minimum when all these modes are occupied. It implies that the ground state corresponds to $\hat{\mathbf{K}} \neq \emptyset$ and we have discontinuities in the symbol $\hat{\mathcal{G}}(\theta)$. If $h \neq 2$, it has four discontinuities of the type MI, which corresponds to the situation represented in

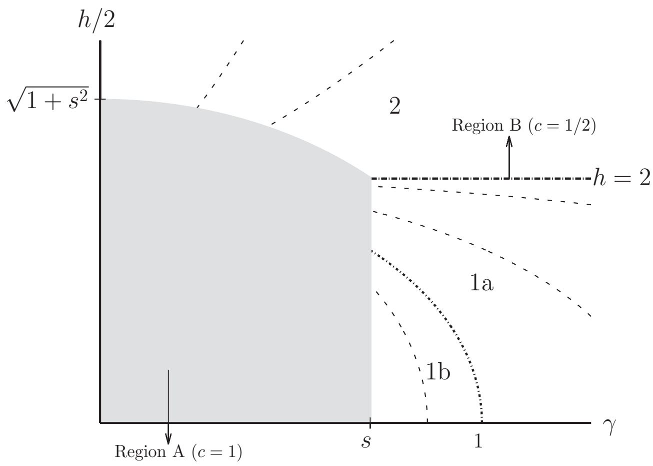

FIG. 3. Phase diagram for $H_{\rm DM}$ in the (γ,h) plane for $t = 1$ and fixed s. The shaded region A is gapless with central charge $c = 1$ (XX universality class) while the dashed line region B has central charge $c = 1/2$ (Ising universality class). In the unshaded area, the Hamiltonian has a gap and there are conical curves with the same entropy. The dashed ellipses and hyperbolas depict some of them.

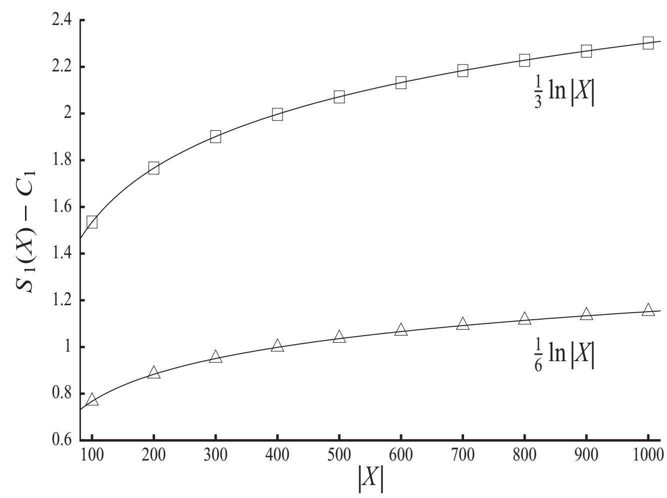

FIG. 4. Numerical logarithmic contribution to the von Neumann entropy ($\alpha = 1$) for two sets of couplings of $H_{\rm DM}$. We have subtracted the constant term $C_1 = S_1(100) - c/3\ln(100)$ with $c = 1$ or $1/2$. The $\square$ correspond to $s = 0.75$, $\gamma = 0.5$ and $h = 0.5$, so it belongs to region A. The $\triangle$ represent $s = 0.75$, $\gamma = 1.5$ and $h = 2$, so we are in region B. The solid lines depict our prediction in each region.

Fig. 2(a). For $h = 2$ one of the zeros of the dispersion relation is at $\theta = \pi$ and it corresponds to Fig. 2(b). Hence, we have two discontinuities of the type MI and one of the type II. In both cases, applying (26) we obtain an asymptotic behavior for the entropy given by

$$S_\alpha(X) = \frac{\alpha+1}{6\alpha}\ln|X| + \dots$$

In the points of region B $\Lambda(\theta)$ is positive except at $\theta = \pi$ where it vanishes. This implies that we have a single discontinuity of the type MM as we discussed before and it is represented in Fig. 2(d). The entropy in this region is

$$S_\alpha(X) = \frac{\alpha+1}{12\alpha}\ln|X| + \dots.$$

In Fig. 4 we check numerically these scalings for the von Neumann entropy ($\alpha = 1$).

We should discuss now the asymptotic behavior of the entropy for the points in the (γ,h) plane outside the critical regions A and B. In this region the dispersion relation is always positive and

$$\hat{\mathcal{G}}(\theta) = M(\theta),$$

which besides is continuous, because $\Lambda^S(\theta) > 0$.

Notice that in our case γ is real and therefore $\overline{\Xi}(z) = \Xi(\overline{z})$, hence we can follow the general procedure in terms of the Riemann surface and theta functions that we mentioned in the previous section. This has been actually carried out in Ref. [5] for the von Neumann entropy and in Ref. [6] for the Rényi entropy. The final results can be stated in a very simple way.

Let us introduce

$$x = \frac{1-(h/2)^2}{\gamma^2}.$$

Now we should distinguish three regions outside the critical ones 1a, 1b, and 2. They are represented in Fig. 3. In every region the von Neumann entropy is constant with $|X|$ and has a different expression.

(i) Region 1a: $0 < x < 1$, $\gamma^2 > s^2$.

$$S_1 = \frac{1}{6}\left[\ln\left(\frac{1-x}{16\sqrt{x}}\right) + \frac{2(1+x)}{\pi}I(\sqrt{1-x})I(\sqrt{x})\right] + \ln 2.$$

(ii) Region 1b: $x > 1$, $\gamma^2 > s^2$.

$$S_1 = \frac{1}{6}\left[\ln\left(\frac{1-x^{-1}}{16\sqrt{x^{-1}}}\right) + \frac{2(1+x^{-1})}{\pi}I(\sqrt{1-x^{-1}})I(\sqrt{x^{-1}})\right] + \ln 2.$$

(iii) Region 2: $x < 0$, $\gamma^2(1-x) > s^2$.

$$S_1 = \frac{1}{12}\left[\ln(16(2-x-x^{-1})) + \frac{4(x-x^{-1})}{\pi(2-x-x^{-1})} \times I\left(\frac{1}{\sqrt{1-x}}\right)I\left(\frac{1}{\sqrt{1-x^{-1}}}\right)\right].$$

Here $I(z)$ is the complete elliptic integral of the first kind

$$I(z) = \int_0^1 \frac{dy}{\sqrt{(1-y^2)(1-z^2y^2)}}.$$

The first observation is that the entropy only depends on the constant $x = (1-(h/2)^2)/\gamma^2$. This fact was first noticed in Ref. [15] where the case of $s = 0$ was discussed. The curves of constant x are ellipses in zones 1a and 1b and hyperbolas in zone 2, they are plotted in Fig. 3. It is clear that (if $s = 0$ and region A shrinks to a line) all curves intersect at $h = 2$, $\gamma = 0$, which implies that the entropy does not have a well-defined limit at that point. It has been called the essential critical point in Ref. [15]. From the expression for the von Neumann entropy, one also observe a duality between the zones 1a and 1b by transforming x into x^{-1}. In this way a curve in the region 1a is transformed into another one in 1b while maintaining the same value for the entropy. One can show that the curves of constant entropy as well as the duality also hold for Rényi entropy.

When we turn on the DM coupling ($s \neq 0$) the critical line at $\gamma = 0$ in Fig. 3 blows up and transforms into region A. The curves of constant entropy in the plane (γ, h) still persist, but only the portion of them outside region A. On the other hand the entropy at the essential critical point is well defined. As it is inside the critical region, it grows like the logarithm of the size of the interval and in the limit of large $|X|$ it becomes

$$S_\alpha(X) = \frac{\alpha+1}{6\alpha} \ln\left(\frac{4s^2}{1+s^2}|X|\right) + \mathcal{I}_\alpha,$$

where $\mathcal{I}_\alpha$ is a constant independent of s whose expression is

$$\mathcal{I}_\alpha = \frac{1}{\pi i}\int_{-1}^{1} \frac{df_\alpha(1,\lambda)}{d\lambda} \ln\left\{\frac{\Gamma[1/2-\beta(\lambda)]}{\Gamma[1/2+\beta(\lambda)]}\right\} d\lambda,$$

where Γ represents the Euler gamma function, f_α is defined in (10) and $\beta(\lambda)$ in (20).

Another special point is $\gamma = 1$, $h = 2$ where, as was noted in Ref. [9] by Kádar and Zimborás, $H_{\rm DM}$ is Kramers-Wannier self-dual. In that case, the correlation matrix reduces to a Toeplitz matrix with scalar symbol and employing the Fisher-Hartwig theorem they can obtain not only the logarithmic contribution but also the constant term. For the von Neumann entropy they have

$$S_1(X) = \begin{cases} \frac{1}{3}\ln(2|X|) + \frac{1}{12}\ln\left(1-s^{-2}\right) + \mathcal{I}_1; & s > 1 \\ \frac{1}{6}\ln(4|X|) + \frac{\mathcal{I}_1}{2}; & s \leqslant 1. \end{cases}$$

Note that the logarithmic term agrees with our general result.

Another interesting property of this theory is that when we approach the critical zone B from 1a or 2, the entropy saturates at a larger and larger value that grows logarithmically with the correlation length (or the inverse of the mass gap). This is the expected behavior that has been predicted from the properties of conformal field theories [16] and has been verified numerical and analytically in many models.

As for the boundary of region A, it can be reached from inside the region or from outside. These two limits are completely different. Of course, inside the critical region the entropy diverges logarithmically with the length of the interval and, what matters for us, the coefficient of this term is constant throughout all the region. Contrary to this behavior, the constant coefficient in the asymptotic expansion of the entropy does change inside region A and it indeed diverges with negative values when we tend to any boundary. If, we now study the case in which we approach zone A from any of the noncritical ones (1a, 1b, or 2) we find that the entanglement entropy of the interval saturates in the limit at a finite value, which is different at any point of the boundary but independent of the path (always inside the noncritical region) that we follow to reach the point. Note that this behavior is anomalous in the sense that, as we mentioned before, one expects an exponential divergence of the entropy with the inverse of the mass gap. Recall that in the noncritical regions 1a, 1b, and 2 the ground state is the Fock space vacuum for the Bogoliubov modes; the same occurs in the critical region B. On the contrary, in region A the ground state has all Bogoliubov modes with negative energy occupied (the Dirac sea). The above behavior of the entropy near the transition could be a sign of this discontinuity in the ground state. In fact, we find a similar issue in the XX spin chain (i.e., when $s, \gamma = 0$). In that case, the entropy always vanishes when $h > 2$, it does not diverge with the inverse of the mass gap when we approach the critical point $h = 2$, and the ground state is the Fock space vacuum. On the contrary, when $h < 2$, the von Neumann entropy scales like $1/3 \ln|X|$ while the constant correction diverges to negative values when we approach the essential critical point. In this region a Dirac sea develops and the ground state has occupied all the modes with negative energy. The situation is, therefore, very similar to what we obtained for the DM model.

From a global point of view, this behavior in the border of region A can be interpreted as a blow up of the essential critical point of Ref. [15]. The different possible values for the limit of the entropy at that point (for $s = 0$) are obtained at different points of the boundary of region A for $s \neq 0$ and the singularity at $h = 2$, $\gamma = 0$ disappears in this case.

VI. EXAMPLE 2: KITAEV CHAIN WITH LONG RANGE PAIRING

As a further application of the previous results we shall discuss the case in which the couplings extend throughout the whole chain. The example is adapted from Ref. [18] and it serves to illustrate how to use the tools of the preceding sections to determine the scaling behavior of the entropy in a theory with long-range couplings.

The Hamiltonian represents a Kitaev chain with powerlike decaying pairing, i.e.,

$$H_{\rm K} = \sum_{n=1}^{N}(a_n^\dagger a_{n+1} + a_{n+1}^\dagger a_n + h a_n^\dagger a_n) + \sum_{n=1}^{N}\sum_{l=-N/2}^{N/2} l|l|^{-\zeta-1}(a_n^\dagger a_{n+l}^\dagger - a_n a_{n+l}) - \frac{Nh}{2}, \quad (29)$$

where the exponent $\zeta > 0$ characterizes the dumping of the coupling with distance. Its value will happen to be critical to determine the scaling behavior of the entropy.

Following the discussion in Sec. IV and taking the thermodynamic limit, $N \to \infty$, we define

$$\Phi^S(z) = \Phi(z) = z + h + z^{-1} \quad (30)$$

$$\Xi_\zeta(z) = \sum_{l=1}^{\infty}(z^l - z^{-l})l^{-\zeta} = {\rm Li}_\zeta(z) - {\rm Li}_\zeta(z^{-1}), \quad (31)$$

where ${\rm Li}_\zeta$ stands for the polylogarithm of order ζ. This is a multivalued function, analytic outside the real interval $[1,\infty)$ and, what is going to be most important for us, has a finite limit at $z = 1$ for $\zeta > 1$ while it diverges at that point for $\zeta < 1$.

If we introduce now $G_\zeta(\theta) = \Xi_\zeta(e^{i\theta})$, which is a purely imaginary function, the dispersion relation reads

$$\Lambda(\theta) = \sqrt{(h + 2\cos\theta)^2 + |G_\zeta(\theta)|^2},$$

and vanishes at $\theta = \pi$ for $h = 2$ and at $\theta = 0$ for $h = -2$ and $\zeta > 1$. These are the two instances in which the mass gap is

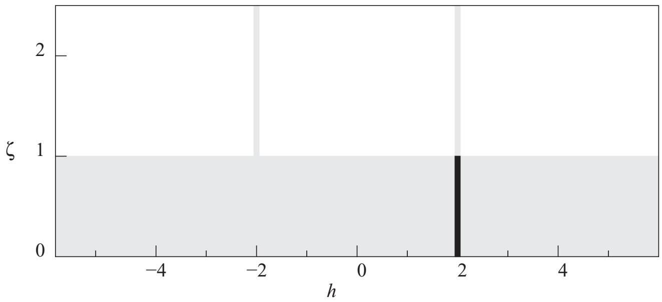

FIG. 5. Plot of the different regions in the (h,ζ) plane according the the coefficient of the logarithmic scaling for the entanglement entropy. White area stands for $c = 0$, gray region for $c = 1/2$ and the black one for $c = 1$.

zero. An interesting feature of this model is that, as we shall see, it may have logarithmic scaling of the entropy even when it has nonzero mass gap.

Notice that $\overline{G(\theta)} = -G(\theta)$ and therefore the formalism of Sec. IV can be applied, we also have $\Lambda^A(\theta) = 0$, which corresponds to cases c or d in Sec. IV. Hence, to uncover the possible logarithmic scaling of the entropy we must simply look for discontinuities of the matrix

$$M(\theta) = \frac{1}{\Lambda(\theta)}\begin{pmatrix} h + 2\cos\theta & G_\zeta(\theta) \\ -G_\zeta(\theta) & -h - 2\cos\theta \end{pmatrix}.$$

One source of discontinuities comes from the zeros of the dispersion relation, this corresponds to the cases in Figs. 2(c) and 2(d) discussed in Sec. IV. In our model the only zeros appear at $\theta = 0$ for $h = -2$ or $\theta = \pi$ for $h = 2$ and the two lateral limits of M at the discontinuity are $\pm\sigma^y$. Therefore they contribute to the effective central charge for the scaling of the entanglement entropy with $c = 1/2$. Note that this contribution has its origin in the absence of mass gap, i.e., it is connected to the universality class of a conformal field theory.

The other possible discontinuities are related to the divergences of $G(\theta)$ at $\theta = 0$; these happen for $\zeta < 1$ and any value of h. The two lateral limits are also $\pm\sigma^y$ and the discontinuity contributes with $c = 1/2$ to the scaling of the entropy. If $h = 2$ this contribution must be added to the one coming from the zero of the dispersion relation at $\theta = \pi$, therefore the total effective central charge is $c = 1$. When $h = -2$ such an addition does not happen as the two discontinuities are actually the same and the total effective central charge is $c = 1/2$.

All these results are summarized in Fig. 5 where the different regions, according to the value of c, are shown. The white region where $c = 0$ corresponds to $\zeta > 1$ and $h \neq \pm 2$; in black we represent the region with $c = 1$, i.e., $h = 2$ and $\zeta < 1$; the rest in gray corresponds to $c = 1/2$.

Our analytic results are very much compatible with the numeric findings of Ref. [18], where the regions we have determined appear smeared somehow. We interpret this fact as the consequence of finite-size corrections to the thermodynamic limit that we are presently considering. Note that for comparison with Ref. [18] one should bear in mind that their parameters α and μ correspond to ζ and $h/2$ in our paper.

Another interesting remark is that the results above can be applied to any family of long-range couplings with the same asymptotic behavior for large l and constant sign. In fact, our discussion was based on the limiting behavior of G at $\theta = 0$ and the latter is governed solely by the asymptotic behavior of the power series.

VII. CONCLUSIONS

In this paper, we extend further the understanding of entanglement entropy in spinless fermionic chains considering translational invariant Hamiltonians with finite-range couplings breaking the fermionic number, the reflection, and the charge conjugation symmetries. The first violation implies dealing with block Toeplitz determinants while the second one can create Bogoliubov modes with negative energy. The latter breaking leads to discontinuities in the symbol of our block Toeplitz matrix. Here, we have performed a systematic analysis of their physical origin, nature, and contribution to the entanglement entropy of a set of contiguous sites in the thermodynamic limit. For the last point, we have carried out a heuristic study based on the fact that the contribution of each discontinuity only depends on the value of the symbol at each side of the jump. Thereby, we conclude that each of them adds a logarithmic term with the size of the interval to the entropy. This method also allows us to determine its coefficient, which informs about the universality class of the critical theory. From a mathematical point of view, our result requires that the two lateral limits of the symbol at the discontinuity commute. Although this is enough for our physical problem, it will be a very interesting mathematical question to study the case in which the two lateral limits do not commute.

When the reflection symmetry breaking does not produce Bogoliubov modes with negative energy, the expressions found by Its, Mezzadri, and Mo can still be applied. Here we have also shown that it can be extended to certain cases where the charge conjugation symmetry is broken.

We have applied this general analysis to an XY spin chain with transverse magnetic field and Dzyaloshinski-Moriya coupling. This system has two critical regions as was previously pointed out in Refs. [9,17]. Here we determine that one region belongs to the Ising universality class while another region corresponds to the XX universality class. The latter can be seen as a blowing up, produced by the DM coupling, of the XX critical line of the XY spin chain with only magnetic coupling.

We have also tested our formula in a theory with long-range couplings, a Kitaev fermionic chain with powerlike decaying pairing. In this case, the logarithmic scaling of the entropy is affected by the dumping of the coupling with the distance. For sufficiently small values, it produces a discontinuity in the symbol of the correlation matrix. As a result, for zero mass gap and positive chemical potential, the universality class of the critical theory changes from the XX class (for small values of the dumping) to the Ising class (when the dumping is sufficiently large). In addition, this discontinuity implies that the entropy may have a logarithmic scaling when the mass gap is not null. Our analytical study agrees a great deal with the numeric results obtained in Ref. [18]. The difference is that the regions we have precisely delimitated here, appear blurred in Ref. [18]. We interpret this fact as a consequence of finite-size corrections to the thermodynamic limit we consider here.

In Refs. [19,20] Keating and Mezzadri established a relation between certain symmetries of one-dimensional quadratic fermionic Hamiltonians and classical compact Lie groups by means of entanglement entropy. This is analogous to the Altland-Zirnbauer classification [21]. In particular, they find that translational invariant Hamiltonians preserving fermionic number, i.e., when the correlation matrix reduces to a scalar Toeplitz matrix, are related with the U(N) group. It would be nice to extend their classification when the fermionic number symmetry is broken, therefore when there appear block Toeplitz matrices. Furthermore, in this case, the discrete symmetries, such as reflection or charge conjugation, would certainly play a crucial role for such classification. This interesting matter deserves a further detailed investigation.

ACKNOWLEDGMENTS

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[1] P. Deift, A. Its, and I. Krasovsky, Toeplitz matrices and Toeplitz determinants under the impetus of the Ising model: Some history and some recent results, Commun. Pure Appl. Math. **66**, 1360 (2013).
[2] E. L. Basor, A localization theorem for Toeplitz determinants, Indiana Math. J. **28**, 975 (1979).
[3] B.-Q. Jin and V. E. Korepin, Quantum spin chain, Toeplitz determinants and Fisher-Hartwig conjecture, J. Stat. Phys. **116**, 79 (2004).
[4] F. Ares, J. G. Esteve, F. Falceto, and E. Sánchez-Burillo, Excited state entanglement in homogeneous fermionic chains, J. Phys. A: Math. Theor. **47**, 245301 (2014).
[5] A. R. Its, B. Q. Jin, and V. E. Korepin, Entropy of XY spin chain and block Toeplitz determinants, Fields Institute Communications, Universality and Renormalization, Vol 50, page 151, 2007.
[6] F. Franchini, A. R. Its, and V. E. Korepin, Rényi entropy of the XY spin chain, J. Phys. A: Math. Theor. **41**, 025302 (2008).
[7] A. R. Its, F. Mezzadri, and M. Y. Mo, Entanglement entropy in quantum spin chains with finite range interaction, Commun. Math. Phys. **284**, 117 (2008).
[8] I. Peschel, On the entanglement entropy for an XY spin chain, J. Stat. Mech. (2004) P12005.
[9] Z. Kádar and Z. Zimborás, Entanglement entropy in quantum spin chains with broken reflection symmetry, Phys. Rev. A **82**, 032334 (2010).
[10] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Entanglement in Quantum Critical Phenomena, Phys. Rev. Lett. **90**, 227902 (2003).
[11] I. Peschel, Calculation of reduced density matrices from correlation functions, J. Phys. A: Math. Gen. **36**, L205 (2003).
[12] F. Ares, J. G. Esteve, and F. Falceto, Entanglement of several blocks in fermionic chains, Phys. Rev. A **90**, 062321 (2014).
[13] V. Alba, M. Fagotti, and P. Calabrese, Entanglement entropy of excited states, J. Stat. Mech. (2009) P10020.
[14] H. Widom, Asymptotic behavior of block Toeplitz matrices and determinants, Adv. Math. **13**, 284 (1974).
[15] F. Franchini, A. R. Its, B.-Q. Jin, and V. E. Korepin, Ellipses of constant entropy in the XY spin chain, J. Phys. A: Math. Theor. **40**, 8467 (2007).
[16] P. Calabrese and J. Cardy, Entanglement entropy and quantum field theory, J. Stat. Mech. (2004) P06002.
[17] W. DeGottardi, M. Thakurathi, S. Vishveshwara, and D. Sen, Majorana fermions in superconducting wires: Effects of long-range hopping, broken-time reversal symmetry, and potential landscapes, Phys. Rev. B **88**, 165111 (2013).
[18] D. Vodola, L. Lepori, E. Ercolessi, A. V. Gorshkov, and G. Pupillo, Kitaev chains with long-range pairings, Phys. Rev. Lett. **113**, 156402 (2014).
[19] J. P. Keating and F. Mezzadri, Random matrix theory and entanglement in quantum spin chains, Commun. Math. Phys. **252**, 543 (2004).
[20] J. P. Keating and F. Mezzadri, Entanglement in Quantum Spin Chains, Symmetry Classes of Random Matrices, and Conformal Field Theory, Phys. Rev. Lett. **94**, 050501 (2005).
[21] J. Hutchinson, J. P. Keating, and F. Mezzadri, Random matrix theory and critical phenomena in quantum spin chains, Phys. Rev. E **92**, 032106 (2015).
[22] A. P. Balachandran, T. R. Govindarajan, A. R. de Queiroz, and A. F. Reyes-Lega, Entanglement and Particle Identity: A Unifying Approach, Phys. Rev. Lett. **110**, 080503 (2013).
[23] A. P. Balachandran, T. R. Govindarajan, A. R. de Queiroz, and A. F. Reyes-Lega, Algebraic approach to entanglement and entropy, Phys. Rev. A **88**, 022301 (2013).